Reducing the Propagation Losses of Slab Photonic Crystal Waveguides for Active Photonic Devices

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ROMAN KAPPELER

MSc EEIT ETH Zurich
born April 4, 1979
citizen of Schwyz SZ, Switzerland

accepted on the recommendation of

Prof. Dr. Heinz Jäckel, examiner
Prof. Dr. Christian Hafner, co-examiner
Prof. Dr. Daniel Erni, co-examiner

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to Conny
Abstract

Line-defect photonic crystal waveguides are considered for integrated photonic circuits, because they promise to overcome the integration density limits established by Kogelnik in 1981. These limits are given by a minimum cross-section of a dielectric waveguide in the order of the wavelength of the light, i.e., $\sim 0.5 \, \mu m \times 0.5 \, \mu m$, and a device length in the order of $0.5 \, mm$. The minimum device length is given by the strength of the light-matter interaction. This interaction strength is determined by the properties of the host material and the intensity of the light confined to this material. Line-defect PhC waveguides exhibit frequency regimes of slow light propagation. These so-called slow waves are characterized by strongly enlarged light intensities, i.e., the light-matter interaction is enhanced in these waveguides. This effect can be exploited to reduce the device lengths. It is expected that line-defect PhC waveguides allow us to reduce the device length by roughly one order of magnitude which leads to a device length below $100 \, \mu m$.

Since the introduction of photonic crystals in the late 80-ies, the photonic crystal technology has been rather successful in the sense that many passive integrated photonic components have been experimentally demonstrated. However electrically pumped active line-defect PhC waveguides are lacking so far. Active photonic components with a net gain are essentially required for an all-embracing integrated photonic circuit technology. The main challenge is to find a design that allows for an efficient current injection and that simultaneously provides low optical propagation losses. Vertically pumped substrate-type line-defect PhC waveguides suffer from substantial lateral current leakage and large propagation losses in the order of $600-1000 \, dB/cm$. On the other hand, free-standing membrane PhC waveguides support single-mode operation with propagation losses below $10 \, dB/cm$. But, in these devices, the current has to be pumped laterally through the perforated membrane, which is very inefficient. After a decade of research, a general disillusionment is spreading; the current opinion is that an efficient current injection scheme and low propagation losses are mutually exclusive.

This dissertation deals with i) the improvement of the understanding of the origin of the large propagation losses of waves propagating in line-defect PhC waveguides and, with ii) the reduction of the propagation losses. The thesis gives concrete answers to many hitherto open questions. The first part of the thesis is devoted to the question of the origin and the physical process behind the observed propagation losses. It is demonstrated that the large propagation losses are caused by the excitation of the PhC waveguide beyond the cutoff frequency, i.e., with a
frequency for which the waveguide does not support a guided mode. On the other hand, if a waveguide is excited with a frequency for which a guided mode exists, the waveguide is theoretically loss-free. Identifying the cutoff frequency in a dispersion diagram of the line-defect PhC waveguide is hence of crucial importance. Therefore, the concept of the background-line is introduced as a tool to identify frequency regions, for which the line-defect PhC waveguide is loss-free.

The second part of the dissertation elucidates a new numerical model to accurately compute propagation losses. The numerical model reliably delivers propagation losses that agree well with experimentally measured propagation losses. For this reason, the method can be used to give an ultimate answer to the questions of ‘What limits the propagation losses in terms of fabrication imperfections?’ and ‘Can the process technology be further improved to reduce the propagation losses?’ We find that the angled-side walls of the cylindro-conical holes are responsible for the fabrication related propagation losses. Based on this insight, two post treatment processes were developed to reduce the angled-sidewalls of the etch holes and to yield more cylindrical holes. The first process consists of a thermal driven annealing step under a phosphine atmosphere that enables a mass transport of the InP at the exposed surfaces of the etched holes. This process reduces the hole depth slightly in exchange for a more cylindrical hole at the bottom of the hole. The second process is a highly selective wet-etch process with an ultra slow etch-rate. This process enlarges the radius in the substrate layer only, and thus is able to compensate for the smaller radius of the holes in the substrate layer. With these first minor improvements of the process, we were already able to experimentally demonstrate propagation losses as low as 154 dB/cm for single-mode line-defect PhC waveguides with a weak vertical layer structure. This represents a four times lower propagation loss than previously reported for similar waveguides (600-1000 dB/cm).

The theoretical understanding of the mechanism behind the propagation losses, together with the possibility to accurately compute the propagation losses for a specific design, were the key ingredients that led to this promising result. With these tools at hand we pursued strategies to reduce the propagation losses even further by i) optimizing the thickness of the vertical layer stack, ii) using alternative waveguide designs that have inherently lower propagation losses and iii) engineering of the substrate layer to suppress radiation leakage into the substrate. We find waveguides with propagation losses as low as 80 dB/cm, theoretically.

Finally, we tackle the question of ‘whether the PhC technology can keep the promise of a denser integration density of photonic circuits with respect to the integration density stipulated by Kogelnik?’ and ‘under which conditions PhCs can provide a higher integration density?’. Therefore, a hypothetical device design – the cross-hair structure – is presented. It exhibits ultra low propagation losses for single-mode operation and simultaneously provides efficient vertical carrier injection. The cross-hair device is the first single-mode PhC waveguide design that can be used for the implementation of an electrically pumped broad-band semiconductor optical amplifier. Furthermore, the design has the potential to enable the exploitation of the benefits offered by slow light modes and therefore to reduce the device length below 100 µm.
Zusammenfassung

Kogelnik hat im Jahre 1981 fundamentale Grenzen der Integrationsdichte von integrierten optischen Schaltungen aufgestellt: der Querschnitt eines integrierten optischen Wellenleiter kann nicht viel kleiner als die Wellenlänge des Lichts (d.h. \( \sim 0.5 \mu m \times 0.5 \mu m \)), und die Länge des Wellenleiters nicht viel kürzer als 0.5 mm gemacht werden. Die Länge des optischen Bauteils ist dabei durch die Stärke der Interaktion zwischen der Lichtwelle und dem Material geben. Eine Verbesserung versprechen Liniendefekt-Photonenkristallwellenleiter. Diese haben ein Frequenzband, für welches die Gruppengeschwindigkeit der propagierenden Welle klein ist. Diese langsamigen Moden weisen hohe Lichtintensitäten auf, welche zu einer Verstärkung der Licht-Material Interaktion führen. Diese Verstärkung der Licht-Material Interaktion erlaubt es nun, die Interaktionslänge und damit auch die Länge der optischen Komponenten um etwa eine Grössenordnung auf weniger als 100 \( \mu m \) zu verkürzen.


Die vorliegende Arbeit beschäftigt sich mit der Frage nach dem Grund der hohen Propagationsverluste von planaren Photonenkristallwellenleitern und wie man diese verkleinern kann. Viele offene, relevante Fragen im Zusammenhang mit den Propagationsverlusten werden in der vorliegenden Schrift beantwortet. Im ersten Teil wird der Ursprung der Verluste und der dazugehörige physikalische Prozess diskutiert. Es stellte sich folgendes heraus: wird ein Wellenleiter mit einer Frequenz angeregt, für welche kein geführter Mode existiert, so entsteht eine Leck-


Dieses vielversprechende Resultat konnte im Wesentlichen durch das verbesserte theoretische Verständnis des Verlustmechanismus und durch die Möglichkeit, die Propagationsverluste zuverlässig zu berechnen, erreicht werden. Die beiden Errungenschaften bilden die Basis, um noch bessere Photonenkristallwellenleiter zu finden, welche Propagationsverluste von nur noch 80 dB/cm aufweisen. Dazu haben wir folgende Strategien verfolgt: i) Optimierung der Schichtstruktur für eine gegebene Lochform, ii) alternative Liniendefekt-Photonenkristallwellenleiter-Anordnungen mit geringeren Verlusten und iii) die Entwicklung von anderen Hintergrundstrukturen, welche die Abstrahlung in das Substrat unterbinden.

Contents

Abstract v
Zusammenfassung vii

1 Introduction 1
  1.1 Integrated Optics for Communication Photonics . . . . . . . . . . . . 1
  1.2 Signal Processing: Integrated Optics vs. Integrated Electronics . . . . 3
    1.2.1 Switching . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 3
    1.2.2 Interconnects . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 6
    1.2.3 Integration Density . . . . . . . . . . . . . . . . . . . . . . . . . 7
  1.3 Requirements for Integrated Optical Devices . . . . . . . . . . . . . . 8
    1.3.1 Minimum Required Functionality . . . . . . . . . . . . . . . . . 8
    1.3.2 Requirements on the Device and the Technology . . . . . . . 9
  1.4 Photonic Crystals - A Promising Candidate for Integrated Optics . . . 10
    1.4.1 Comparison of PhCs and PhWs for Communication Photonics 11
    1.4.2 Miniaturized SOA with Electrical Current Injection . . . . . . 13
  1.5 Objectives and Contributions of this Work . . . . . . . . . . . . . . . 14
    1.5.1 Scope of this Thesis . . . . . . . . . . . . . . . . . . . . . . . . 15

2 Theory of Slab Photonic Crystal Waveguides 19
  2.1 Asymmetric Slab Waveguide . . . . . . . . . . . . . . . . . . . . . . . . 20
    2.1.1 Ray Optics Model . . . . . . . . . . . . . . . . . . . . . . . . 20
    2.1.2 Mode Theory . . . . . . . . . . . . . . . . . . . . . . . . . . . . 24
    2.1.3 Conclusion . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 33
  2.2 Photonic Crystals . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 33
    2.2.1 Photonic States Physics . . . . . . . . . . . . . . . . . . . . . 34
    2.2.2 Photonic Crystal Waveguides . . . . . . . . . . . . . . . . . . 40
    2.2.3 Fourier Optics . . . . . . . . . . . . . . . . . . . . . . . . . . . 46
  2.3 Slab Photonic Crystal Waveguides . . . . . . . . . . . . . . . . . . . . 52
    2.3.1 Polarization of the Slab PhC Waveguide Modes . . . . . . . . 53
    2.3.2 Effective Index Approximation . . . . . . . . . . . . . . . . . 54
    2.3.3 Conclusions . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 55
# Contents

3 Computation of Dispersion Diagram of PhCs 57

3.1 Methods to Compute the Photonic Bands 58

3.2 Super-Cell Approach 59

3.2.1 Super-Cell Approach for Line-Defect PhC Waveguides 60

3.2.2 3D MPB Simulations of Slab PhC Waveguides 63

3.3 Mode-Maps for Line-Defect PhC Waveguides 66

3.3.1 Method for Computing the Mode-Maps of Line-Defect PhC Waveguides 66

3.3.2 Sensitivity Analysis of the W1 PhC Waveguide Mode Using Mode-Map Plots 69

3.4 Photonic Band Computation Using hp-FEM 72

3.4.1 The Finite Element Formalism 74

3.4.2 Weak Formulation for TE Modes for Systems with a 1D-Periodicity of the Permittivity 74

3.4.3 Discretization by Means of Finite Elements 77

3.4.4 Matrix Eigenvalue Problem 82

3.4.5 Verification for a Test Structure with an Analytical Solution 84

3.4.6 Realistic Test Case: W1 PhC Waveguide 85

3.4.7 Implementation in Concepts 87

3.4.8 Efficiency Analysis 89

3.5 PhC Band Diagram Computations Using Dispersive Material Models 93

3.5.1 Influence of a Dispersive InP Material Model on the PhC properties 94

3.5.2 Outlook 97

3.6 Conclusion 98

4 Loss Mechanism in Substrate-Type Photonic Crystal Waveguides 99

4.1 Waveguide Losses 100

4.1.1 Absorption Losses 101

4.1.2 Scattering Losses 101

4.1.3 Waveguide Losses 105

4.2 The Loss Mechanism in Line-Defect Slab PhC Waveguides 110

4.3 Existing Loss Theories Based on Perturbation Theory 112

4.3.1 Perturbation by a Small Wall Distortion Function 112

4.3.2 \( \varepsilon'' \)-Model 114

4.3.3 Concluding Remarks on the Scattering Process in Strongly Modulated Periodic Structures 117

4.4 Plane Wave Expansion for a Slab with 1D Periodicity 119

4.4.1 Description of the Mode Solutions 120

4.4.2 Solving the Helmholtz Equation in the Cladding Layer 121

4.4.3 Solving the Wave Equation in the Core Layer 123

4.4.4 Boundary conditions 124

4.4.5 Conclusion 125

4.4.6 The Loss Mechanism 127

4.5 The Background Concept 127

4.5.1 Failure of the Light Line Concept for Substrate-Type PhCs 128

4.5.2 The Background Line Concept 128
4.5.3 The Background Line Concept for a Slab Waveguide with a
1D Periodic Substrate ........................................... 129
4.5.4 Finite Etch Depth - Approximate Background Line ........ 132
4.5.5 The Background Line Concept Applied to Line-Defect Slab
PhC Waveguides .................................................. 135
4.6 Full 3D Simulation of a Membrane-Type W1 PhC Waveguide .... 136
4.6.1 Setup of the Membrane-Type W1 PhC Waveguide Simulation 137
4.6.2 Radiating Spatial Fourier Component Above the Light Line . 138
4.6.3 Exponential Decay of the Fourier Components in the Cladding 141
4.6.4 Backward Radiation ....................................... 142
4.7 Simple Loss Model by Means of Ray Optics ..................... 144
4.7.1 Propagation Losses of a Leaky Wave of a Slab Waveguide .. 144
4.7.2 Estimation of the Propagation Losses of a Membrane Type
PhC W1 Waveguide ............................................. 146
4.8 Conclusions ................................................. 148

5 Computation of the Propagation Losses of PhC Waveguides 151
5.1 Introduction .................................................. 152
5.2 The Cutback-Method ....................................... 154
5.2.1 The Exponential Decay ................................... 155
5.2.2 Geometry of the Model ................................. 156
5.2.3 Transmission and Reflection Coefficient ................. 158
5.2.4 Method A: The Cutback-Method of Transmissions ....... 159
5.2.5 Method B: The Flux Distribution Method ............... 160
5.2.6 Method of Least Squares and the Coefficient of Determina-
tion ............................................................. 161
5.3 Results and Discussion .................................. 161
5.3.1 Comparison of the Cutback-Methods .................... 161
5.3.2 Comparison of the Computed Propagation Loss to Other
Simulation Results: The Membrane-Type W1 PhC Waveguide 163
5.3.3 Comparison of the Computed Propagation Loss to Opti-
cally Measured Propagation Losses: The InP/InGaAsP/InP
Substrate-Type W1 PhC Waveguide .......................... 165
5.3.4 Accuracy of the Simulation Results ....................... 167
5.4 Conclusions .................................................. 173

6 Structural Imperfections in Slab PhC Waveguides 175
6.1 Phenomenological Loss Channels ........................... 176
6.1.1 Material Absorption ..................................... 176
6.1.2 Out-of-Plane Losses ..................................... 177
6.1.3 Lateral Radiation Leakage ............................... 177
6.1.4 Losses Due to Mode Coupling Caused by the Asymmetry 178
6.1.5 Scattering at Geometric Non-Uniformity ................ 178
6.1.6 Interface Losses ......................................... 178
6.2 Structural Properties, Loss Channels and Loss Mechanisms .... 179
6.3 Influence of the Structural Imperfections on the Propagation Loss 180
6.3.1 The W1 PhC Waveguide of Interest ..................... 181
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.3.2 Intrinsic Propagation Loss</td>
<td>182</td>
</tr>
<tr>
<td>6.3.3 Propagation Losses Originating From Periodic Imperfections</td>
<td>183</td>
</tr>
<tr>
<td>6.3.4 Propagation Losses Originating From Randomly Distributed</td>
<td>196</td>
</tr>
<tr>
<td>Imperfections</td>
<td></td>
</tr>
<tr>
<td>6.4 Discussion</td>
<td>199</td>
</tr>
<tr>
<td>6.4.1 The Limiting Structural Imperfection</td>
<td>199</td>
</tr>
<tr>
<td>6.4.2 Intrinsic Propagation Losses of the PhC Waveguide Design</td>
<td>201</td>
</tr>
<tr>
<td>6.5 Conclusion</td>
<td>203</td>
</tr>
<tr>
<td>7 Reducing the Propagation Losses of Substrate-Type PhC Waveguides</td>
<td>205</td>
</tr>
<tr>
<td>7.1 Optimization of the Layer Stack</td>
<td>207</td>
</tr>
<tr>
<td>7.2 Alternative PhC Waveguide Designs</td>
<td>209</td>
</tr>
<tr>
<td>7.3 Suppressing Radiation Into the Substrate</td>
<td>214</td>
</tr>
<tr>
<td>7.4 Improving the Process Technology to Yield a Better Hole Shape</td>
<td>219</td>
</tr>
<tr>
<td>7.4.1 Reducing the Sidewall-Angle of the Etched Holes</td>
<td>220</td>
</tr>
<tr>
<td>7.4.2 Increasing the Radius of the PhC Waveguide in the Substrate Layer</td>
<td>221</td>
</tr>
<tr>
<td>7.5 Discussion</td>
<td>224</td>
</tr>
<tr>
<td>7.6 Conclusion</td>
<td>227</td>
</tr>
<tr>
<td>8 The Cross-Hair Device</td>
<td>229</td>
</tr>
<tr>
<td>8.1 Vertical vs. Horizontal Current Injection Schemes</td>
<td>230</td>
</tr>
<tr>
<td>8.2 Theoretical Foundations to Obtain Low Propagation Losses</td>
<td>231</td>
</tr>
<tr>
<td>8.3 Optical Design Considerations</td>
<td>233</td>
</tr>
<tr>
<td>8.3.1 Photonic Crystal Waveguide Design</td>
<td>233</td>
</tr>
<tr>
<td>8.3.2 Material and Free-Carrier Absorption</td>
<td>238</td>
</tr>
<tr>
<td>8.4 Electronic Design Considerations</td>
<td>239</td>
</tr>
<tr>
<td>8.4.1 Depletion Width and Surface Space Charge Density of Our Etching Process</td>
<td>239</td>
</tr>
<tr>
<td>8.4.2 Gain of the Active Device</td>
<td>240</td>
</tr>
<tr>
<td>8.4.3 Self-Heating and Heat Dissipation</td>
<td>241</td>
</tr>
<tr>
<td>8.5 Summary of the Parameters and Performance of the Cross-Hair Device</td>
<td>244</td>
</tr>
<tr>
<td>8.6 Discussion</td>
<td>246</td>
</tr>
<tr>
<td>8.7 Conclusion</td>
<td>248</td>
</tr>
<tr>
<td>9 Conclusions and Outlook</td>
<td>249</td>
</tr>
<tr>
<td>9.1 Achievements and Contributions of this Work</td>
<td>249</td>
</tr>
<tr>
<td>9.2 Conclusions</td>
<td>252</td>
</tr>
<tr>
<td>9.3 Outlook</td>
<td>253</td>
</tr>
<tr>
<td>A Appendix</td>
<td>255</td>
</tr>
<tr>
<td>A.1 Governing Maxwell’s Equations</td>
<td>255</td>
</tr>
<tr>
<td>A.2 Remark on the Power Flux of a Superposition of Modes</td>
<td>257</td>
</tr>
<tr>
<td>A.3 Reciprocal Lattice Vectors for a 2D Photonic Crystal</td>
<td>258</td>
</tr>
<tr>
<td>A.4 Plane Wave Expansion</td>
<td>259</td>
</tr>
<tr>
<td>A.5 Analysis of Lattice Disorder and Radius Variations in our PhC Waveguides</td>
<td>261</td>
</tr>
<tr>
<td>A.6 Free Carrier Absorption Models</td>
<td>262</td>
</tr>
<tr>
<td>-----------------------------------</td>
<td>-----</td>
</tr>
<tr>
<td>Bibliography</td>
<td>265</td>
</tr>
<tr>
<td>Nomenclature</td>
<td>285</td>
</tr>
<tr>
<td>Index</td>
<td>287</td>
</tr>
<tr>
<td>Curriculum Vitae</td>
<td>289</td>
</tr>
<tr>
<td>Publications</td>
<td>291</td>
</tr>
<tr>
<td>Acknowledgements</td>
<td>293</td>
</tr>
</tbody>
</table>
1

Introduction

1.1 Integrated Optics for Communication Photonics

Optical data transmission has become the backbone of modern communication for two main reasons: (i) optical fibers offer propagation losses below 0.2 dB/km for the telecom wavelength ($\lambda = 1550$ nm) while (ii) providing unrivaled broad bandwidths (roughly 58 THz with low-loss for the AllWave fiber of Lucent Technologies). In practice, it is challenging to aggregate and prepare this huge amount of data to be transmitted over a single fiber. The signal processing is almost exclusively performed by high-speed electronic circuits that are limited in speed (currently limited to about 100 GHz) due to the finite mobilities of the carriers in the materials and due to capacitive loads. The broad bandwidth of optical systems is best used by wavelength division multiplexing (WDM) techniques [32, 79], where the spectrum is divided into narrow frequency channels having a bandwidth limited by the electronic circuits (50 – 100 GHz). Recently, an optical fiber link of 240 km length with a transmission rate of 25.6 Tb/s was demonstrated by Gnauck et al. [78] using WDM. They used 160 channels of 50 GHz bandwidth while exploiting the two independent polarizations and both L- and C-band. The highest reported transmission rate to date using WDM is 69.1 Tb/s by NTT [230]. Together with the development of broad-band erbium doped fiber amplifiers (EDFA) [174, 56] and their appropriate pump lasers [130], WDM optical links have revolutionized optical fiber communication [129]. WDM requires the usage of many lasers and its fine-tuning to the optical transmission channels and thus is relatively expensive if the number of channels is increased. As opposed to WDM, optical time division multiplexing (OTDM) [284] employs ideally only one transmission channel. The highest transmission rate employing OTDM is actually 10.2 Tb/s [223]. OTDM is not as successful [190] as WDM in terms of aggregated data rate, mainly due to the lack of an all-optical signal processing technology providing all required devices beyond 100 GHz. Apart from the re-amplification, the processing is mainly performed electronically and only the final link to/from the fiber is realized by a semiconductor laser, modulator or detector. Shifting more signal processing functionalities from the electronic into the
optical domain [36] would allow to replace their parallel operated electronic (speed limited) signal processing units by a single optical processing unit [101, 306, 204]. In the future, OTDM and WDM are expected to be employed in conjunction: OTDM will be used to reduce the number of individual channels by increasing and exploiting the bandwidth of each individual channel. WDM will be used to take advantage of the complete bandwidth provided by the fiber.

Many signal processing steps have already been implemented with high speed all-optical components such as e. g., all-optical transparent 3R signal regeneration systems [29, 208, 151]. However, those all-optical signal processing systems are typically realized off-chip by combining individual components, such as modulators, fiber and diode lasers. Those systems are thus still large, bulky and costly. The electronic integrated circuit industry was boosted by pursuing a miniaturization strategy of monolithically integrated devices. The transistor device sizes and the cross-sections of the connecting wires were continuously reduced for every new technology increment. The simultaneous development of new technologies to handle the complexity of circuits consisting of millions of transistors led to the enormous integration density of electronic circuits as we have it today. It is expected that a similar evolution for integrated photonic circuits would happen if all required optical components could be monolithically integrated on a single chip. Then a similar miniaturization strategy could be pursued to reduce costs per functionality. The integration of different types of optical devices on a single semiconductor chip was already demonstrated [188, 221, 293]. This effort has resulted in sophisticated semiconductor laser diodes and semiconductor optical amplifiers [86, 191, 266]. Nagaranjan et al. [188, 189] reported on the development of a commercial transmitter chip containing all the devices required for 10[188]/40 channels [189] (> 50/ > 200 optoelectronic devices, respectively). Raring et al. [221] demonstrated a 40 Gbit/s wide tunable transceiver by monolithic integration of a distributed Bragg reflector laser (DBR laser) a quantum well electro-absorption modulator (EAM) a low confinement SOA and an uni-traveling carrier (UTC) photo diode. This was achieved by combining MOCVD regrowth steps with multiple band-gap quantum well intermixing (QWI) processes. Even so, integrated all-optical signal processing is still in its infancy.

The next section continues the discussion of electronic and optic signal processing with a focus on current limitations of both technologies. Thereafter, we define the required basic building blocks for optical communication systems and basic requirements for integrated optical devices. Photonic crystals (PhC) and photonic wires (PhW) are considered to be promising technologies for satisfying the request of high density optical integration, since theoretically, they allow for shrinking the footprint of both, passive and active photonic devices to the wavelength scale. This is explained in Sec. 1.4. The last section outlines the contributions and achievements of this thesis towards the aim of developing electrically pumped PhCs for communication photonics.
1.2 Signal Processing: Integrated Optics vs. Integrated Electronics

The large discrepancy between available bandwidth of the optical fiber in the order of several 10 Tbps and the low throughputs of several 10 Gbps of electronic driver circuits is was already referred to as the electronic bottleneck in 1988 [284]. The argument is commonly used to motivate a shift of the signal processing from the electronic to the optical domain. Nowadays, integrated optics still have not replaced electronic circuits to aggregate the data for the transmission, although optical interconnects are already considered for board-to-board, chip-to-chip and on-chip communication [20, 179]. The reason is that optics has the potential advantage of high bandwidth, low power, low latency and noise immunity. The following paragraphs elucidate these potential benefits of optical signal processing. We start with a rather rough comparison of physical limits of both, electronic signal processing and optical signal processing in table 1.1.

1.2.1 Switching

- **Switching speed**: Since transistors rely on carrier transport, the maximum speed is linked to the saturation velocity and the mobility of either the electron or the holes in the semiconductor. Moreover, the switching speed is related to the $RC$-delay of the transistor. A reduction of the device dimensions reduces the gate capacitance and consequently increases the switching speed. The fastest transistor to date can be operated at 340 GHz [84, 268]. However, the switching speed of the transistors is not limiting the speed-performance of electronic circuits, but instead the wires connecting

<table>
<thead>
<tr>
<th>‘carrier’ frequency</th>
<th>Electronics moderate (GHz)</th>
<th>Optics high (THz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>waveguide material</td>
<td>metals</td>
<td>dielectrics</td>
</tr>
<tr>
<td>waveguide loss</td>
<td>high resistive losses for high frequencies</td>
<td>low dielectric losses</td>
</tr>
<tr>
<td>method of information transfer</td>
<td>voltage swing</td>
<td>transmission of photons</td>
</tr>
<tr>
<td>signal carrier</td>
<td>electrons (have a charge and a rest mass)</td>
<td>photons (no charge and no rest mass)</td>
</tr>
<tr>
<td>integration density</td>
<td>extremely high ($&gt;10^9$ devices per chip)</td>
<td>low ($&lt;10^3$ devices per chip)</td>
</tr>
<tr>
<td>memory device</td>
<td>available</td>
<td>lacking</td>
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the transistors are.
As opposed to electronic switches, for all-optical switches the potential
switching speed is given by the involved photon-electron interaction. Table 1.2 gives an overview of the response times $\tau$ of some typical non-linear
processes and lists the magnitude of the intensity induced refractive index
change $\Delta n$ where appropriate. The corresponding maximum bandwidth $B$
is inversely related to the response time $B = 1/\tau$. The currently fastest all-optical switch is based on four wave mixing (FWM) in a silicon waveguide [102]. They demonstrated optical sampling and optical demultiplexing for a data rate of 1.28 Tb/s.

- **Switching energy**: For electronic devices the generated heat and the required power scales with the operating speed of electronic devices. The energy required for a switching operation with an electronic switch was compared to the required energy for an all-optical switch by Tucker and Hinton [285]. They approximated the energy used for a logic operation with a CMOS device by energy involved in the charging and discharging of the capacitance of the transistor $C_{\text{gate}}$ and the interconnect wires ($L_w$ length of the wire, $C_w$ capacitance per unit length of the wire) according

$$E_{\text{device}} = \frac{1}{2}(C_{\text{gate}} + C_w L_w) V_{DD}^2,$$

where $V_{DD}^2$ is the supply voltage. Leakage currents of the transistors are neglected because, currently, the interconnecting wires are limiting the performance. The average wire length between devices is roughly $L_w \approx 3 \mu m$ and the energy per bit is roughly at $E_{\text{device}} \approx 2 \text{ fJ}$ [285] by 2010. It is expected that the average wire length will be reduced to $L_w \approx 1.5 \mu m$ and the energy per bit will decrease to $E_{\text{device}} \approx 0.2 \text{ fJ}$ by 2020[285].
The energy of an optical switch $E_{\text{opt}}$ depends strongly on the switch design and has to include, both the energy of the optical signal $E_S$ and the supply energy $E_{\text{supply}}$, that can either be an electronic supply (semiconductor

<table>
<thead>
<tr>
<th>Mechanism</th>
<th>$\Delta n$ (cm$^2$/W)</th>
<th>$\chi^{(3)}$ (m$^2$/V)</th>
<th>Response Time $\tau$ (sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electronic polarization</td>
<td>$10^{-16}$</td>
<td>$10^{-22}$</td>
<td>$10^{-15}$</td>
</tr>
<tr>
<td>Intersubband transition</td>
<td>-</td>
<td>-</td>
<td>$10^{-13}$</td>
</tr>
<tr>
<td>Molecular orientation</td>
<td>$10^{-14}$</td>
<td>$10^{-20}$</td>
<td>$10^{-12}$</td>
</tr>
<tr>
<td>Direct band gap transitions</td>
<td>-</td>
<td>-</td>
<td>$10^{-12}$</td>
</tr>
<tr>
<td>Electrostriction</td>
<td>$10^{-14}$</td>
<td>$10^{-20}$</td>
<td>$10^{-9}$</td>
</tr>
<tr>
<td>Saturated atomic absorption</td>
<td>$10^{-10}$</td>
<td>$10^{-16}$</td>
<td>$10^{-8}$</td>
</tr>
<tr>
<td>Thermal effects</td>
<td>$10^{-6}$</td>
<td>$10^{-12}$</td>
<td>$10^{-3}$</td>
</tr>
</tbody>
</table>
optical amplifier (SOA)) or an optical pump power

\[ E_{\text{opt}} = E_S + E_{\text{supply}}. \]

In a first order approximation, the \( E_{\text{opt}} \) is independent of the ‘wire-length’ since the interconnect losses are typically small in optical circuits. A comparison of different all-optical switches has been made by Y. Fedoryshyn [68] with a focus on high-speed switching and by Nozaki et al. [199] with a focus on switching energy and device size. Table 1.3 summarizes their findings. Furthermore Tab. 1.3 shows that the usage of photonic crystal cavities allows to reduce the switching energy to energies that are comparable to the switching energies of electronic switches. However, the low switching energy of the PhC-based high-Q cavity switches is obtained at the expense of lower switching speeds [81].

Table 1.3: Comparison of the performance of various on-chip all-optical switches [199, 68].

<table>
<thead>
<tr>
<th>Device</th>
<th>Mechanism</th>
<th>Switching energy [fJ]</th>
<th>Switching frequency [Gb/s]</th>
<th>Size [( \mu m^2 )]</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \chi^{(3)} )-waveguide</td>
<td>FWM</td>
<td>1070</td>
<td>&gt;1000</td>
<td>550</td>
<td>[132]</td>
</tr>
<tr>
<td>ISBT waveguide</td>
<td>ISBT</td>
<td>6800</td>
<td>&gt;1000</td>
<td>240</td>
<td>[43]</td>
</tr>
<tr>
<td>Si waveguide</td>
<td>FWM</td>
<td>&gt;10000</td>
<td>1280</td>
<td>675</td>
<td>[102]</td>
</tr>
<tr>
<td>Ring cavity</td>
<td>carrier induced refractive index change</td>
<td>1000</td>
<td>40</td>
<td>4</td>
<td>[292]</td>
</tr>
<tr>
<td>PhC MZI</td>
<td>QDs acting as a nonlinear phase-shift source</td>
<td>100</td>
<td>70</td>
<td>45</td>
<td>[92]</td>
</tr>
<tr>
<td>1D PhC</td>
<td>carrier induced refractive index change</td>
<td>6</td>
<td>2/200*</td>
<td>4</td>
<td>[235]</td>
</tr>
<tr>
<td>2D PhC waveguide**</td>
<td>THG</td>
<td>&lt; 22</td>
<td>640</td>
<td>8.5</td>
<td>[45]</td>
</tr>
<tr>
<td>PhC cavity</td>
<td>carrier induced refractive index change</td>
<td>0.42***</td>
<td>20 − 40</td>
<td>0.025***</td>
<td>[199]</td>
</tr>
</tbody>
</table>

THG: third harmonic generation  FWM: four wave mixing  ISBT: intrasubband-transition
* the relaxation time is \(~ 500\) ps and the switch-on time is a few ps, i.e., \( (~ 2 − 200 \) Gb/s)
** using slow light
*** calculated switching energy (only absorbed energy). Measured switching energies range from 1.4 fJ to 5.4 fJ.
**** the nano-cavity size. A realistic size would include the surrounding holes as well as a part of the access waveguides and would amount to about 10 \( \mu m^3 \).
1.2.2 Interconnects

- **Interconnect density**: The resistive loss in the electrical interconnect lines (without repeaters) is responsible for the attenuation and the limited bandwidth of electrical transmission lines. The maximum bit rate for electrical lines can be approximated \( B \leq B_0 \frac{A}{L^2} \),

where \( A \) is the cross-section and \( L \) is the length of the wire and \( B_0 \) is a constant representing the maximum bit rate of a specific line. For instance, \( B_0 \approx 10^{16} \text{ b/s} \) is the characteristic bit rate for the \( RC \) lines on a chip and \( B_0 \approx 10^{17} - 10^{18} \text{ b/s} \) is the characteristic bit rate for off-chip \( RLC \) lines. To visualize the bottleneck, let us consider an example: Let’s imagine that we need a bit rate of 100 Gb/s to wire two processing units on the same chip but separated by 1cm. Thus, the cross-section of the wire required to provide this data rate would be \( A = B/B_0 \cdot L^2 \approx 30 \times 30 \mu \text{m}^2 \). To double the bit rate from 100 Gb/s to 200 Gb/s, the cross-section has to be doubled as well. As opposed to electronic interconnects, the cross-section of optical interconnects is small (\( \approx 5 \times 5 \mu \text{m}^2 \)) and independent of the length \( L \) of the interconnect.

- **Interconnect energy**: For electronic data transmission, the entire transmission line is charged to at least the signaling voltage \( V_S \). Therefore, the total energy for transferring one bit \( E_S \) can be estimated by \( E_S \geq C_w V_S^2 \),

where \( C_w \) is the total capacitance of the transmission line. The easiest way to reduce the energy required for transferring a bit with an electronic line is to reduce the signal voltage \( V_S \) since the bit energy scales quadratically with the signal voltage \( V_S \). Reducing the bit energy by reducing the capacitance \( C_w \) is challenging because the capacitance \( C_l \) per length is similar for all lines (\( \approx 200 \text{ aF/\mu m} \)). For optical data transmission, photons have to be created by a source. Then they are transmitted through the dielectric waveguide to be absorbed by a detector. Light can propagate in dielectric waveguides with very high carrier frequencies without generating heat, i.e., the power dissipation is approximatively independent of the transmission length. The relevant energy for the comparison is thus given by the electrical input and the optical energy required to discharge the total capacitance \( C_d \) of the photo-detector \( E_p \geq C_d V_S \frac{\hbar \omega}{e} \),

where \( \frac{\hbar \omega}{e} \approx 0.8 \text{ V} \) is the energy of a photon and \( V_S \) is the signaling voltage. By equating Eq. 1.2 and Eq. 1.3, we can compute the break-even length \( L_{be} \)

\[
L_{be} = \frac{C_d}{C_l V_S} \frac{\hbar \omega}{e}
\]
For $C_d = 1 \text{ff}$, $C_w = 200 \text{aF/}\mu\text{m}$ and $V_S \approx 100 \text{mV}$ a break-even length $L_{be} = 40 \mu\text{m}$ is obtained. In other words, optical interconnects can potentially be more energy efficient for interconnect lengths $L > L_{be}$. The conditions are clearly in favor of optics (single photon transmission is assumed), however, it shows the potential of lower interconnect energies of optical interconnects for on-chip communication.

- **Propagation delay:** In an electronic interconnect, the propagation delay $\tau$ scales *quadratically* with propagation distance $L$ \cite{178}

\[ \tau \approx R_l C_l \cdot L^2, \]

where $R_l$ and $C_l$ are the resistance and the capacitance per unit length of the electronic interconnect, respectively. A common technique to reduce the propagation delay in electrical interconnects is to use repeaters. With optimized repeater circuits, a *linear* behavior of the propagation delay with respect to the propagation distance $l$ is obtained. One of the most important parameters in designing repeater circuits for electrical interconnects is the width of the wires. By optimizing the width of the wires, very efficient power repeater circuits can be designed \cite[Chap.4, pp.85]{212}. But, the power consumption increases with increasing number of repeaters \cite{63} (and hence with interconnect length) as well as with the data rate \cite{126}.

As opposed to electronic signals, optical pulses (down to a few ps) do not spread substantially for propagation distances in the order of a few centimeters, which are typical for on-chip interconnects. Additionally, optical pulses have low latencies \cite{3}. Therefore, optical interconnects are considered for clock distribution and signaling networks on-chip as well as I/O \cite{125, 158}. For optical interconnects, the limiting delays originate from the length-independent opto-electronic components, such as modulators, laser diodes and detectors \cite{91}.

### 1.2.3 Integration Density

By end of 2011, the Xilinx Vertex 7 has the highest count of transistors on a single chip (6.8 billion transistors) \cite{1}. The integration density of electronic devices is thus extremely high. Even though that all-optical switches have footprints now of only a few $4 \mu\text{m}^2$ \cite{199, 235} there are a few essential techniques missing for integrated optical devices: efficient and high density memory and an efficient and simple multi-layer wiring technology.

Conventional integrated photonic devices based on silica-on-silicon or III-V compounds are reliable but rather large: waveguide couplers are typically of millimeter length and bending radii are in the order of hundreds of micrometers. Until lately, high refractive index contrast systems have not been used for optical wave-guiding, mainly due to the low resolution of the fabrication technology. This changed rapidly in the early 90-ties, when semiconductor strips of about 300 nm could be fabricated. The continuous progress of CMOS technology – and particularly the invention of silicon-on-insulator (SOI) technology – finally led to silicon
waveguides with low-losses (< 3 dB/cm). Those devices have a waveguide cross-section smaller than 0.1 \(\mu\text{m}^2\) and bending radii below 1 \(\mu\text{m}\) but they require demanding smooth surfaces (surface roughness < 2 – 3 nm). The integration density of passive photonic waveguides has been improved considerably by the SOI technology. Nevertheless, for active devices, still millimeter-long interaction lengths are needed [128] due to the weak interaction of light with material. The concept of slow light in photonic crystals (PhC) waveguides promises a considerable reduction of the device size (length) in exchange for bandwidth [12, 255, 156] as it can already be observed in Table 1.3. This is further detailed in Sec. 1.4 and Sec. 2.2.2.3).

1.3 Requirements for Integrated Optical Devices for Optical Communication Systems

The MOS-FET transistor is clearly the basic electronic building block permitting the implementation of all elements required for signal processing. Such a single fundamental component does not exist for integrated optics. This device would have to fulfill the following basic requirements for an integrated optical device technology as defined by Miller [181]:

- cascadability: the output of one stage must have the correct form to drive the input
- fan-out: the output of one stage must be able to drive at least two inputs of the next stage
- logic-level restoration: the quality of the logic signal must be restored
- input/output isolation: the reflections at the input must be negligible
- absence of critical biasing: the operational point of the devices must not depend on critical tuning
- the logic level must be independent of loss

According to Miller [181] the only all-optical transistor that fulfills the basic requirements above for optical logic in analogy to electronic logic was implemented by Lentine et al. [153]. This all-optical transistor consists of two symmetric multiple quantum-well p-i-n diodes and is known as the self-electro-optic effect device (SEED) [182].

1.3.1 Minimum Required Functionality

We approach the problem with a more specific focus on optical communication: by defining the elementary functionalities by those required for 3R signal regeneration. Leclerc et al. [151] defined the basic building blocks for optical 3R signal regeneration systems from a functional point of view to be a decision element and clock-recovery block. We prefer to adopt a device oriented view: we consider waveguides, bends and power splitters as the three elementary functions for the passive wave-guiding; we single out the semiconductor optical amplifier (SOA) [226, 243]...
as the fourth required element [266]. Furthermore, lasers and detectors are essentially required for optical communication. But the detector is not required for the 3R signal regeneration. A laser is obtained by combining an SOA with a resonant cavity, e.g., two mirrors. Therefore we consider the SOA together with the waveguides, bends and power splitters to be the four elementary functions to be integrated on a single chip for optical 3R signal regeneration. For instance, Slovak [244] studied novel techniques for all-optical 3R signal regeneration and many of the reported techniques solely rely on the strong non-linearity of SOAs: Re-amplification requires an optical amplifier; re-shaping requires a non-linear gate device, e.g., a Mach Zehtender Interferometer (MZI) and SOAs; and re-timing requires clock extraction circuitry, e.g., a mode locked laser and an SOA.

The passive elementary devices have already been implemented using PhCs [261, 263] or photonic wires (PhWs) [227, 62]. But so far, miniaturized electrically pumped SOAs are still lacking. Currently, there is no PhC device design that exhibits simultaneously efficient current injection and low optical propagation losses.

### 1.3.2 Requirements on the Device and the Technology

In a next step, we define necessary requirements for the technology and the device design.

- **In-plane-guiding:** From the demand of cascadability and the rather long interaction lengths in the order of $\sim 500 \mu m$ we deduce the requirement of *in-plane guiding* of the light.

- **Monolithic integration:** The cascadability of passive and active devices as it is required for an optical 3R regeneration system requires *monolithic integration* of active and passive devices on the same chip. Silicon is increasingly used for light guiding at the telecom wavelength because of the relatively high refractive index ($n \approx 3.4$) and the low absorption losses. The most important reason for the choice of silicon is the mature process technology due to the superior optical lithography processes. But silicon lacks the capability to provide gain for active devices. Furthermore, silicon exhibits only weak electro-optical effects. On the other hand, III/V-semiconductor compounds (InP, GaAs, GaN) are convenient for optoelectronic devices: InP is transparent for the telecom wavelength range and allows epitaxial growth of active quaternary InGaAsP layers. As opposed to silicon, the InP/InGaAsP system provides stronger electro-optical effects and direct band gaps and thus efficient radiative recombination processes for the telecom wavelength. By using selective regrowth techniques [160] or quantum-well intermixing [33, 221] active and passive devices can be realized on the same chip.

- **High-integration density:** The all-optical 3R regeneration system proposed by Nolting [194] requires a cascadability of ten all-optical components in a row. The 3R regeneration system of Nolting [194] further requires five active components (four SOA and one laser). Integrated SOAs in InGaAsP/InP currently have a length of the active region ranging from 300 $\mu m$ to 2 mm [236, 221]. Already in 1981, Kogelnik [128] anticipated the minimum device size: the
confinement is limited to roughly the $\lambda/2$ and the minimum device length is given by the interaction length to exploit a specific physical effect and amounts to roughly $L_{\text{device}} = 500 \mu m$. Therefore, a maximum number of 30 SOA can be cascaded on a 1.5 cm-long chip, optimistically.

What integration density is actually required? To answer this question, we consider the experiment performed by NTT [230]. They used 432 channels at 171 Gb/s to achieve a transmission rate of 69.1 Tb/s. If we were about to perform all-optical 3R signal regeneration for all 432 channels on a single chip, we would need 16 elements (5 active and 11 passive components) per channel. Thus, the required integration density would be 2160 active components and 4752 passive components. But, the current state-of-the-art of the integration density of optoelectronic devices is roughly 200 devices per chip [189]. Therefore, we need an improvement of the integration density of all-optical integrated devices of at least one order of magnitude.

1.4 Photonic Crystals - A Promising Candidate for Integrated Photonic Circuits

In 1987, two pioneering papers from Yablonovitch [299] and John [105] were published. Therein, Yablonovitch discovered the inhibited spontaneous emission and John discovered the strong localization of light in materials having a periodic modulation of the refractive index in the order of the wavelength of the light. Those two papers are usually associated with the term ‘photonic crystals’ (PhC). Even so, the PhC concept is not completely new. 1D periodic structures, such as Bragg-gratings, have been investigated for years. Nevertheless, those two papers triggered extensive research on two and three dimensional periodic structures. Thenceforward, many exciting new phenomena have been discovered, such as the possibility for high Q cavities [257, 145], enhanced spontaneous emission [30], negative index of refraction [54, 195], super-prism effect [133], slow-light phenomena [59, 44, 138, 139, 239, 12] and dispersion engineering [14, 257, 73, 156, 142].

Today, PhCs are considered to be one of the most promising technologies to realize the vision of integrated photonic circuits [11]. The reasons are the following:

- **Passive device components**: All passive device components as listed in Sec. 1.3.1 are viable for the 2D slab PhCs technology: line-defect waveguides [175, 177, 248, 15], bends [282, 224, 263] and power splitters (e. g., waveguide couplers [278, 261] and add-drop filters [134, 217, 307]).

- **Slow light**: Line-defect PhC waveguides exhibit slow light modes. Those modes have a low group velocity and an enhanced field amplitude. Slow light modes allow to trespass the integration density limit anticipated by Kogelnik [128] of the device length in the sub-mm-range due to the weak interaction: first, the interaction is enhanced due to the intensity enhancement of the slow light mode and secondly the higher intensity stays longer in the waveguide due to the low group velocity [256, 255]. In other words, the interaction length $L$ can be reduced by a factor $(c/v_{gr})^2$ – proportional to the square of the slow down factor of the group velocity (cf. 2.2.2.3). Therefore,
slow light modes promise to enhance nonlinear effects [138, 44, 45] and the gain [193] of line-defect PhC waveguide based lasers and SOAs. Furthermore, slow light waveguides have been proposed for all-optical buffering [13, 162].

- **Dispersion tailoring**: The high speed operation of integrated optical components requires waveguides with a low group velocity dispersion. Line-defect PhC waveguides can be engineered to obtain broad band slow light modes with low group velocity dispersion [142]. Furthermore, the tailoring of the dispersion relation of PhC waveguide modes also allows for fine-tuning of frequency features of PhC waveguide to a specific wavelength.

Note that slow light modes and dispersion properties are solely obtained by nanostructuring a material and not by using different materials. The PhC waveguide technology thus represents a generic solution to improve the performance of integrated optical devices for any material system.

### 1.4.1 Competing Technologies: Comparison of PhCs and PhWs for Communication Photonics

A photonic wire (PhW) is a dielectric waveguide that consists of a core with high refractive index (usually silicon with $n \approx 3.4$) and claddings with very low refractive indices, such as air, SiO$_2$ or BCB. A typical PhW is shown in Fig. 1.1 (left). The high contrast of the permittivities of the waveguide core and the surrounding claddings leads to small dimensions of the waveguide core for single-mode operation: The cross-section of a rectangular waveguide has a height of about 200 – 250 nm and width of about 500 nm [62, 26, 80]. The strong light confinement in the small core allows the realization of small bending radii of about a 1 $\mu$m [62] and for high optical power densities. For instance, a 1000-fold enhancement of the optical power density from that of a conventional single-mode fiber can be achieved [300]. Besides the strong confinement of the light, PhW also provide low propagation losses. Propagation losses as low as $\alpha_{dB} = 2.4$ dB/cm have been measured by Dumon et al. [61].

In the following, the PhC technology is compared to the PhW technology regarding the requirements defined above: in-plane operation, monolithic integra-

![Figure 1.1](image_url) Left: Photonic wires typically consists of a silicon dielectric waveguide with a rectangular cross-section on a SiO$_2$ or BCB substrate. Right: Membrane-type photonic crystal waveguide. The corresponding PhC waveguides are manufactured by dry-etching holes in about a 250 nm silicon membrane carried by a SiO$_2$ or BCB substrate.
Table 1.4: Comparison of the PhC and the PhW technology.

<table>
<thead>
<tr>
<th></th>
<th>line-defect PhC waveguide</th>
<th>PhW waveguide</th>
</tr>
</thead>
<tbody>
<tr>
<td>integration density</td>
<td>+ slow light effects</td>
<td>+ ‘continuous’ designs</td>
</tr>
<tr>
<td></td>
<td>- ‘discrete’ designs</td>
<td></td>
</tr>
<tr>
<td>group velocity dispersion</td>
<td>high (depends on the design)</td>
<td>low (4400 ps/(nm·km) at 1550 nm)</td>
</tr>
<tr>
<td>propagation losses (membrane)</td>
<td>2 dB/cm [197]</td>
<td>2.4 dB/cm [61]</td>
</tr>
<tr>
<td>dispersion tailoring</td>
<td>possible</td>
<td>‘linear’ dispersion</td>
</tr>
<tr>
<td>device optimization</td>
<td>laborious</td>
<td>relatively dispersion easy</td>
</tr>
</tbody>
</table>

...tion, and footprint of the device. Both technologies inherently comply with the first requirement, since they are both based on planar geometric structuring (one lithographic step). The two technologies have also the same premises for the second requirement of monolithic integration.

The third request of miniaturization requires a more in-detail discussion, since both PhWs and PhCs provide a tight confinement of light within a region of about half the wavelength [128]. Dai et al. [48] performed a comparative study of the integration density for passive photonic circuits. They compared the minimal decoupling separation between two parallel waveguides and investigated the respective area of a low-loss (less than 0.1 dB loss) 90 degree bend for PhC waveguides and PhWs. The conclusion from that study is that PhWs provide the higher integration density. But, the potential benefits of line-defect PhC waveguides, such as slow light operation, have not been considered in the study. Furthermore, it was not realized that there is indeed a fundamental difference in the degree of freedom of the design of PhCs and PhWs. The periodic pattern that is the basis of PhCs, only allows for ‘discrete’ designs, i.e., in a hexagonal lattice only bends of 60 and 120 degrees can be realized. As opposed to PhCs, the PhW technology permits ‘continuous’ designs, i.e., a bend of any desired angle can be realized. Also the separation distance $d_{PhC}$ between two parallel waveguides can take an arbitrary value for the PhW technology, whereas for the PhC technology the separation distance must be a multiple $n$ of the lateral lattice constant (e.g., $d_{PhC} = n \cdot \sqrt{3}/2 \cdot a$ for line-defect PhC waveguides in a hexagonal lattice).

For instance, Dai et al. [48] determined the minimum separation distance $d$ between two waveguides of 1 cm length by requiring less then 30 dB cross-talk. Because the separation distance $d_{PhW}$ between two PhW can be chosen from a continuum set of separation distances, the separation distance $d_{PhW}$ between PhW waveguides can be designed such that it just meets the given requirements. As opposed to that, the separation distance $d_{PhC}$ of two PhC waveguides has to be chosen from the discrete set of separation distances $d_{PhC} = n \cdot \sqrt{3}/2 \cdot a, n \in \mathbb{N}$. Thus, generally, the separation distance $d_{PhC}$ between two line-defect PhC waveguides is larger than the separation distance between to two PhWs to fulfill the same requirements. The PhW technology always wins in these competitions. Therefore, we modify the experiment as follows: We determined the cross-talk for a specific...
separation distance between the line-defect PhC waveguides, e.g., $d_{\text{PhC}}(n = 3)$. Then we compute the required separation distance $d_{\text{PhW}}$ for the PhW such that the same value for the cross-talk is obtained: We find $d_{\text{PhW}} \approx d_{\text{PhC}}(n = 3)$. Our investigations hence suggests that in terms of integration density the two technologies are comparable, but the PhW technology offers the higher design flexibility.

An essential argument in favor of line-defect PhC waveguides is the possibility of slow light operation that can be use to reduce the device lengths (cf. Sec. 2.2.2.3) and hence increases the integration density. However, slow light modes typically require more lateral layers of holes to guide the light efficiently (cf. 6.3.3.2). A reduction of the device length leads to a moderate enlargement of the lateral dimension of the line-defect PhC waveguides. It is hence very difficult to make an ultimate conclusion about the superiority of one of the technologies. Table 1.4 lists the most notable difference between the two technology competitors.

It is possible to combine the two technologies to design new devices. For instance, it was shown that the radiation losses of a sharp PhW bend can be largely suppressed with a small local pillar-type PhC in the bend area [224, 298] (cf. Fig. 1.2, A). Another example is the double trench waveguide (cf. Fig. 1.2, B) proposed by Lau and Fan [149]. This waveguide has a guided mode with a linear dispersion (from the PhW) and simultaneously a photonic band gap (from the surrounding 2D PhC). Vlasov et al. [288] demonstrated that the bandwidth $\Delta \nu = c/\lambda^2 \Delta \lambda$ for low-loss propagation ($< 50 \text{ dB/cm}$) can be significantly expanded to about $\Delta \lambda \approx 250 \text{ nm}$ for these double trench waveguides. However, a PhC can also be incorporated in a PhW. A typical example is the so-called nano-beam waveguide design (cf. Fig. 1.2, C). This waveguide consists of a PhW containing additional periodic holes. The design was proposed by Deotare et al. [55, 305] to realize very high Q-cavities in the framework of the PhW technology.

1.4.2 Miniaturized SOA with Electrical Current Injection

Currently, membrane-type PhC waveguides (cf. Fig. 1.1(right)) figure among the most successful integrated optics technologies due to their low propagation losses in the order of less than 10 dB/cm [203, 173, 60, 197, 267]. But yet an efficient carrier injection scheme for electrically driven active PhC devices is lacking for the membrane technology. Currently, for membrane-type PhCs the current is pumped later-
Figure 1.3: Left: Membrane-type W1 PhC waveguide with four QW’s. The current flows laterally through the suspended membrane. Right: Substrate-type W1 PhC waveguide with four QW’s. The current flows vertically through the line-defect PhC waveguide.

ally through the PhC [65, 211] as illustrated in Fig. 1.3 (left). Lateral carrier injection has the disadvantage that the ohmic resistance increases with the radius of the holes of the PhC [23]. Furthermore, etching holes into a planar layer stack enlarges the surface area. The enlarged surface area gives rise to additional carrier losses due to surface recombination [93]. As opposed to membrane-type PhC waveguides, the weak vertical layer structure resulting from an epitaxial growth allows a straightforward realization of a PIN diode. Those so-called substrate-type PhC waveguides can be contacted similarly to conventional semiconductor lasers and amplifiers with a vertical current injection scheme and is shown in Fig. 1.3(right).

Electrically pumped PhC lasers based on line-defect PhC waveguides using vertical carrier injection scheme have already been fabricated [165, 120, 272, 53]. However, those devices are all multimoded ($W_x \geq 3$) in order to keep the losses at a minimum. As mentioned above, the potential benefit of PhC waveguides rely almost exclusively on slow light modes. Therefore, the single-mode operation is an essential requirement. The high propagation losses of single-mode line-defect slab PhC waveguides with a weak vertical refractive index confinement in the order of $600-1000$ dB/cm [274, 117] so far prevented the realization of an efficient PhC based SOA. The reduction of the propagation losses is thus of key importance for the development of efficient electrically pumped active PhC waveguides.

1.5 Objectives and Contributions of this Work

The original goal of this project was the theoretical analysis and implementation of electrically pumped PhC devices. A major issue towards that goal is the large propagation losses in the order of $\alpha_{dB} = 600 - 1000$ dB/cm observed in single-mode substrate-type PhC waveguides. These large propagation losses make the implementation of an electrically pumped single-mode PhC waveguide with an net-gain almost impossible. To the best of our knowledge, the smallest working
electrically pumped line-defect PhC lasers in our material system have a waveguide width of \( w \approx 1.4 \mu m \) of the multimode PhC waveguide [120, 272]. In order that a single-mode line-defect PhC waveguide device can exhibit a net gain, the propagation losses must be reduced substantially. The focus of this work therefore lies on the question whether the propagation losses of a single-mode substrate-type PhC waveguides can be reduced to the level of the propagation losses of a line-defect PhC waveguide mode with a width \( w \approx 1.4 \mu m (\approx W_3) \), i.e., \( \alpha_{dB} < 50 \) dB/cm (cf. Fig. 5.9).

1.5.1 Scope of this Thesis

The main obstacle in the path of the successful implementation of a PhC-based SOA is the large propagation loss of substrate-type W1 PhC waveguides. Moreover, the reason for this large propagation loss is not well understood. This thesis tries to fill those missing gaps by (i) advancing the theory of the loss mechanisms in slab PhC waveguides, (ii) by developing numerical methods to accurately model the propagation losses and by (iii) proposing alternative PhC waveguide designs that have lower propagation losses.

The content of the thesis is as follows:

- **Chapter 2 – Theory of Slab Photonic Crystal Waveguides** introduces fundamental concepts of waveguide theory at the example of a slab waveguide. The aim of this introduction is two-fold: First a slab waveguide is used as the vertical guiding structure of planar PhC waveguides. Second, we aim at a proper introduction of the mode theory terms that are used in the following chapters. Furthermore, we give a short introduction to slab PhCs and line-defect PhC waveguides. A particularity of this introduction is the Fourier representation of a Bloch wave.

- **Chapter 3 – Computation of Dispersion Diagram of PhCs** The optimization of PhCs and line-defect PhC waveguides is a key issue for successfully engineering PhC devices. This design task is computationally expensive. Therefore, we present two contributions to improve the design process. First, mode-map plots for line-defect PhC waveguides are introduced. The aim of mode-map plots is to determine the relevant PhC parameters that can be used to modify the mode of the line-defect PhC waveguide according the specific needs. The process largely reduces the computational design task. Second, the available codes to compute the dispersion relation are reliable but not very efficient. This is even more pronounced for dispersive materials. Therefore, we present a new method based on higher order finite elements with curved cells that allows to solve for the band structure taking dispersive materials into account. This is accomplished by reformulating the wave equations as a linear eigenproblem in the complex wave vectors \( k(\omega) \). The high numerical efficiency for the computation of guided PhC waveguide modes is demonstrated by a convergence analysis.

- **Chapter 4 – Loss Mechanism in Substrate-Type Photonic Crystal Waveguides** presents a theory about the loss mechanism in slab PhC waveguides. The
theory consists of five hypotheses and is based on two concepts: i) the Fourier representation of a Bloch wave (cf. Sec. 2.2.3) and the ii) background concept (cf. Sec. 4.5 and Kaspar et al. [121]) that describes the region in the dispersion diagram of oscillatory fields in the (infinite) cladding layers. We test the hypotheses for a number of examples including slab waveguides, weak periodic modulations (Bragg grating), membrane-type W1 PhC waveguide and substrate-type PhC waveguides. So far no falsification of the hypotheses was found.

- **Chapter 5 – Computation of the Propagation Losses of PhC Waveguides** The theory that we introduce in chapter 4 does not provide a simple analytical formula for the propagation losses of line-defect PhC waveguides. Instead, we have reasons to believe that quantitative numbers of the propagation losses can only be obtained by advanced numerical methods. Therefore, a numerical method was developed to accurately compute the propagation losses. Currently, our efficient FEM method presented in chapter 3 supports only 2D and thus is not appropriate to compute out-of-plane losses. The 3D finite difference time domain (FDTD) method software package MEEP [206] provides a highly efficient parallel electromagnetic solver. The propagation losses are computed by implementing the experimentally employed cutback-method on the numerical transmission spectra obtained from 3D FDTD simulations. A remarkable agreement is found between the computed propagation losses and experimental data for almost the entire single-mode regime of the line-defect PhC waveguide. The method is of key importance to i) identifying the origins of the large propagation losses in substrate-type PhC waveguides and ii) to verify the propagation loss characteristics of new promising low-loss designs.

- **Chapter 6 – Structural Imperfections in Slab PhC Waveguides** presents a numerical study of the influence of fabrication imperfections on the propagation losses of a substrate-type line-defect PhC waveguide. The developed numerical method allows to accurately compute the propagation losses for a large number of structural imperfections and design considerations of the PhC waveguides. The performed set of numerical experiments allowed us to identify the angled-sidewalls of the hole shape resulting from the dry-etching process to be responsible for the fabrication related propagation losses.

- **Chapter 7 – Reducing the Propagation Losses of Substrate-Type PhC Waveguides** From the previous chapters (chapter 4 - chapter 6), a number of strategies can be deduced to reduce the propagation losses. All strategies are explored and discussed: the vertical layer stack is optimized for a realistic hole shape and we find an improvement of the propagation losses from about 1000 dB/cm to about 600 dB/cm. Then, we elaborate on the question if there are other line-defect PhC waveguide designs that have intrinsically lower propagation losses. Thereafter, we discuss the idea to modify the background to reduce the propagation loss. We find that enlarging the holes in the substrate results in propagation losses as low as 100 – 150 dB/cm. Finally, two processes are developed: the first aims at reducing the side-
Objectives and Contributions of this Work

wall angle of the etched hole-shape and the second complies with the most promising idea to increase the radius in the substrate layer. By using the two new processes, we experimentally demonstrate propagation losses as low as $\alpha_{dB} = 154$ dB/cm.

- **Chapter 8 – The Cross-Hair Device** Although substantially lower propagation losses ($\alpha_{dB} \approx 100$ dB/cm) can be achieved by relatively small modifications of the design and the fabrication process, the results of chapter 7 suggest that substrate-type line-defect PhC waveguides are limited to about $\alpha_{dB} \approx 70$ dB/cm in the best case. Therefore, we propose a new single-mode line-defect PhC waveguide design that is not yet compatible with our existing process, but that is promising for electrically pumped active PhC devices. As such the proposed PhC waveguide design allows for vertical carrier injection and simultaneously exhibits low propagation losses in the order of $\alpha_{dB} < 20$ dB/cm.

- **Chapter 9 – Conclusions and Outlook** summarizes the achievements and answers some hitherto open questions. We conclude about the initially posed question about the feasibility of electrically pumped single-mode line-defect PhC waveguides.
Theory of Slab Photonic Crystal Waveguides

Slab PhC waveguides are based on two different concepts for guiding the light: vertical index guiding and lateral band gap guiding as it is depicted in Fig. 2.1. This chapter consists of a critical review of the well-established theories of ray optics and mode theory to describe the propagation of light in a slab waveguide and of PhC theory to describe the propagation of light in a line-defect slab PhC waveguides. At the same time we introduce the terms, definitions and concepts that are required.

Figure 2.1: Guidance of light in a slab line-defect PhC waveguide (A): the lateral confinement of the light is due to band-gap guiding (B) and vertical confinement of the light is due to index guiding of the slab waveguide (C).
for the description of propagation losses and radiation phenomena in dielectric waveguides. However, the theory of propagation losses in line-defect slab PhC waveguides is not yet completely established and is discussed later in a separate chapter (chapter 4).

2.1 Asymmetric Slab Waveguide

A slab waveguide consists of at least three stacked planar layers: a high refractive index core layer is sandwiched between two cladding layers having a lower refractive index than the core layer and is shown in Fig. 2.4. Light is guided in the core of the slab waveguide due to index guiding [104]. Index-guiding originates from the notion of a propagating ray that is totally internally reflected every time the ray impinges on the dielectric interface of the slab waveguide. Ray optics is capable to deliver a necessary condition for loss-free propagation of light in a slab waveguide. Furthermore, if the phase and polarization information is added to the rays, the eigenvalue equation describing the guided modes is obtained. Another reason for the introduction of ray optics is that it is the traditional concept to describe the phenomenon of leaky waves (as defined later in Sec. 4.7) observed in fibers [249, 253, 251, 252] and in slab waveguides [170, pp. 31][275].

Thereafter we introduce the mode theory. Mode theory results in the same eigenvalue equation for the guided modes and the same necessary condition for loss-free propagation of light in slab waveguides as it results from ray optics. Furthermore, mode theory provides a complete basis set that can be used to model propagation losses and radiation phenomena.

2.1.1 Ray Optics Model

Ray optics is typically applied to geometries that are larger than the wavelength of the light and thus its application to single-mode slab waveguides and to PhCs is questionable. However, in the case of slab waveguides, ray optics has successfully been applied to describe the guiding of light.

2.1.1.1 Foundations of Ray Optics

- **Assumption:** A ray can represent the propagation of light by a narrow straight beam. A ray is strongly localized, since it’s lateral dimension is neglected. The propagation velocity of a ray in a given medium is characterized by the refractive index \( n \geq 1 \), which is the ratio of the speed of light in free space \( c_0 \) to the one in the medium \( c_m \). \( n = c_0 / c_m \)

- **Assumption:** Scatterer \( \gg \lambda \). Ray optics is usually applied for objects and structures that are a lot larger than the wavelength of the light. For those cases, phenomena such as transmission, reflection and refraction can be accurately described by rays. If it comes to smaller objects, where the wave nature of the light is important, then ray optics fails to describe phenomena such as interference or diffraction, because of the missing phase infor-
mation. This can be cured if the phase information and the polarization is attached to the ray.

- **Snell’s law.** If light impinges with an angle $\theta_1$ on an interface formed by two different dielectric materials ($n_1, n_2$), then Snell’s law describes the geometrical continuation of the light propagation (refraction)

  \[ n_1 \sin(\theta_1) = n_2 \sin(\theta_2). \] (2.1)

- **Total internal reflection and guidance of light.** From Eq. 2.1 it follows that there is an incident angle $\theta_1$, for which the outgoing angle $\theta_2$ becomes imaginary. In this case, the light is totally internally reflected. The critical angle $\theta_c$, where total internal reflection sets in is given by $\theta_1 = \theta_c \geq \arcsin \left( \frac{n_2}{n_1} \right)$. If light propagates between two such interfaces, such that it is totally internally reflected at both interfaces, then the light is guided without loss. This is illustrated in Fig. 2.2 c).

### 2.1.1.2 The Representation of Modes in the Ray Optics Concept

We consider an asymmetric planar layer consisting of a substrate layer with refractive index $n_2$, a core layer of thickness $d$ and refractive index $n_1$ and a cover layer with refractive index $n_3$ as shown in Fig. 2.2. Furthermore, we assume that $n_1 > n_2 > n_3$. The path of the ray is sketched in Fig. 2.2 by ray optic principles for three distinct cases of incident angles

- **a) Two-sided radiation modes** : $\theta_r < \arcsin \left( \frac{n_3}{n_1} \right)$. The light impinges with a small angle $\theta_r$ such that the light is partially transmitted through the three layers and partially reflected at the interfaces. No total internal reflection occurs. If the rays are locally perceived as plane waves, then the incoming field of the ray interferes with the field of the reflected ray and forms a transverse standing wave in the top-cladding and the substrate.

- **b) Single-sided radiation modes (also referred to as substrate modes)** : $\theta_s < \arcsin \left( \frac{n_2}{n_1} \right)$. The incident angle $\theta_s$ is such that the light is totally internally reflected at the interface formed by the core and the top-cladding, but thereafter is transmitted back to the substrate. A transverse standing wave

![Figure 2.2](image-url)  

Figure 2.2: The superposition of the incoming and reflected rays leads to standing waves in the three regions. The standing wave pattern depends on the incident angles $\theta_r, \theta_s$. 


is established in the substrate by the interference of the incoming with the reflected rays.

- **c) Guided modes**: \( \theta_g \geq \arcsin \left( \frac{n_2}{n_1} \right) \). If a ray in the core travels with an angle \( \theta_g \), the ray is totally internally reflected at both interfaces and is hence guided in the waveguide core. Note that the impinging angle of a ray from the outside would have to be increased beyond \( \frac{\pi}{2} \) in order that the requirement \( \theta_g \geq \arcsin \left( \frac{n_2}{n_1} \right) \) can be fulfilled. Hence, a guided mode requires a ray with a source located in the core layer.

### 2.1.1.3 Derivation of the Eigenvalue Equation for Guided Modes

For the mathematical description of modes, we already need to extend ray optics by the concept of local plane waves [250, p. 666]. Plane waves have a well defined phase and are of infinite lateral extent, such that they overlap and interfere. In this way a phase is attached to the ray by the notion of the optical path length [170, p. 4]. Figure 2.3 shows the guided mode by using rays and their corresponding local plane wave representation. The wave number \( k \) of the plane wave in the slab waveguide core is given by the refractive index of the core medium \( k = \frac{\omega n_1}{c} = n_1 k_0 \).

The accumulated transverse phase for one round trip (indicated by the two red arrows in Fig. 2.3) must add up to a multiple of \( 2\pi \), and thus the condition (eigenvalue equation) for constructive interference reads

\[
2k_0 n_1 d \cos(\theta_g) = m 2\pi,
\]

where \( m \) is an integer number. While the plane wave undergoes the total internal reflection, a phase-shift is added to the propagating light. This phase shift depends on the polarization of the plane wave [100, p.386] and is given by the Fresnel coefficients rather than by Snell’s law. Thus, a different discrete guided mode set is obtained for the two cases of an electric field perpendicular or parallel to the plane.

Figure 2.3: A guided mode is formed by the interference of the propagating light with its total internal reflection. The interference process results in a propagating wave that propagates along the \( e_x \)-direction with propagation constant \( \beta_x \).
of incidence. The phase shift per interface is given by [100, p.386]:

$$\phi_{TE\,2,3} = \arctan \left( \frac{\sqrt{n_1^2 \sin^2(\theta_g) - n_{2,3}^2}}{n_1 \cos(\theta_g)} \right)$$ (2.3)

$$\phi_{TM\,2,3} = \arctan \left( \frac{n_1^2 \sqrt{n_1^2 \sin^2(\theta_g) - n_{2,3}^2}}{n_{2,3}^2 \ n_1 \cos(\theta_g)} \right)$$ (2.4)

and hence the final eigenvalue equations for the TE and the TM modes are

**TE-Mode:**

$$k_0 n_1 d \cos(\theta_g) = m\pi - \phi_{TE\,2} - \phi_{TE\,3}$$ (2.5)

**TM-Mode:**

$$k_0 n_1 d \cos(\theta_g) = m\pi - \phi_{TM\,2} - \phi_{TM\,3}$$ (2.6)

The propagation constant $\beta_{x,m}$ of the guided modes is oriented in horizontal direction $e_x$ and is obtained by

$$\beta_x = \sqrt{k^2 - k_z^2} = \sqrt{k(1 - \cos^2 \theta)} = \frac{\omega n_1}{c} \sin \theta$$

(cf. Fig. 2.3), where $k = k_0 n_1$ is the wave number of the local plane wave in the core. Guided modes are obtained, if the angle $\theta_g$ is larger than the critical angle $\theta_c$, i.e.,

$$\beta_x > \frac{\omega n_1}{c} \max(n_3, n_2) \frac{n_1}{n_1} = \max(n_3, n_2) \cdot \frac{\omega}{c}. \quad (2.7)$$

If Eq. 2.7 holds, then the rays are totally internal reflected and a wave propagates without loss. If $\beta_x < \max(n_3, n_2) \cdot \frac{\omega}{c}$, then the ray is partially reflected back into the core and partially transmitted into the cladding layers. The propagating wave radiates energy from the core to the cladding: The wave propagating in the core is attenuated. Eq. 2.7 is thus a necessary condition for loss-free guidance of light in the slab waveguide core. This condition defines the so-called light-line

$$\beta(\omega) = \max(n) \frac{\omega}{c}.$$

### 2.1.1.4 Conclusion

We discussed the index-guiding mechanism by means of propagating rays that are totally reflected at the boundaries of the dielectric interfaces. Ray optics provide a intuitive notion for the mode concept if the rays are locally replaced by plane waves with a proper phase and wave number $k$. The interference of two plane waves with alternating directions form standing waves patterns in transverse direction $e_z$. We will see in the following sections that the condition Eq. 2.7 for the existence of loss-free guided modes as well as its description by the eigenvalue equation is equivalent to the results obtained by the mathematically more rigorous mode theory. Furthermore, a radiative wave is excited, if the incident angle $\theta_g < \theta_c$. The excitation of a radiative wave (we will call this wave a leaky wave) represents the main loss mechanism in substrate-type PhC waveguides and is discussed in detail
2.1.2 Mode Theory

A more rigorous approach is to seek solutions of Maxwell’s equations that satisfy the boundary conditions defined by the slab waveguide. As opposed to ray optics, mode theory results in modes that form a complete basis set. In other words, any wave phenomena of the slab waveguide with non-absorbing materials can be expressed in terms of these modes. In this chapter, an overview of all types of possible modes is put together along with its formal descriptions. The detailed derivation of the mode solutions can be found in the textbooks of Marcuse [170, 169] and Chuang [40].

For this analysis, only loss-less materials ($\varepsilon(r) = \Re\{\varepsilon(r)\}$) in the absence of electric charges ($\varrho = 0$) and currents ($\mathbf{J} = 0$) are considered.

2.1.2.1 TE and TM Modes

The asymmetric slab waveguide as depicted in Fig. 2.4 is invariant in propagation direction $e_x$. Because of that, the modes of the asymmetric slab waveguide can be classified according to two independent polarizations: TE modes (TM modes) have a magnetic (electric) field component in the propagation direction, i.e., $E_x = 0$ ($H_x = 0$). Note that these two types of modes can be associated with two different boundary conditions. For TE-modes ($E_x = 0$) the tangential magnetic field components are continuous at the interface ($\mu \frac{\partial H_x}{\partial n} |_{S = 0}$ is fulfilled on the dielectric interface $S$) whereas for the TM-modes ($H_x = 0$) the tangential electric field components are matched at the interface ($E_x |_{S = 0}$ is fulfilled) [100].

Without loss of generality, we can assume that the propagation is exclusively along the $e_x$-direction, i.e., the fields are independent of $y$, i.e., $\partial/\partial y = 0$ and it follows that $E_z = H_y = 0$. This assumption is not a restriction, since it is always

![Figure 2.4: Sketch of a slab waveguide, where $x$ is the propagation direction. The refractive index depends only on the $z$-coordinate $n(r) = n(z)$.](image-url)
possible to rotate the coordinate system in the \(x\)-\(y\) plane such that the propagation direction is \(e_x\). For this particular case, the scalar homogeneous Helmholtz equation (Eq. A.15) for the electric field may be used to solve for the TE eigenmodes:

\[
- \Delta E_y(x, z, t) + \varepsilon(z) \left( \frac{\omega^2}{c^2} \right) E_y(x, z, t) = 0
\]

(2.8)

Once \(E_y\) is found, the remaining non-zero field components \((H_x, H_z)\) can be computed by using Faraday's law (Eq. A.6)

\[
H_x = \frac{i}{\omega \mu_0} \frac{\partial}{\partial z} E_y
\]

(2.9)

\[
H_z = \frac{1}{\omega \mu_0} \frac{\partial}{\partial x} E_y = -\frac{\beta_x}{\omega \mu_0} E_y
\]

(2.10)

Analogous to the TE case, it can be shown that \(E_y = H_z = 0\) for the TM case. Therefore, to compute TM modes, the scalar Helmholtz equation (Eq A.16)

\[
- \Delta H_y(x, z, t) + \left( \frac{\omega^2}{c^2} \right) H_y(x, z, t) = 0
\]

(2.11)

has to be solved in every layer. The remaining non-zero field components \((E_x, E_z)\) can be calculated from the resulting \(H_y\) by using Ampere’s law (Eq. A.5)

\[
E_x = -\frac{i}{n^2 \omega \varepsilon_0} \frac{\partial}{\partial z} H_y
\]

(2.12)

\[
E_z = -\frac{\beta}{n^2 \omega \varepsilon_0} H_y
\]

(2.13)

In the following, we focus on the TE Modes only. The procedure to obtain the TM modes is analogous to the one for TE modes.

### 2.1.2.2 The Description of Modes

The electric field \(E_y\) can be separated as an ‘ansatz’ into a transverse and a longitudinal function

\[
E_y(x, z, t) = e(z) e^{i(\omega t - \beta_x x)}.
\]

(2.14)

for the case of time harmonic fields propagating along \(e_x\). The transverse function \(e(z)\) is independent of the propagation distance \(x\) and time \(t\). This means that the transverse mode profile will maintain its shape along the propagation direction \(e_x\) except for a phase change [170, p. 33]. We have seen in the previous section that the incident and reflected rays form standing waves in the cladding and in the core layer. The used function prototypes for the transverse function \(e(z)\) are motivated by this notion and reflect the three possible cases: a decaying transverse function \(e(z)\) (i.e., \(\lim_{|z| \to \infty} e(z) = 0\)), standing waves in the claddings (radiation modes) or a growing transverse function \(e(z)\) (leaky modes).
The Helmholtz equation

$$\frac{d^2}{dz^2} e(z) - \left[ \beta_x^2 - n^2(z) k_0^2(\omega) \right] e(z) = 0.$$  \hfill (2.15)

for the amplitude of the transverse electric fields $e(z)$ is obtained, if the separation ansatz Eq. 2.14 is inserted into Eq. 2.8 and if $\varepsilon(z) = n^2(z)$ and $\frac{\omega^2}{c^2} = \omega^2 \varepsilon_0 \mu_0 = k_0^2(\omega)$ are used.

### 2.1.2.3 Guided TE Modes

We start by discussing solutions of the Helmholtz equation that satisfy the boundary conditions and decay in the cladding $e(z \pm \infty) = 0$:

$$e(z) = \begin{cases} 
A e^{-\delta z} & z > d \\
A \cos(\kappa z) + B \sin(\kappa z) & -d < z < 0 \\
(A \cos(\kappa d) + B \sin(\kappa d)) e^{\gamma(z+d)} & z < -d 
\end{cases}$$  \hfill (2.16)

where $\kappa = \sqrt{k_i^2 - \beta_x^2}$, $\gamma = \sqrt{\beta_x^2 - k_0^2 n_i^2}$ and $\delta = \sqrt{\beta_x^2 - k_0^2 n_i^2}$ and $k_i = n_i \omega/c = n_i k_0$. We follow here the notation used by Marcuse [170]. The equations above already satisfy the boundary conditions for the tangential electric fields. By applying the boundary conditions for the tangential magnetic fields, an eigenvalue equation with eigenvalue $\kappa$ results (the detailed mathematical treatment can be found in the appendix A.1)

$$dk = \arctan \left( \frac{(\gamma + \delta) \kappa}{k_i^2 - \gamma \delta} \right) + m \cdot \pi.$$  \hfill (2.17)

This eigenvalue equation is usually solved numerically. Note that the eigenvalue equation results in a discrete set of eigenvalues $\kappa_m$ and hence discrete values for the propagation constant $\beta_{x,m} = \sqrt{k_i^2 - \kappa_m^2}$. Further note that an exponential decay is only obtained for $\beta_{x,m} > k_0 n_i$ and $\beta_{x,m} > k_0 n_3$. Thus, a mode is only confined to the core of the slab waveguide and guided loss-free if $\beta_{x,m} > \max(n_2, n_3) \cdot k_0$. This is equivalent to the light-line condition (Eq. 2.7).

The electric field of a guided mode $E_m$ can thus be modeled with

$$E_m := E_y(x, z, t) = e(z) e^{i(\omega t - \beta_{x,m} x)},$$

where $\beta_{x,m}$ is determined by Eq. 2.17.

### 2.1.2.4 TE Radiation Modes

Next, we consider the two different kinds of radiation modes of the asymmetric slab waveguide (cf. Sec. 2.1.1.2). A radiation mode is characterized by spatially oscillating fields in at least one of the cladding layers.

**a) Single-sided radiation modes** ($k_0 n_2 > |\beta_x| > k_0 n_3$): represent the situation in ray optics (cf. Sec. 2.2), where light is impinging from the bottom with an angle $\theta'$, such that the light is totally internally reflected at the interface between region
and region 3. This leads to evanescent fields in the cover layer and to oscillating fields in the substrate. The ansatz for the transverse function $e(z)$ reflecting our notion from ray optics is (we strictly follow the notation of Marcuse [170, p. 22])

$$e(z) = \begin{cases} 
A_r e^{i\Delta z} & z > 0 \\
A_r \cos(\sigma z) + B_r \sin(\sigma z) & -d < z < 0 \\
[A_r \cos(\sigma d) + B_r \sin(\sigma d)] \cos(\rho(z + d)) + \bar{C}_r \sin(\rho(z + d)) & z < -d 
\end{cases} (2.18)$$

where

$$\Delta = \sqrt{k_3^2 - \beta_x^2} \quad (2.19)$$
$$\sigma = \sqrt{k_1^2 - \beta_x^2} \quad (2.20)$$
$$\rho = \sqrt{k_2^2 - \beta_x^2}. \quad (2.21)$$

The choice of the amplitude coefficients $A_r$, $B_r$ and $\bar{C}_r$ keep the field expression general and simultaneously guarantee that Eq. 2.18 satisfies the boundary conditions given by the slab waveguide. By further imposing the boundary conditions for $H_x$ for $z = 0$ and $z = -d$, two additional conditions are obtained

$$-i\sigma B_r = \Delta A_r \quad (2.22)$$
$$\sigma \cos(\sigma d) B_r - \rho \bar{C}_r = -\sigma \sin(\sigma d) A_r. \quad (2.23)$$

The coefficients $B_r$ and $\bar{C}_r$ directly depend on $A_r$. The coefficient $A_r$ however cannot be determined from the available equations. Thus, the eigenmode $E$ is determined except for a factor $A_r$. For any eigenvalue $\beta_x$ within the range $k_0 n_2 > |\beta_x| > k_0 n_3$, an $A_r$ can be found such that the combination of $A_r$, $B_r$ and $\bar{C}_r$ satisfies Eq. 2.18-Eq. 2.23. Hence, the eigenmodes $E$ form a continuum of modes.

b) Two-sided radiation modes $k_0 n_3 \geq |\beta|$: represent the situation in ray optics (cf. Sec. 2.2), where the impinging light interferes with its reflection forming a standing wave in the top and in the bottom layer. The transverse function $e(z)$ that satisfies Maxwell’s equations and the boundary condition is [170, p. 25]

$$e(z) = \begin{cases} 
C_r [\cos(\Delta z) + (\sigma / \Delta) F_i \sin(\Delta z)] & z > 0 \\
C_r [\cos(\sigma z) + F_i \sin(\sigma z)] & -d < z < 0 \\
C_r \{(\cos(\sigma d) - F_i \sin(\sigma d)) \cos(\rho(z + d)) + ... \\
... + (\sigma / \rho) \{(\sin(\sigma d) + F_i \cos(\sigma d)) \sin(\rho(z + d)) \} & z < -d 
\end{cases} (2.24)$$

The transverse field $e(z)$ given in Eq. 2.24 oscillates in all three layers.
Let us discuss the transverse wave number $\rho$. $\rho$ describes the oscillation of the standing wave in the bottom cladding. The standing wave is given by the superposition of the impinging ray with incident angle $\theta'$ and its reflection at the interfaces of the slab waveguide and is essentially defined by the incident wave. Therefore, $\rho$ is allowed to assume all real values from 0 to $\infty$. Three different domains of $\rho$ can be identified

\begin{align}
0 \leq \rho & \leq \sqrt{n_2^2 - n_3^2k} \\
\sqrt{n_2^2 - n_3^2k} \leq \rho & \leq n_2k \\
n_2k \leq \rho & \leq \infty
\end{align}

The first domain ($0 \leq \rho \leq \sqrt{n_2^2 - n_3^2k}$) represents single-sided radiation modes that have only oscillatory fields in the bottom layer and an exponentially decaying function in the top cladding (cf. Fig. 2.5 C). The second domain ($\sqrt{n_2^2 - n_3^2k} \leq \rho \leq n_2k$) corresponds to double-sided radiation modes that have oscillatory fields in the top and the bottom cladding (cf. Fig. 2.5 D). These two types of radiation modes have real propagation constants $\beta_x$. The last domain $n_2k \leq \rho$ represents another type of radiation modes. Those radiation modes have purely imaginary propagation constants $\beta_x = \sqrt{k_2^2 - \rho^2}$ for $\rho > n_2k$. These radiation modes decay along the propagation direction $e_x$ and oscillate along the transverse direction $e_z$. Therefore, they are called evanescent radiation modes. These modes represent waves that propagate laterally across the slab waveguide. Because of the exponential decay in propagation direction, they are irrelevant for the propagation of light along the propagation direction of infinitely long slab waveguides. The transverse wave number $\rho$ in the bottom cladding is a good parameter to characterize radiation modes.

The electric field of a radiation mode $E(\rho)$ is modeled with

$$E(\rho) := E_y(x, z, t, \rho) = e(z, \rho)e^{i(\omega t - \beta_x(\rho)x)},$$

where the propagation constant $\beta_x(\rho)$ depends on the parameter $\rho$.

### 2.1.2.5 Leaky Modes

There is another type of mode that fulfills the eigenvalue equation for guided modes (Eq. 2.17).

$$d\kappa = \arctan\left(\frac{(\gamma + \delta)\kappa}{\kappa^2 - \gamma\delta}\right) + m \cdot \pi$$

These so far undiscussed mode solutions have a complex eigenvalue $\kappa$. A complex eigenvalue $\kappa$ automatically leads to a complex propagation constant $\beta_x$ because of $\beta_x = \sqrt{k_2^2 - \rho^2}$ and hence to an exponentially decaying or increasing function in propagation direction $e_x$. Let $\beta_{r,x}$ denote the real part of $\beta_x$ and $\beta_{i,x}$ the imaginary part of $\beta_x$, i.e., $\beta_x = \beta_{r,x} + i\beta_{i,x}$. Actually, we did not explicitly allow for complex propagation constants. Therefore we investigate now the possible consequences
for the case of complex propagation constants in the ansatz (Eq. 2.14). If the propagation constant is a complex number, then the longitudinal dependence of the fields is $e^{i(\omega t - \beta_{r,x} x - i\beta_{j,x} z)}$ and the transverse dependence is $e^{i\zeta_m z}$, where $\zeta_m$ is the transverse wave number for the regions $m \in \{1, 2, 3\}$. Because of the imaginary part of the propagation constant, the mode solution either grows or decays exponentially in propagation direction. Therefore, this mode is called leaky modes. By inserting the ansatz into the wave equation Eq. 2.8, a condition for the transverse wave number $\zeta_m$ is obtained

$$\zeta_m^2 = n_m^2 k_0^2 - \beta_{r,x}^2 + \beta_{j,x}^2 - i2\beta_{r,x}\beta_{j,x} = u_m + i \cdot w_m,$$

(2.29)

where $u_m = n_m^2 k_0^2 - \beta_{r,x}^2 + \beta_{j,x}^2$ is the real part of $\zeta_m^2$ and $w_m = -2\beta_{r,x}\beta_{j,x}$ is the imaginary part of $\zeta_m$. The real and imaginary part of $\zeta_m$ can be given analytically as follows

$$\Re\{\zeta_m\} = \frac{1}{\sqrt{2}} \sqrt{\sqrt{u_m^2 + w_m^2} + u_m},$$

(2.30)

$$\Im\{\zeta_m\} = \frac{\text{sgn}(w_m)}{\sqrt{2}} \sqrt{\sqrt{u_m^2 + w_m^2} - u_m},$$

(2.31)

where $\text{sgn}(w_m)$ is the sign of $w_m$ (+1 if $w_m \geq 0$ and −1 if $w_m < 0$).

We start by considering a forward propagating wave ($\beta_{r,x} > 0$) that decays ($\beta_{j,x} < 0$) along the propagation direction $e_x$. In this case $w_m > 0$ and $u_m > 0$ for $\beta_{r,x}^2 + \beta_{j,x}^2 < n_m^2 k_0^2$. It directly follows from Eq. 2.30 and Eq. 2.31 that $\Re\{\zeta_m\} > 0$ and $\Im\{\zeta_m\} > 0$. That means that an exponentially growing transverse function $e(z) = e^{-i\zeta_m z} = e^{-i\Re\{\zeta_m\} z + \Im\{\zeta_m\} z}$ is obtained in the cladding for a forward propagating wave.

### 2.1.2.6 Comparison of the Mode Types

There are five different types of solutions of Maxwell’s equation that fulfill the boundary conditions for the asymmetric slab waveguide: guided modes, leaky modes, one-sided radiation modes, two-sided radiation modes and evanescent radiation modes. The transverse function of the five different modes is shown in Fig. 2.5. The propagation constant $\beta_x$ and the transverse wave number $\gamma, \rho$ and $\zeta_m=2$ for the bottom cladding layer are plotted in the complex plane for the five types of modes for a specific frequency $\omega_0$ in Fig. 2.6 (left) (cf. [152]). Guided modes and leaky modes have a discrete set of eigenmodes and their eigenvalues are depicted as ♦ and x in Fig. 2.6. On the other hand radiation modes have strictly real propagation constants $\beta_r$ and a continuum of modes. They are represented by the red and blue lines in Fig. 2.6. Note that the real part $\beta_{x,r}$ of the complex propagation constant $\beta_x$ of the leaky modes lies within the domain of radiation modes.

The dispersion diagram – the propagation constant $\beta_x(\omega)$ plotted as a function of the frequency $\omega$ – is shown in Fig. 2.7 and displays only the modes that have a real propagation constant $\beta_x$. The guided modes are characterized by a discrete set of propagation constants $\beta_{x,i}$ in the range $k_1 > \beta_x > \max(k_2, k_3)$. The dispersion curves of the guided modes end at the line given by $\max(k_2, k_3)$. These
Figure 2.5: $E_y$ for the five types of modes. A: guided mode with exponentially decaying fields in the cladding, B: leaky mode with exponentially increasing fields in the cladding (transverse direction) and with an exponentially decaying field in propagation direction $e_x$, C: substrate mode with oscillating fields only in the bottom cladding, D: radiation mode with oscillatory fields in both claddings and E: an evanescent radiation mode with oscillatory fields in both claddings and with an evanescent field in propagating direction $e_x$.

Figure 2.6: The five types of modes of a slab waveguide: propagating radiation modes have a real propagation constant $\beta_x$ that is bound by the range $-k_2 < \beta_x < k_2$ and a positive, real wave number in the cladding. Evanescent radiation modes decay in propagation direction, i.e., have a purely imaginary $\beta_x$ and are characterized by a $\rho > k_0 n_2$. Guided modes have discrete, real propagation constants in the range $|k_1| > |\beta_x| > |k_2|$ and decay in the cladding, i.e., $\gamma$ and $\delta$ are negative and purely imaginary. Finally, leaky modes have both a complex propagation constant $\beta_x$ and a complex transverse wave number $\zeta_m$. 
Figure 2.7: The first three guided TE modes are shown. For an asymmetric planar waveguide, there is a cut-off, which intersects with the line given by $\omega = \frac{c \cdot k}{\max(n_2, n_3)}$.

‘intersection’ points represent the mode cutoffs that are observed in asymmetric slab waveguides. For very high frequencies $\omega$, the dispersion curve of the guided modes approach the core light-line $\omega = \frac{c k}{n_1}$. The red area in the dispersion diagram represents the continuum of radiation modes that oscillate only in the bottom cladding ($k_0 n_2 > |\beta_x| > k_0 n_3$) and the orange area represents the continuum of radiation modes that have oscillatory fields in the top and bottom cladding ($k_0 n_3 \geq |\beta_x|$). The two areas are bounded by the lines given by $\omega = \frac{c k}{n_2}$ and by $\omega = \frac{c k}{n_3}$. The line given by

$$\omega = \frac{c k}{\max(n_2, n_3)}$$

marks the boundary that separates confined modes (guided modes) from unconfined modes (radiation modes). This boundary is referred to as the light-line or the separatrix. The same separatrix has already been obtained by the ray optics model (Eq. 2.7) and hence the mode cutoff can also be interpreted as the point, where the guided modes lose guidance by total internal reflection. Note that for more complex waveguide structures, the connections between light-line, separatrix and loss of total internal reflection is not straightforward.

**Practical Relevance of the Modes** Legitimately, one may ask about the practical relevance of the five different types of modes. Approximately, an individual guided mode may be excited by a localized, finitely extended source that approximates the mode profile of the guided mode. But, the required source to excite an individual radiation mode cannot be approximated by a source of finite extent. The physical interpretation of radiation modes should therefore not be on a single radiation mode but on the sum of many radiation modes. Any finite source excites infinitely many radiation modes and guided modes. The reason is that the radia-
tion modes and the guided modes form a complete basis set, such that any field pattern of the perfect slab waveguide can be decomposed in radiation modes \( \mathcal{E}(\rho) \) and guided modes \( \mathcal{E}_n \) according to [166]

\[
E_y = \sum_m C_m(x) \mathcal{E}_m + \int_0^\infty g(\rho, x) \mathcal{E}(\rho) d\rho.
\] (2.33)

The first term represents the summation of all guided modes \( \mathcal{E}_m \) weighted by a coefficient \( C_m \). The second term takes the continuum of all radiation modes \( \mathcal{E}(\rho) \) weighted by a factor \( g(\rho, x) \) into account. Marcuse [166, 167, 168] used this expansion along with a perturbation approach to compute the radiation losses originating from distortions of the dielectric interfaces of the slab waveguide. Numerically, this approach is inefficient, since an integration over a continuum of radiation modes has to be performed. The rigorous proof of the completeness of the basis set is not simple because the radiation modes do not have a finite energy. To proof the completeness, first an appropriate transformation has to be applied to map the modes with infinite energy to modes that have a finite energy. Then, the completeness of the transformed system can be proven by using the Sturm-Liouville theorem [164].

Because the radiation modes and the guided modes form a complete set of basis functions, the leaky modes can also be obtained by a superposition of radiation and guided modes. Recently, Liu [159] proved that guided modes and leaky modes also form a complete basis set. The expansion in guided and leaky modes has the advantage that only a finite set of modes is required for a good approximation. An expansion of the fields of an open waveguide in terms of leaky modes and guided modes was already proposed by Synder [250, ch. 24] and Shevchenko [242]. Lee et al. [152] applied the proposed expansion in leaky and guided modes of a multilayer slab waveguide and they found that a few leaky modes are sufficient to approximate the fields of the excited mode very accurately. A similar result was obtained by Lenz et al. for the case of a rectangular waveguide [154].

**Radiation Losses of the Waveguide** Guided modes and radiation modes share the property that their Poynting vectors are directed in propagation direction \( \mathbf{e}_x \) exclusively. Thus, one may ask how lateral radiation phenomena can be described by such a basis set. However, the summation of the electromagnetic fields of only two radiation modes already results in a Poynting vector that has a non-zero components along \( \mathbf{e}_z \). This is shown analytically in appendix A.2. To demonstrate that a summation of radiation modes is capable to model radiation phenomena of a slab waveguide, we numerically compute the electric field \( E_y(x, z) \) and the Poynting vector for a summation of 51 radiation modes. Figure 2.8 shows the resulting electric field \( E_y(x, z) \). The plot clearly shows a radiation field pattern. The inset depicts the Poynting vector for a small cut-out. A sum of radiation modes is thus able to describe out-going radiation with respect to the slab waveguide.
Figure 2.8: Electric field $E_y$ obtained by a superposition of 51 radiation modes in a slab waveguide (horizontal lines at $z = 0$ and $z = -d$). The inset shows the Poynting vector for a small cut-out. The Poynting vector clearly points away from the slab waveguide. The radiation modes $\mathcal{E}(\rho)$ were selected according to a Gaussian distribution in the wave vector space $g(\rho,z) = e^{-(\beta_x - \beta_x,i)/(2\sigma')}$. Following parameters were used: $n_1 = 3.5$, $n_2 = 2.8$, $n_3 = 1$, $d = 261$ nm, $\lambda = 1550$ nm, $\beta_x = 0.95 \cdot k_0 \cdot n_2$, $\beta_x,i = \{-0.048, \ldots, 0.048\} \cdot k_0 \cdot n_2$ and $\sigma' = 0.024 \cdot k_0 \cdot n_2$.

2.1.3 Conclusion

Ray optics is not suitable for the investigation of a slab waveguide in a traditional sense. However, by using the concept of local plane waves to represent rays, i.e., replacing the propagating ray in the waveguide core with a local plane wave [250, ch.35,p.666], an eigenvalue equation and a condition for loss-free guiding are obtained that describe the phenomenon of light guidance in slab waveguides adequately. We can conclude so because the same eigenvalue equation and guiding-condition are found by using a separation ansatz that satisfies both, the Maxwell equations and the boundary conditions imposed by the slab waveguide. Loss-free guided modes are found, if the dispersion of the guided modes is located below the light-line. The obtained set of guided modes and radiation modes represent a complete basis set that can be used to describe radiation phenomena of the slab waveguide.

The common perception of the guiding mechanism of slab PhC waveguides is that the slab provides the vertical index guiding due to total internal reflection and the PhC provides the lateral confinement due to the photonic band gap [137]. A propagation constant $\beta_x < k_0 n_{cladding}$ leads to a loss of total internal reflection and the propagating mode becomes lossy. We will see in section 4.5 that this notion is not strictly correct for substrate-type PhC waveguides.

2.2 Photonic Crystals

PhCs are characterized by a spatially periodic modulation of the refractive index in the order of the wavelength of the light [104]. In analogy to semiconductor
materials whose periodic electrical lattice potential gives rise to a band of forbidden electron energies (frequencies) for electron waves, in PhCs the periodic refractive index modulation creates forbidden bands of photon frequencies for optical waves. Within these forbidden frequency ranges – the photonic band gap (PBG) – the propagation of light is prohibited (cf. Sec. 2.2.1.4). Similar to the electronic counterpart, defects in the lattice result in additional, localized photonic states. Energy states that emerge within the photonic band gap lead to strongly localized modes at this defect. A single defect in the lattice forms a cavity. An entire row of defects corresponds to a channel for photons – a waveguide. Since no propagation is allowed at frequencies within the band gap of the crystal, the light has to follow the defect line, even around sharp corners [186, 224] or is reflected in backward direction.

PhCs can be built either in one, two or three dimensions (cf. Fig. 2.9). Although three-dimensional PhCs are the most favorable because of their property to exhibit a complete photonic band gap in all directions, their fabrication remains challenging. To simplify the fabrication, the concept of planar PhCs is usually employed. The PhC pattern is reduced to two dimensions (horizontal plane), whereas the light guiding in the vertical dimension is achieved by conventional index guiding. Commonly, one distinguishes between strong index guiding – membrane-type PhC (cf. Fig. 2.20 a) – and weak index guiding – a substrate-type PhC waveguide structure (cf. Fig. 2.20 b)).

![Figure 2.9: Generic examples for one (A), two (B) and three (C) dimensional PhCs having a rectangular lattice. The different colors represent a different permittivity $\varepsilon_r(r)$.](image)

2.2.1 Photonic States Physics

Photonic states – electromagnetic eigenmodes of the PhC – share the symmetry properties of the periodic permittivity pattern. Therefore, the eigenmodes of the PhCs are best characterized by their symmetry properties.
2.2.1.1 Translational Symmetry: The Floquet-Bloch Theorem

We consider a periodic modulation of the permittivity \( \varepsilon(r) \) such that

\[
\varepsilon(r) = \varepsilon(r + a), \tag{2.34}
\]

where \( r \) is the position vector and \( a \) is a translation vector. The system has a discrete translational symmetry, i.e., it is invariant under a translation by \( a \). The Floquet-Bloch theorem states that the eigenfunctions of the Helmholtz equation in a system of a periodic permittivity \( \varepsilon(r) \), can be written as the product of a plane wave \( e^{i k r} \) and a periodic envelope function \( u_k(r) = u_k(r + a) \) that shares the periodicity of the permittivity [127, p.167]

\[
\psi_k(r) = u_k(r) \cdot e^{i k r}. \tag{2.35}
\]

\( \psi_k \) is called a Bloch wave or a Bloch state and stands either for the electric field \( E \) or the magnetic field \( H \) in case of a PhC and \( k \) is the Bloch index. Note that only the envelope function \( u_k(r) \) is periodic with periodicity \( a \), and not the Bloch wave \( \psi_k(r) \) itself [127, p.171] [192, p.133].

2.2.1.2 The Reciprocal Lattice

We first expand the periodic function \( u_k(r) \) and \( u_k(r + a) \) in spatial harmonics

\[
u_k(r) = \int g(b) e^{i b r} d^3b \tag{2.36} \]

\[
u_k(r + a) = \int g(b) e^{i b r} e^{i b a} d^3b \tag{2.37} \]

where \( g(b) \) are the coefficients of the ‘space harmonics’ \( e^{i b r} \) and \( b \) its wave vector (cf. Joannopoulos et al. [104, Appendix B]). The condition \( u_k(r) = u_k(r + a) \), i.e., \( \int g(b) e^{i b r} d^3b = \int g(b) e^{i b r} e^{i b a} d^3b \) is only satisfied for \( e^{i b \cdot a} = 1 \). For a given lattice vector \( a \), a wave vector \( b \) is obtained such that

\[
b \cdot a = 2\pi. \tag{2.38}\]

is fulfilled. This specific wave vector \( b \) is referred to as the reciprocal lattice vector. A 3D PhC is defined by three lattice vectors \( a_1, a_2 \) and \( a_3 \) and its correspondent reciprocal lattice vectors are

\[
b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot a_2 \times a_3} \tag{2.39} \]

\[
b_2 = 2\pi \frac{a_3 \times a_1}{a_2 \cdot a_3 \times a_1} \tag{2.40} \]

\[
b_3 = 2\pi \frac{a_1 \times a_2}{a_3 \cdot a_1 \times a_2}. \tag{2.41} \]

The derivation of the reciprocal lattice vectors for a 2D PhC can be found in ap-
pendix A.3. The reciprocal lattice vectors span the wave vector space of the Bloch modes. Thus, the wave vectors \( \mathbf{b}_i \) of the Bloch modes are periodic with the periodicity of the reciprocal lattice.

**Translational Symmetry of the Reciprocal Lattice**  
The importance of the periodicity of the wave vectors of the Bloch mode is best explained by an example. Therefore, we consider a 1D periodic system with periodicity \( a \) in \( x \)-direction. The wave vectors \( k_x \) of the Bloch mode are periodic with \( 2\pi/a \), i.e., \( k_x = \hat{k}_x + m2\pi/a \), where \( m \in \mathbb{Z} \). Consider the following mathematical conversions

\[
\psi_{k_x}(r) = u_{\hat{k}_x}(x) \cdot e^{ikx}
\]

\[
= e^{ik_x x} \sum_m A_m e^{im2\pi/a x}
\]

\[
= e^{i(\hat{k}_x + l2\pi/a)x} \sum_m A_m e^{i(m-l)2\pi/a x}
\]

\[
= e^{i(\hat{k}_x + l2\pi/a)x} \sum_{p=m-l} A_{p+l} e^{ip2\pi/a x}
\]

\[
= e^{i(\hat{k}_x + l2\pi/a)x} u_{\hat{k}_x + l2\pi/a}(x)
\]

(2.42)

\( \sum_{p=m-l} A_{p+l} e^{ipKx} \) is a different periodic function with periodicity \( 2\pi/a \) and is associated with the wave vector \( k_x = \hat{k}_x + l2\pi/a \). Thus, the any wave vector \( \hat{k}_x + l2\pi/a \) produces the same Bloch function \( \psi_{\hat{k}_x} \). From this it follows that only one wave vector \( \hat{k}_x \) is required to compute the Bloch mode. Usually, the wave vector in the first Brillouin zone is used to determine the Bloch mode and we refer to it as the **Bloch index** \( \hat{k}_x \).

### 2.2.1.3 Crystal Symmetries and the First Brillouin Zone

The symmetries of the periodic permittivity pattern appear in the electromagnetic modes of the system and can thus be used for a categorization of the modes. In the following, we discuss the symmetries for the example of a hexagonal lattice of circular air holes as shown in Fig. 2.10. The lattice is given by the fundamental (or primitive) lattice vectors

\[
\mathbf{a}_1 = \left( \begin{array}{c} \sqrt{3}/2 \\ 1/2 \end{array} \right) a \quad \mathbf{a}_2 = \left( \begin{array}{c} \sqrt{3}/2 \\ -1/2 \end{array} \right) a.
\]

and are shown in the left sketch of Fig. 2.10. Note that this choice is not unique (cf. chapter 3.2). The reciprocal lattice vectors \( \mathbf{b} \) spanning the wave vector space is obtained using Eq. A.29 and Eq. A.30

\[
\mathbf{b}_1 = \frac{2\pi}{a} \left( \begin{array}{c} 1 \\ -1/\sqrt{3} \end{array} \right) \quad \mathbf{b}_2 = \frac{2\pi}{a} \left( \begin{array}{c} -1 \\ 1/\sqrt{3} \end{array} \right)
\]

(2.43)

Figure 2.10 (right) displays the reciprocal lattice vectors \( \mathbf{b}_1 \) and \( \mathbf{b}_2 \) and the re-
Figure 2.10: Left: hexagonal lattice of circular holes. Right: the associated reciprocal lattice (red) and the irreducible Brillouin zone (gray colored area).

ciprocal lattice. The hexagonal reciprocal lattice shares the symmetry properties of the permittivity $\varepsilon(\mathbf{r})$. All symmetries of the permittivity are found again in the wave vector space: For example, the angle between the vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ is conserved in the reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$. The hexagonal lattice has six different mirror symmetries and five different rotational symmetries [228, p.75]. Actually, the rotation symmetries and mirror symmetries are only obtained because of the circular hole shape, i.e., they would not exist for quadrilateral holes. Operators can be defined for all symmetries. For example, if a lattice has a mirror symmetry with respect to the $x - z$ - plane, then the symmetry is reflected in the wave function $\hat{\psi}_\mathbf{k}$ according to

$$\hat{\psi}_\mathbf{k}(-\mathbf{r}) = \sigma_y \hat{\psi}_\mathbf{k}(\mathbf{r})$$

where the mirror operator $\sigma_y$ is defined as

$$\sigma_y : \left( \begin{array}{c} x \\ y \end{array} \right) \rightarrow \left( \begin{array}{c} x \\ -y \end{array} \right).$$

Table 2.1 lists all symmetry properties of the hexagonal lattice of circular holes.

Let’s imagine that we have computed the magnetic field for the hexagonal lattice as shown in Fig. 2.10 and for a Bloch index $\hat{\mathbf{k}}$. It is clear that we would find the exact same solution for the magnetic field for the same lattice, but rotated by $\pi/3$. Or in other words, we only need to compute one magnetic field and we get five more solutions for free just by rotating the solution by $m \cdot \pi/3$, where $m \in \{0, 1, 2, 3, 4, 5\}$. For every rotated mode solution, the corresponding wave vector is rotated by $-m \cdot \pi/3$ in the reciprocal lattice.

The crystal view from the origin in $\mathbf{a}_1$-direction is identical to the view in $-\mathbf{a}_1$-direction, hence, the physical properties on the $\mathbf{b}_1$-axis in the reciprocal space must be symmetric to the mirror axis $(-1/2, \sqrt{3}/2)$ going through $\Gamma$. Because of the additional translational invariance with periodicity $|\mathbf{b}_1|$, the dispersion from $\Gamma$ to $-\mathbf{b}_1$ is identical to the one from $\mathbf{b}_1$ to $\Gamma$. If both symmetry properties are combined – the mirror symmetry and the translational invariance by $\mathbf{b}_1$ – one can conclude that the dispersion is symmetric to $M' = \mathbf{b}_1/2$, i.e., the physical information is con-
Table 2.1: The symmetries of a two-dimensional hexagonal lattice of circular holes [228].

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Description</th>
<th>Point</th>
<th>Axis</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>Identity Operation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>σ₁</td>
<td>Mirror Symmetry ((a₁ = −(−a₁)))</td>
<td>Γ</td>
<td>((-1/2, \sqrt{3}/2))</td>
</tr>
<tr>
<td>σ₂</td>
<td>Mirror Symmetry ((a₂ = −(−a₂)))</td>
<td>Γ</td>
<td>((1/2, \sqrt{3}/2))</td>
</tr>
<tr>
<td>σ₃</td>
<td>Mirror Symmetry</td>
<td>Γ</td>
<td>((1, 0))</td>
</tr>
<tr>
<td>C₁</td>
<td>Rotation by (α = \pi/3)</td>
<td>Γ</td>
<td>(Γ)</td>
</tr>
<tr>
<td>C₂</td>
<td>Rotation by (α = 2\pi/3)</td>
<td>Γ</td>
<td>(Γ)</td>
</tr>
<tr>
<td>C₃</td>
<td>Rotation by (α = π)</td>
<td>Γ</td>
<td>(Γ)</td>
</tr>
<tr>
<td>C₄</td>
<td>Rotation by (α = −\pi/3)</td>
<td>Γ</td>
<td>(Γ)</td>
</tr>
<tr>
<td>C₅</td>
<td>Rotation by (α = −2\pi/3)</td>
<td>Γ</td>
<td>(Γ)</td>
</tr>
<tr>
<td>σ₄</td>
<td>Mirror Symmetry</td>
<td>Γ</td>
<td>((\sqrt{3}/2, 1/2))</td>
</tr>
<tr>
<td>σ₅</td>
<td>Mirror Symmetry</td>
<td>Γ</td>
<td>((0, 1))</td>
</tr>
<tr>
<td>σ₆</td>
<td>Mirror Symmetry</td>
<td>Γ</td>
<td>((\sqrt{3}/2, −1/2))</td>
</tr>
</tbody>
</table>

tained in half the length of the \(b₁\) starting in \(Γ\). This conclusion can be applied for all three distinct directions of the hexagonal lattice. This leads to a hexagonal area as drawn in red in the right illustration in Fig. 2.10 right. This so-called reduced Brillouin zone or first Brillouin zone can be obtained for any lattice by intersecting the perpendicular bisectors of the reciprocal lattice vectors \(b_i\). Furthermore, the hexagonal lattice is invariant under rotations of \(α_m = m \cdot \pi/3\). Hence the physical information in the Brillouin zone is still contained 6-fold redundant in the Brillouin zone. Exploiting the last symmetry – the mirror symmetry given by the mirror axis \((0, 1)\) going through \(Γ\) – a triangle spanned by the points

\[
Γ = \left( \begin{array}{c} 0 \\ 0 \end{array} \right), \quad M = \frac{2\pi}{a \sqrt{3}} \left( \begin{array}{c} 1 \\ 0 \end{array} \right) \quad \text{and} \quad K = \frac{4\pi}{3a} \left( \begin{array}{c} \sqrt{3}/2 \\ 1/2 \end{array} \right)
\]

is obtained. This triangle is called the irreducible Brillouin zone and is depicted by the gray triangle in Fig. 2.10 (right). It is thus sufficient to compute the eigenfrequencies \(ω\) only for the Bloch indices \(\hat{k}\) in the irreducible Brillouin zone. All other solutions can be generated by applying symmetry operations on the obtained solution. We denote the dispersion diagram depicting the frequency as a function of \(\hat{k}\) as the ‘folded’ band diagram (cf. Fig. 2.11 for an example).

A generally desired property of a PhC is an isotropic behavior, i.e., the same optical properties of the PhC regardless of the incident angle of the light. A completely angle-independent behavior of a PhC would require a circular reduced Brillouin zone. It is noteworthy that the hexagonal Brillouin zone obtained for a hexagonal lattice of circular holes is the best possible approximation of such an ideal circular Brillouin zone\(^1\). Furthermore, the hexagonal lattice is the only one allowing

\(^1\)There are no more than five different lattices for a 2D crystal: the rhombic lattice, the hexagonal lattice, the square lattice, the rectangular lattice and the parallelogrammic lattice. The hexagonal lattices is the only one with a \(C_6\) space group, and thus has the highest num-

to design identical waveguides with three different propagation directions. There is another symmetry that was not discussed so far: the two dimensional crystal has an invariance in the out-of-plane direction $e_z$. Thus the solutions of the Maxwell equations can be classified into distinct polarizations (TE and TM). The TE(TM)-mode has a magnetic (electric) field component $H_z(E_z)$ in the out-of-plane direction $e_z$ and only electric (magnetic) field components for the in-plane directions $e_x$ and $e_y$.

### 2.2.1.4 The Photonic Band Gap

In a 1D PhC, there are two possibilities to align waves whose field pattern share the same periodicity as the one of the periodic permittivity: The field pattern can be overlaid with the periodic permittivity, such that its field energy is concentrated in either the high or the low dielectric region. The Bloch indices $\hat{k}_x$ of the two Bloch modes are the same, i.e., on the edge of the first Brillouin zone ($k = \pi/a$). The wave, whose field is concentrated in the high dielectric has a lower frequency than the wave with the energy confined in the low dielectric [104, pp.46]. Between these frequencies, no other modes can be found and a mode free frequency range is formed.

In Fig. 2.11 the frequencies for all Bloch indices $\hat{k}$ in the reduced Brillouin zone are computed for the case of a hexagonal lattice of air holes ($\varepsilon_r = 1$) of radius $r = 0.34 \cdot a$ in a dielectric material with $\varepsilon_r = 11.25$. It can clearly be seen that there is a frequency range, where no solutions for the wave vector $\hat{k} = (k_x, k_y)$ can be found. TE polarized light with a frequency within that range is not allowed to propagate.

![Figure 2.11: The TE Modes of a hexagonal lattice of air holes of radius $r = 0.34 \cdot a$ are plotted for all Bloch indices $\hat{k}$ within the first Brillouin zone (see perspective view, left figure). The photonic band gap of the TE modes is clearly visible in the center figure. The extrema of the bands are always found on the boundary of the irreducible Brillouin zone that is spanned by the $\Gamma$-M-K-$\Gamma$ points (to the best of our knowledge, there is no proof of this property). The right figure shows both, TE (blue) and TM (red) modes along the boundary of the irreducible Brillouin zone. A band gap exists only for the TE modes.](image-url)
Theory of Slab Photonic Crystal Waveguides

in the photonic crystal independent of the in-plane propagation direction. This forbidden frequency range is called the **photonic band gap** (PBG).

### 2.2.1.5 Gap Maps

An important figure for the design process of PhCs is the so-called gap map plot as shown in Fig. 2.12. In a gap map plot, the photonic band gap is plotted for both polarizations as a function of the hole radius \( r \). For a radius of \( r = 0.34 \cdot a \) it can be seen that there is only a TE band gap (cf. Sec. 2.11). However, there is a radius range, for which the hexagonal lattice of air holes in InP exhibit both, a TE and a TM band gap (shown in yellow in Fig. 2.12). A 2D PhC hence can exhibit a complete in-plane photonic band gap.

The gap map graphically illustrates the possible choices of the radius \( r \) and the lattice constant \( a \) such that a band gap is obtained. Since both parameters can be chosen freely, it is possible to design devices in a straightforward manner. For example a TE notch filter that blocks wavelengths from \( \lambda_1 \) to \( \lambda_2 \) is obtained by choosing the lattice constant \( a \) and radius \( r \) in such a way that \( \lambda_1 \) and \( \lambda_2 \) match the boundaries of the band gap.

### 2.2.2 Photonic Crystal Waveguides

#### 2.2.2.1 Line-Defect Modes in Photonic Crystals

A waveguide is obtained if a line of holes is omitted in an otherwise perfect hexagonal lattice of air holes. The missing line of holes introduces defect mode solutions. The frequencies of those defect modes may have values outside and inside the photonic band gap of the defect-free PhC. In Fig. 2.13 three different types of line defects are shown: one missing row of holes along the \( \Gamma - K \) direction is called a W1 waveguide (Fig. 2.13, left), three missing rows of holes is called a W3 waveguide.
Figure 2.13: Three different types of line defects in PhC: (left) W1 waveguide, (center) W3 waveguide and (right) a waveguide along the $\Gamma - M$ direction.

(Fig. 2.13, center). The last example shows a removed pattern of holes along the $\Gamma - M$ direction (Fig. 2.13, right).

By introducing a line-defect in a two dimensional lattice, the periodic system is changed from a two dimensional periodic system to a one dimensional periodic system. The line-defect PhC waveguide is only periodic in propagation direction $e_x$. It follows that the reciprocal lattice is also one-dimensional. The Bloch index $\hat{k}_x$ of the line-defect modes are periodic with periodicity $2\pi/a$. The irreducible Brillouin zone is is given by $k_x \in [-\pi/a, \pi/a]$. Furthermore, the number of crystal symmetries are reduced from 12 symmetries of the hexagonal lattice of the defect-free PhC to four symmetries for the W1 PhC waveguide (cf. Tab. 2.2). Note that the edge ($K$-point) of the irreducible Brillouin zone for the $\Gamma - K$ direction for a defect-free hexagonal lattice is located at $K = 4\pi/3a$, whereas the edge of the irreducible Brillouin zone for a line-defect PhC with a hexagonal lattice is $K = \pi/a$. For instance, this is relevant for the correct sampling of the Bloch index $\hat{k}_x$ for the numerical computation of the eigenfrequencies $\omega$.

Because of the invariance in the out-of-plane direction $e_z$, the modes can further be separated into TE ($H_z, E_x, E_y$) and TM ($E_z, H_x, H_y$) modes. Furthermore, the modes of the line defect are usually further classified into even and odd modes, due to the mirror symmetry at the $x$-$z$-plane. Traditionally, the classification of even and odd is made with respect to the electric field of the modes of the dielectric waveguide. In the PhC community, however, the classification is usually made with respect to the out-of-plane field component, e.g., the magnetic field $H_z$ in case of a TE mode. Unfortunately an even mode with respect to the magnetic field is an

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Description</th>
<th>Point</th>
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<tbody>
<tr>
<td>$E$</td>
<td>Identity Operation</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\sigma_y$</td>
<td>Mirror Symmetry</td>
<td>$\Gamma$</td>
<td>(1, 0)</td>
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<tr>
<td>$C_1$</td>
<td>Rotation by $\alpha = \pi$</td>
<td>$\Gamma$</td>
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<tr>
<td>$\sigma_x$</td>
<td>Mirror Symmetry</td>
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odd mode with respect to the electric field. The classification of the modes by using the symmetry operators \( \sigma_y \) and \( \sigma_z \) — also called \( y \)-parity and \( z \)-parity — has the advantage of being unambiguous. For example, the \( y \)-parity directly refers to the mirror symmetry at the \( x-z \) plane and is defined as the ‘flip’ of the \( y \)-coordinate

\[
\sigma_y : \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} x \\ -y \\ z \end{pmatrix}
\]

A mode has thus an odd \( y \)-parity if \( \sigma_y = 1 \), i.e.,

\[
E(\sigma_y r) = \sigma_y E(r) \text{ and } H(\sigma_y r) = -\sigma_y H(r)
\]

The classification of the PhC waveguide modes according to the parity notation is given in Fig. 2.14. An even TE mode has hence an odd \( y \)-parity and an odd \( z \)-parity, whereas an odd TE mode has an even \( y \)-parity and an odd \( z \)-parity.
2.2.2.2 Line-Defect Modes Used for Waveguiding

The dielectric core of a PhC line defect is laterally bounded by two semi-infinite PhCs. For frequencies within the band gap of the PhCs, the PhC boundaries prohibit the propagation of light in lateral direction with respect to the waveguide. A propagating wave in a PhC waveguide (a line defect mode) is thus guided laterally by the PhC band gap – also referred to as gap-guided. The ‘perfect’ reflection properties of the PhC boundaries allow even the guidance of the light around sharp corners [186, 224, 175, 263]. In Fig. 2.15 the band diagrams for the lowest two even (red) and odd (blue) TE modes are shown for the W1 PhC waveguide (left) and the 2D hexagonal lattice PhC (right). Odd and even denotes the symmetry with respect to a $x$-$z$-plane. The photonic band gap of the PhC is shaded gray and extends over both diagrams. The PhC defect modes which are located within the band gap are gap-guided by the PhC boundaries.

The dispersion curves of the PhC waveguide modes (Fig. 2.15, left) are substantially different to the ones of conventional waveguides. First, there are also band gaps in the dispersion of the waveguide mode. Band gaps at the edge of the one-dimensional Brillouin zone (cf. even TE mode gap for $k_x = \pi/a$ in Fig. 2.15) are called mode gaps [177], whereas band gaps occurring inside the Brillouin zone are called mini-stop bands (cf. Sec. 2.2.2.4). Secondly, the dispersion curve is both symmetric about the origin (Γ-point) and periodic with periodicity $2\pi/a$. There are frequency ranges, where the dispersion is flat, i.e., where $\partial \omega / \partial \hat{k}$ is small. $\partial \omega / \partial \hat{k}$ represents the group velocity $v_{gr}$ of a Bloch mode. Typically, the slope of the PhC mode dispersion reaches zero towards the edges of the Brillouin zone, and thus – theoretically – the propagation of light can be stopped completely.

Figure 2.15: Right: the TE modes of a PhC with a hexagonal lattice is shown. The gray area denotes the band gap of the PhC. Left: The TE-modes of a PhC W1 waveguide is shown. The PhC waveguide modes having frequencies within the band gap of the PhC (gray area) are laterally guided by the surrounding PhC.
2.2.2.3 Slow Light Regime in PhC Waveguides

The slow light regime of line-defect PhC waveguide is one of the main advantages of PhCs for integrated optics [138], since it potentially allows to reduce the devices lengths of integrated photonic components. For example, light pulses having a very low group velocity can be used for optical buffering: if two optical pulses arrive at the same time at a node, one of the pulses has to be buffered so that both packages can be transmitted on the same fiber sequentially [297]. Conventionally, a delay line is realized by adding loops to a straight waveguide. By using slow light waveguides, some of the loops can be spared, since the low group velocity $v_{gr}$ saves a factor of $\approx c/v_{gr}$ in device length. A further benefit of slow light waveguides is the reduction of the input power for non-linear devices. A pulse entering a slow light waveguide is spatially compressed. While the pulse enters a slow light waveguide, the front end of the pulse gets slowed down before the back end of the pulse has arrived in the slow light waveguide. Thus, the length of the pulse shrinks by a factor of $\approx c/v_{gr}$. Because of the energy conservation of the pulse, its energy is now distributed over a volume that is reduced by $\approx c/v_{gr}$. Many, in particular non-linear, effects depend on strong light intensities. For instance, the operational power of a device exploiting the Kerr-effect ($\delta n \propto |E|^2$, where $E$ is the electric field of the optical control signal) can be reduced by a factor $\approx c/v_{gr}$ and simultaneously the length can be reduced by another factor $\approx c/v_{gr}$. Both saving effects can be traded for each others and in the case of the Kerr-effect device a quadratic $\approx (c/v_{gr})^2$ increase of its performance with the group velocity $v_{gr}$ is expected [256, 255]. By using PhC waveguides, the group velocity can be designed to almost any value [301]. Slow down factors from 33 ($v_{gr} = 0.03c$) [98], 90 ($v_{gr} = 0.90c$) [198] and to 300 [289] have been demonstrated experimentally. The positive influence of the slow down factor on the intensity enhancement has been exploited experimentally and theoretically: Nojima [193] identified the gain enhancement factor to be uniquely determined by the product of the time of the light to pass the gain region and the confinement factor of the light in the active region. Corcoran et al. [44] could enhance third harmonic generation by using the field enhancement phenomena of slow light PhC waveguides.

Exploiting the slow light mode of PhC waveguides however has some limitations. First, one is confronted with a fundamental trade-off between slow-down factor and bandwidth: since the bands are flat, the slow light regime exists only for a small frequency range [66, 14]. For example, the frequency range of the slow light regime has to cover all wavelengths from 1542nm to 1558nm to process an optical signal with a bandwidth of 2THz used at the telecom wavelength of 1550nm. This has been shown experimentally by Settle et al. [239] for a moderate slow-down factor of the light of about 12 for a bandwidth of 2.5THz.

The second limitation is the efficient coupling into slow light waveguides. The mismatch of the mode profiles of the guided modes at the interface from the access structure and the slow light PhC waveguide results in large modal reflection coefficients. This high reflection coefficient prevented Vlasov et al. [289] from

---

2According to [138], a photon does still have a velocity of $n/c$, but it is scattered multiple times in forward and backward propagation direction. The velocity of the pulse is the average speed of this scattering process.
demonstrating experimentally even lower group velocities than $n_{gr} = 300$. Recently much effort was put into developing interfaces to couple efficiently into slow light waveguides [96, 287, 171, 216] and it was shown that negligible small reflection coefficients into slow light modes can be obtained if the interfaces are properly designed.

Often PhC waveguides suffer from large group velocity dispersion [9, 66, 77]. Engelen et al. [66] measured optical pulses propagating in slow light PhC waveguides using phase-sensitive and time-resolved near-field microscopy. The measured pulse shape is not only broadened, but also spatially skewed. The dispersion of the PhC waveguide modes can be tailored such that group velocity dispersion is negligible [213, 73, 239].

In conclusion, the slow light operation has successfully been demonstrated. Limitations, such as inefficient coupling into slow light modes and large group velocity dispersion can be mastered by carefully optimizing the PhC waveguide dispersion and the waveguide interfaces.

2.2.2.4 Mini-Stop Bands

Frequency gaps at the edge of the first Brillouin zone are expected not only for the PhC but also for line-defect PhC waveguides. For line-defect PhC waveguides another similar phenomenon can be observed within the irreducible Brillouin zone: the dispersion of line-defect PhC waveguide modes with the same parities do not cross each others in the folded band diagram, but instead, a mini-stop band opens. Various mini-stop bands in the band diagram of a W3 PhC waveguides can be seen in Fig. 2.16. Figure 2.16 further shows the magnetic field plots of the ‘crossing’ of two even PhC waveguide modes. It can be seen that the modes with the same parities start to blend into each other. To the best of our knowledge, the physics behind this phenomenon is not understood completely. Instead, we list some of the main

![Figure 2.16: Even and odd modes of a W3 PhC waveguide. There are several mini stop bands within the band gap. For each symmetry a pronounced mini stop band is indicated in the plot.](image)
observations in literature. Qiu et al. [219] investigated mini-stop bands numerically and found that they occur due to the contra-directional coupling between different order of modes with the same symmetry. Agio et al. [4] further discovered that the frequency position of the mini-stop bands of PhC waveguide modes coincide with the resonances of the cavity that is formed in the lateral direction. Hence they infer that the physical processes consists of coupling between the crossing modes enabled by the lateral cavity resonance. Vaslov et al. [288] found that mini-stop bands can also exist at anti-crossing points of TE and TM like modes for their asymmetric double-trench PhC waveguides.

We conclude that there are very narrow frequency regions within the photonic bands of anti-crossing PhC waveguide modes, where light propagation of certain polarization is impeded.

2.2.3 Fourier Optics

2.2.3.1 The Wave Vector of a Bloch Mode: The Unfolded Band Diagram

The wave vector $k$ of a plane wave has a physical meaning: it has a magnitude (the wave number) and a direction (propagation direction). Physical properties, such as the group velocity $v_{gr} = \frac{\partial \omega}{\partial k}$ and the phase velocity $v_{ph} = \frac{\omega}{k}$ are based on a physically relevant wave vector $k$. But, what is the wave vector $k$ of the Bloch mode that has a physical relevance, i.e., the wave vector from which we can deduce physical properties such as the group and the phase velocity?

We have seen in Eq. 2.42 that the wave vector of the Bloch mode is not unique, i.e., any integer multiple of $\frac{2\pi}{a}$ can be added to $\hat{k}$ and the same Bloch mode results. The Bloch index $\hat{k}$ represents the ‘folded’ wave vector, i.e., the wave vector $k_x$ of the Bloch mode in the first Brillouin zone. The Bloch index $\hat{k}$ labels a Bloch mode and does not have a direct physical meaning as opposed to a wave vector $k$ of a plane wave. There are some confusing ‘inconsistencies’ originating from this subtle difference between $k$ and $\hat{k}$.

This confusion can be illustrated by studying the transition from a periodically modulated permittivity to a homogeneous material. The wave vector $k$ of a homogeneous medium obeys $k = \omega \cdot n/c$ – a straight line in the dispersion diagram. In other words, the dispersion of a 1D PhC should fade to a straight line as we reduce the contrast of the periodic modulation of the permittivity. In the following experiment, a 1D PhC with periodicity $a$ and a refractive index given by $n_{core} = 3.3296$ and $w_{core} = 0.6 \cdot a$ and $n_{hole} = 1$ and width $w_{hole} = 0.4 \cdot a$ is considered as shown in Fig. 2.17. We continuously increase the refractive index $n_{hole} \rightarrow n_{core}$. For the limiting case of $n_{holes} = n_{core}$, the periodic permittivity vanishes and the Bloch wave $H_{z,\hat{k}_x}(x) = u_{\hat{k}_x}(x) \cdot e^{i\hat{k}_x x}$ becomes a single plane wave. The dispersion of a plane wave in a homogeneous material is given by $\omega = c \cdot k_x/n_{core}$ and is represented by the red line in Fig. 2.17. The photonic bands of the 1D PhC are shown in the ‘folded band diagram’ representation in the top row. It can be seen that this band diagram does not lead to the linear dispersion of the homogeneous material with $n = n_{core} = n_{hole}$. Furthermore, the sign of the group velocity $v_{gr} = \frac{\partial \omega}{\partial \hat{k}_x}$ changes between two consecutive ‘folded’ modes of the 1D PhC, i.e., the mode would alternate its propagation direction after every folding.
Figure 2.17: Simulation of a 1D PhC as depicted in the top row. The folded band diagram represents the Bloch index $\mathbf{k}_x$ in the first Brillouin zone. The dispersion of the homogeneous system is represented by the red line. In the un-folded band diagram, the principal wave vector $\mathbf{\tilde{k}}_x$ is plotted. The dispersion diagram of the principal wave vector $\mathbf{\tilde{k}}_x$ coincides with the wave vector of a plane wave for the limiting case $n_{\text{hole}} = n_{\text{core}}$ and has only a positive group velocity.

The transition experiment can be used to identify the wave vector that potentially has a physical meaning. If the periodicity is removed ($n_{\text{hole}} = n_{\text{core}}$), then the Bloch wave should be identical to a plane wave, i.e.,

$$\psi_{k_x}(x) = u_{k_x} \cdot e^{i k_x x}$$  \hspace{1cm} (2.44)

with

$$u_{k_x} = \sum_{m} A_{k_x,m} e^{i m 2\pi / a} = A_{k_x,0} = 1. \hspace{1cm} (2.45)$$

If the periodic modulation is very weak, then the Bloch mode is still approximatively a plane wave $u_{k_x} \cdot e^{i k_x x}$, where $e^{i k_x x}$ represents a strongly varying carrier oscillation and $u_{k_x} \approx 1$ is a slowly varying envelope. The wave vector $k_x$ of the carrier is labeled by a breve and is called the principal wave vector [302, p. 202] of the Bloch mode. The principal wave vector $\mathbf{\tilde{k}}_x$ is determined in such a way that

$$|A_{\mathbf{\tilde{k}}_x,0}| \geq |A_{k_x,m}| \forall m \geq 1. \hspace{1cm} (2.46)$$

Note that the band diagram of the principal wave vector $\mathbf{\tilde{k}}_x$ results in a positive group velocity exclusively. Furthermore, the dispersion diagram obtained by plot-
ting \( \hat{k}_x \) coincides with the dispersion line of the homogeneous material for the limiting case of \( n_{\text{hole}} = n_{\text{core}} \). According to Yariv and Yeh [302, p. 202] the principal wave vector \( \hat{k}_x \) has an similar physical meaning as the wave vector \( k \) of a plane wave. They used the principal wave vector \( \hat{k}_x \) to define the phase velocity \( v_{\text{ph}} \) and the group velocity \( v_{\text{gr}} \) of a Bloch mode

\[
v_{\text{ph}} = \frac{\omega}{\hat{k}_x} \quad v_{\text{gr}} = \frac{\partial \omega}{\partial \hat{k}_x}.
\]

(2.47)

We will use the principal wave vector \( \hat{k}_x \) later in chapter 4 to discuss the propagation losses of slab PhC waveguides.

### 2.2.3.2 Plane Wave Expansion

![Figure 2.18: 1D periodic modulation of the refractive index \( n(x) = \sqrt{\varepsilon(x)} \) with periodicity \( a \).](image)

The procedure of the plane wave decomposition analysis is demonstrated here for a 1D PhC as shown in Fig. 2.18. For the extension to 2D and 3D PhC the reader is referred to [215, 110, 49]. Furthermore, we focus on TE modes \( (H_x = H_y = E_z = 0) \) exclusively. The procedure for TM modes is analogous. The magnetic field \( H_{k_x} \) satisfies the Bloch’s theorem and hence \( H_{k_x,\hat{k}_x}(x) \) can be written as the product of a plane wave \( e^{i\hat{k}_x x} \) and an envelope function \( u_{k_x}(x) \) that is periodic with periodicity \( a \) (cf. Eq. 2.35)

\[
H_{k_x,\hat{k}_x}(x) = H_0 u_{k_x}(x) e^{i\hat{k}_x x}.
\]

(2.48)

In the following, we expand the periodic function \( u_{k_x}(x) \) in terms of plane waves of the form \( e^{ik_{m} x} \), where \( k_{m} \) are the wave vectors. The plane wave expansion of a periodic function results in a sequence of equidistant (periodic with wave vector periodicity \( m \cdot 2\pi/a \)) spatial Fourier components with coefficients \( w_{m}(\hat{k}_x) \) in the wave vector space

\[
u_{k_x}(x) = \sum_{m} w_{k_x,m} e^{i(m\frac{2\pi}{a})x}.
\]

(2.49)

The weights of the Fourier components \( w_{k_x,m} \) are decreasing for large values of \( m \). The approximation of \( u_{k_x}(x) \) (Eq. 2.49) with a Fourier series is only exact for \( m \rightarrow \infty \). The Bloch wave is rewritten by replacing \( u_{k_x}(x) \) in Eq. 2.48 by Eq. 2.49 and by additionally by using \( k_{m} = \hat{k}_x + m2\pi/a \)

\[
H_{k_x,\hat{k}_x}(x) = \sum_{m} w_{k_x,m} H_0 e^{i(k_x + m\frac{2\pi}{a})x}.
\]

(2.50)
The Fourier expansion of the Bloch wave must satisfy the master equation (Eq. A.9) that is

\[-\nabla \times \left( \begin{array}{cc}
\frac{1}{\varepsilon(x)} & 0 \\
0 & 0 \\
\end{array} \right) \nabla \times \hat{H}_{k,x,z}(x) + \frac{\omega^2}{c^2} \left( \begin{array}{c}
0 \\
0 \\
H_{k,x,z}(x) \\
\end{array} \right) = \mathbf{0} \quad (2.51)\]

for time harmonic fields. Because \(\varepsilon(x)\) is dependent on the \(x\)-coordinate, it is more convenient to use the inverse of the permittivity \(\frac{1}{\varepsilon(x)}\) instead of \(\varepsilon(x)\) \[215\]

\[\frac{1}{\varepsilon(x)} = \sum_l v_l e^{il\frac{2\pi}{a}x}, \quad (2.52)\]

where \(v_l\) are the coefficients of the plane wave expansion of \(\frac{1}{\varepsilon(x)}\). After some mathematical manipulations (performed in appendix A.4) the following eigenvalue equation for \(\hat{k}_x\) is obtained

\[-\sum_m \left\{ \sum_l \left( \left( l \frac{2\pi}{a} (\hat{k}_x + m \frac{2\pi}{a}) + (\hat{k}_x + m \frac{2\pi}{a})^2 \right) v_l e^{il\frac{2\pi}{a}x} \right) - \frac{\omega^2}{c^2} \right\} \cdot w_{k_x,m} H_0 e^{i(\hat{k}_x + m \frac{2\pi}{a})x} = 0. \quad (2.53)\]

We obtain \(m\) eigenvalue equations for either \(\hat{k}_x\) or \(\omega\) by multiplying both sides of the equation with an orthogonal function \(e^{-i \frac{2\pi}{a} p}\) where \(p \in \mathbb{Z}\), followed by an integration over the unit cell \(\frac{1}{a} \int_{-a/2}^{a/2} dx\)

\[\sum_l \left( (\hat{k}_x + p \frac{2\pi}{a}) (\hat{k}_x + (p - l) \frac{2\pi}{a}) \cdot w_{k_x,p-l} \cdot v_l \right) = \frac{\omega^2}{c^2} w_{k_x,p} \quad (2.54)\]

Once, the eigenvalues \(\hat{k}_x\) are obtained for all \(m\), the magnetic field \(H_{k_x,z}\) is obtained by evaluating the Fourier series given in Eq. 2.50. The electric field \(E_{k_x,y}(x)\) can be derived from the magnetic field by using Ampere’s law

\[E_{k_x,y}(x) = \sum_m E_{k_x,m} e^{i(\hat{k}_x + m \frac{2\pi}{a})x}, \quad (2.55)\]

where the coefficients \(E_{k_x,m}\) are

\[E_m = w_{k_x,m} H_0 \frac{\hat{k}_x + m \frac{2\pi}{a}}{\varepsilon(x)} \frac{1}{\varepsilon(x)}. \]

For the numerical computation, the Fourier series \(\sum_l\) have to be truncated to a finite number of summation terms \(l_s\) as well as to a finite number of equations \(m_s\). This results in the following linear system of equations
\[
\begin{pmatrix}
(k_x - m_s \frac{2\pi}{a}) (k_x + (-m_s + l_s) \frac{2\pi}{a}) v_{-l_s} \\
\vdots \\
(k_x - m_s \frac{2\pi}{a}) (k_x + (m_s - l_s) \frac{2\pi}{a}) v_{l_s}
\end{pmatrix}
\cdot
\begin{pmatrix}
w_{k_x, -n_s} \\
\vdots \\
w_{k_x, n_s}
\end{pmatrix}
= \frac{\omega^2}{c^2}
\begin{pmatrix}
w_{k_x, -n_s} \\
\vdots \\
w_{k_x, n_s}
\end{pmatrix},
\]

that can be solved by an eigenvalue solver. This technique still represents one of the most used numerical method to solve for photonic bands. For example, MIT’s photonic bands (MPB) [110] program essentially solves this eigenvalue equation.

2.2.3.3 The Dominant Fourier Component

In Sec. 2.2.3.1, we introduced the principal wave vector \( \tilde{k}_x \) of a Bloch mode. The Bloch mode consists of the product of two factors: a strongly varying carrier wave \( e^{i\tilde{k}_x x} \) and a slowly varying periodic envelope function \( u_{\tilde{k}_x}(x) \). In this section, we compute the Fourier decomposition of the Bloch mode with COMSOL. We find a strong correlation between the strongest Fourier component of the Bloch mode and the principal wave vector \( \tilde{k}_x \) of the Bloch mode.

In this numerical experiment, we excite the W1 PhC waveguide at the input with a magnetic field \( H_z \) with a specific frequency \( \omega \). A Bloch wave is established in the W1 PhC waveguide. Thereafter, we apply a Fast-Fourier-transform to the complex magnetic field of the excited Bloch wave. Figure 2.19 shows the dispersion diagram in the Bloch representation and the Fourier representation of a W1 PhC waveguide with a hexagonal lattice of air holes with radius \( r = 0.34 \cdot a \) and \( n_{\text{core}} = 3.35 \). The main difference between the two dispersion diagrams is that the magnitudes of the Fourier components are included in the Fourier representation by a color representation (white: weak Fourier component, red: strong Fourier component). This information is missing in the Bloch representation. The location of the strongest Fourier component in the dispersion diagram of the Fourier representation coincides with the location of the principal wave vector \( \tilde{k}_x \) of the Bloch mode in the Bloch representation. It is thus possible to compute the Fourier representation to determine the principal wave vector \( \tilde{k}_x \).

The additional non-zero Fourier components with respect to the principal wave vector \( \tilde{k}_x \) of the Bloch mode can be assigned to the periodic function \( u_{\tilde{k}_x}(x) \). These non-zero Fourier components are relevant for the discussion of the propagation losses of slab line-defect PhC waveguides (cf. chapter 4). However, it is claimed by Lombardet et al. [161] that those non-zero Fourier components are able to modify other physical properties such as the group and phase velocity (cf. Eq. 2.47). Let us quickly discuss the Fourier representation of the photonic bands shown in Fig. 2.19.B. The Fourier component with the largest amplitude is found in the second Brillouin zone. Most of the spatial Fourier components for the even excitation have a positive group velocity and hence are forward propagating. The coefficients of the spatial Fourier components for the flat photonic band sections are distrib-
Figure 2.19: A: The Bloch diagram obtained with a 2D MPB supercell simulation of a W1 PhC waveguide with $n_{\text{core}} = 3.24$ and $r = 0.34 \cdot a$. B: Fourier mode diagram obtained by exciting the W1 PhC waveguide. An even lateral cosine was used for the excitation. C: the Fourier spectrum for $\omega a/(2\pi c) = 0.2895$. 
uted in several Brillouin zones. For the wave vector close to \( k_x = \pi/a \), i.e., close to the edge of the first Brillouin zone, the coefficients of the spatial Fourier components in forward and backward direction is nearly equal. This supports the simplified notion of slow light propagation of Krauss [138]: slow light modes consist of many equally strong forward and backward propagating plane wave components, such that the finally resulting group velocity of the Bloch wave is low.

Generally, the Fourier representation is preferred to discuss the behavior at the PhC/homogeneous material interfaces [161, 52, 195]. Most notably, the Fourier representation is helpful to discuss the existence of loss-free guided PhC waveguide modes: The Fourier representation of the dispersion of the PhC waveguide mode is the natural representation to be compared with the light-line, i.e., the area of oscillatory modes (plane waves) in a homogeneous cladding material. The detailed discussion of this process is in chapter 4.

2.3 Slab Photonic Crystal Waveguides

So far we discussed two dimensional systems exclusively. However, for the realization of practical devices a three dimensional waveguide design is required. Unfortunately, the manufacturing of waveguides based on 3D PhC is very challenging. An alternative concept that is easier to fabricate, is the slab PhC waveguide as shown in Fig. 2.20(right). The lateral confinement of the light is provided by the PhC waveguide and the vertical confinement is provided by the vertical refractive index contrast. The manufacturing of slab PhC waveguides typically involves only a single lithographic step for the 2D patterning. Therefore, slab PhC waveguides have been experimentally realized in many research labs. There are mainly two different types of slab waveguide designs employed for the vertical light confinement: the high index contrast membrane-type PhC waveguide (as shown in Fig. 2.20, left) and the weak index contrast substrate-type PhC waveguide (also shown in Fig. 2.20, right).

Joannopoulos [104, p.135] emphasizes that such structures are not ‘two-dimensional’ PhCs despite the resemblance. The finite thickness of the slab leads to additional phenomena that cannot be observed in 2D structures. For instance, the large out-of-plane radiation loss of slab PhC waveguides as discussed in chapter 4 is a phenomenon that is only observed in slab PhC waveguides, i.e., these

Figure 2.20: A membrane-type (left) and a substrate-type W1 PhC waveguide design.
losses cannot be observed in 2D structures. In this section, we will only point out two exemplary properties – the polarization and the dispersion of line-defect PhC waveguides – that are often treated similarly to 2D PhC waveguides. However, both are strongly modified by the slab waveguide. Even so, the theory of 2D PhC’s can sometimes be used as an approximation. For instance, the polarization defined for the 2D PhC waveguide are exact and turn into approximates for slab PhC waveguides. In any case, it is important to be aware of the limitations of these approximations and to know, where some precaution is required for the interpretation of the results.

2.3.1 Polarization of the Slab PhC Waveguide Modes

A separation into two polarizations can always be made for geometries that have an invariance along one direction. Figure 2.21 shows the 2D PhC waveguide as well as the slab waveguide. The slab waveguide has a structural invariance along the propagation direction $e_x$. Therefore the polarization is defined according to $H_x = 0$ (TM) and $E_x = 0$ (TE) as shown in Fig. 2.21. The 2D PhC waveguide has a structural invariance along the out-of-plane direction $e_z$ and hence the polarization is defined according to $H_z = 0$ (TM) and $E_z = 0$ (TE). The slab PhC waveguides as shown in Fig. 2.20 do not have an invariance and thus the modes of these slab PhC waveguides mode are neither pure TE nor pure TM modes.

From a theoretical perspective this seems to be fatal: all considerations, such as a photonic band gaps, rely on the symmetry properties of the PhC. The slab destroys the $\sigma_z$-symmetry that is used to distinguish between TE and TM modes. If a 2D PhC has a band gap for a TE mode, but not for a TM mode, then it is expected that the ‘TM part’ of the hybrid mode is not guided and hence not confined. Johnson even concluded that there is no longer any band-gap in a slab PhCs [109]. For asymmetric structures, such as the substrate-type PhC waveguide as shown in Fig. 2.20(right), the situation is even worse, since there is no vertical symmetry axis for $z = 0$. However, Johnson’s statement contradicts our experimental obser-

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Figure 2.21: A separation into two polarization can always be made for 2D geometries. Note that polarizations for the slab and the 2D PhC waveguides are not compatible.
vations. For instance, a very sharp mini-stop band is observed in a substrate-type W3 PhC waveguide [241](cf. Fig. 5.9). Qiu [218] investigated numerically the influence on the band gaps of slab PhCs. He only found a small reduction of the band gap for slab PhCs and not the claimed annihilation. We conclude that the band gap is mostly maintained in substrate-type PhC waveguides, even though from a theoretical perspective the distinction in TE and TM polarization is strictly not allowed. The polarizations of slab PhC waveguides are thus approximately TE and TM polarized.

Let us consider a symmetric, membrane-type PhC waveguide as shown in Fig. 2.20(left) and discuss again the symmetry properties. There is a symmetry plane going through the center of the slab at \( z = 0 \). For this symmetry plane the electric and magnetic fields are oriented perfectly to either the \( x \) or the \( z \)-axis as illustrated in Fig. 2.22. For a position close to the symmetry axis, e. g., in the center of the slab waveguide, the fields are still mostly polarized. Such modes that approximate accurately the TE and TM polarization of 2D PhCs are called TE-like and TM-like modes [104, p.130].

### 2.3.2 Effective Index Approximation

The photonic bands of the slab PhC waveguide are not the same as the one for the corresponding 2D PhC waveguide. Slab PhC waveguides are three-dimensional systems and the computation of their photonic bands is a strictly three-dimensional problem. Unfortunately, three-dimensional simulations are currently still very demanding on the computational resources. To reduce the computational costs of PhC waveguide optimizations, an effective refractive index approximation is employed in order to reduce the 3D problem to a 2D problem. We determine the effective refractive index by performing a large number of 2D MPB simulations with different effective refractive indices and superimpose the obtained photonic bands with the photonic band obtained from the 3D MPB super-cell simulation (thick black line in Fig. 2.23 (right). The super-cell and the geometrical parameters are shown in Fig. 2.23 (left). For the substrate-type PhC W1 waveguide an effective index ranging from \( n_{eff} = 3.2 \) to \( n_{eff} = 3.24 \) is found for the even TE-like mode and \( n_{eff} = 3.205 \) for the odd TE-like mode.

Another technique is to approximate the effective refractive index \( n_{eff} \) from the propagation constant of the fundamental TE mode of the vertical slab waveguide [260, pp. 38-39]. P. Strasser found numerically an effective refractive of index
Figure 2.23: Effective index approximation: The black thick line is the photonic band of a substrate-type W1 PhC waveguide obtained from a 3D MPB super-cell simulation. The super-cell with the parameters is shown on the right. The thin, colored lines are the photonic bands of 2D W1 PhC waveguide for various effective refractive indices \( n_{\text{eff}} \) according to the color-bar. For frequencies close to \( \omega a/(2\pi c) = 0.32 \), a refractive index \( n_{\text{eff}} = 3.24 \) yields the best approximation and for frequencies close to \( \omega a/(2\pi c) = 0.24 \), a refractive index \( n_{\text{eff}} = 3.2 \) is the best approximation.

\[ n_{\text{eff}} = 3.245 \text{ to } n_{\text{eff}} = 3.275 \text{ (dependent on the frequency) for the substrate-type PhC waveguide. The advantage of this approach is that no 3D calculations are required at all. However, the effective refractive index } n_{\text{eff}} \text{ obtained from the former method is more accurate for the problem of optimizing the dispersion of a particular PhC waveguide design – e.g., a W1 PhC waveguide – since the effective refractive index is already tailored to the photonic bands of the W1 PhC waveguide design.} \]

### 2.3.3 Conclusions

The purpose of this chapter was to introduce all relevant terms and concepts of mode theory and photonic crystals that will be used in the following chapters. For instance, we will need the concept of the light-line to identify truly guided modes in slab PhC waveguides (cf. 4.5). We will further rely on the plane wave decomposition of a Bloch mode for the discussion of propagation losses in slab PhC waveguides. Also, the definitions of the polarizations in slab waveguides as well as in line-defect PhC waveguides are used throughout the thesis and are revisited in Sec. 8.2. All in all, the presented concepts will serve as a ‘toolbox’ for the subsequent chapters.
3

Computation of the Dispersion Diagrams of Photonic Crystals and Photonic Crystal Waveguides

This chapter covers three different topics related to the super-cell approach for the computation of the dispersion relation of line-defect PhC waveguides. The numeric computation of the dispersion relation of both PhC and line-defect PhC waveguides is a prerequisite for the research of PhCs. However, often, the details about the numeric computation as well as the exact data processing are neither discussed nor scrutinized. Therefore, the computational process to obtain the photonic bands for slab PhC waveguides is documented in detail in the first part of this chapter.

The second part of this chapter addresses the problem of how to design a line-defect PhC waveguide that has a particular dispersion relation for the line-defect waveguide mode. In literature, usually numerical optimization algorithms are applied for the design process [73, 142, 156]. As an alternative to those brute force computations, we introduce mode-map plots for line-defect PhC waveguides. Mode-map plots are an extension of the gap-map plots for defect-free PhCs. Similar to gap-map plots, the mode-map plots are useful to identify the relevant design parameter that can be used to modify the dispersion of the line-defect PhC waveguide according to specific needs.

The last part of this chapter reports on a new FEM method [233] that allows to directly solve for a Bloch index $\hat{k}$ for a given excitation frequency $\omega$. The method was developed in collaboration with K. Schmidt. The initial motivation behind the collaborative effort was to compute the propagation losses of substrate-type PhC waveguides from the complex Bloch index $\hat{k}$ for a given excitation frequency $\omega$. The new method cannot yet be used to compute the out-of-plane radiation losses, since for that purpose 3D super-cells would be required. Nevertheless, the method is highly interesting, because i) it allows to take dispersive materials into account and ii) it exhibits an exponential convergence theoretically.
3.1 Methods to Compute the Photonic Bands

Many different methods and codes are used to compute photonic bands. Johnson [104, Appendix D] distinguishes between three categories of problems in computational photonics: frequency-domain eigenproblems of the form $Ax = \omega^2 Bx$, frequency-domain responses for a given current distribution $J(x)$ of the form $Ax = b$ and time-domain simulations of the electromagnetic fields for a given current source $J(x)$. However, equally important is the classification according the discretization scheme: i) discretization of the space $\Omega$ (finite-element methods and finite-difference methods) and discretization of the boundary $\partial \Omega$ (multipole method, plane wave expansion). Since the computation of the photonic bands of a PhC is essentially a search for eigen-modes of a periodic system, the problem is primarily a frequency-domain eigenproblem.

Thus, one can distinguish between four main types of numerical methods for the computation of photonic bands. For each of the four methods, a typical method is presented in the following:

- **Plane Wave Expansion ($\partial \Omega$-discretization) [155]**: The most prominent code is MIT Photonic Bands (MPB) that has been developed by Johnson et al. [110]. MPB is a method based on a global plane wave expansion (PWM) for loss less periodic systems [215]. Whereas the method gives exponential convergence for smooth potentials e.g., present in quantum-mechanics, it approximates the eigenmodes in PhCs only with a linear rate of convergence due to their discontinuous dielectric spatial distribution.

- **Multipole Method ($\partial \Omega$-discretization)**: The method of auxiliary sources (MAS) [114], the method of moments (MOM), the method of fictitious sources (MFS) [279] are based on the expansion in zero order multipoles. These methods exhibit algebraic convergence rates. Furthermore, the convergence rate critically depends on the spatial distributions of the fictitious current sources. For the multiple multipole method [85, 185, 186, 246] higher order multipoles are used for the expansion and in case of continuous derivatives an exponential convergence is achieved [37]. Multipole methods tend to be very efficient (small matrices), if appropriate basis functions are chosen.

- **Finite Difference Methods ($\Omega$-discretization)**: The finite difference time domain method (FDTD) is ubiquitously used for electromagnetic scattering problems. But most FDTD codes [38, 269, 88] allow also to solve for eigen-modes of periodic systems. A complete set of eigenmodes can be obtained with a single computation for a range of frequencies if the location and pulse of the excitation is properly chosen [259]. Long simulation run-times are typically required for the accurate computation of the photonic bands and the method in the time-domain is rather inefficient. The frequency-domain version of the finite-difference method is more appropriate for the simulation of the photonic bands. Guo et al. [82] showed that the FDFD method is more efficient for the computation of photonic bands than the plane wave expansion method.
• **Finite Element Methods (Ω-discretization):** The finite element method is extremely flexible and is therefore widely applied in all physical domains. Kono and Koshiba [131, 135, 136] used a three dimensional super-cell to compute the photonic bands of line-defect magneto-PhC waveguides. Their code is optimized for the computation of PhCs [136]. For the computation of the PhC band structure it was shown that the $h$-version of the commercially available FEM-code (COMSOL) with polynomial degree two already achieves double the convergence rate of MPB [290]. For material interfaces having continuous contours (continuous also in their derivatives such as e.g., circles) the $p$-version of FEM with curved cells leads to an exponential convergence, i.e., the convergence rate increases continuously. And a limited, but high convergence rate (algebraic convergence) can be achieved for the ‘worst case’ scenario, i.e., geometries with contours with sharp corners [234].

The convergence rate is a characteristic property of a numerical method. But the convergence rate is an insufficient argument to rate the efficiency of a method. Practically, the implementation of the method – i.e., the written code, the used libraries, the required memory and the used compiler – is more relevant for an efficient executable. Further relevant criteria are: licensing and availability, user interface, user support, open source, scripting interfaces and so on. For example, the advantages of MPB are the following

  • open source software and free of charge
  • scripting interface (the same scripting interface can be used for the FDTD program MEEP)
  • a parallelized code exist and thus MPB can be used on distributed memory systems
  • large community of users

We mostly use MPB for the computation of the photonic bands mainly because of the above reasons and because we have access to two large distributed memory systems.

### 3.2 Super-Cell Approach

The primitive cell (unit-cell) is defined as the smallest structure that is able to perfectly fill all space (no overlaps nor voids) if it is translated along the lattice vectors. A primitive unit-cell must contain precisely one lattice point [192]. However, the definition of the primitive unit-cell as well as the lattice vectors are generally not unique. In Fig. 3.1 three different possibilities of the primitive unit-cell are shown for a 2D lattice. All primitive unit-cells have the same volume given by the triple product of the lattice vectors $\mathbf{a}_i$. The reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ depend on the choice of the lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. Even tough the reciprocal lattice vectors may be different, the same reciprocal lattice and the same Brillouin zone is obtained for all primitive unit-cells. The choice of the unit-cell and the lattice vectors is thus not important for determining the Brillouin zone and the reciprocal lattice. Note that an even smaller structure than the primitive unit-cell could be
3.2.1 Super-Cell Approach for Line-Defect PhC Waveguides

The photonic bands of line-defect PhC waveguides are commonly computed by using the super-cell approach [112, 104, 228, 258], where the standard band structure codes for PhCs are applied to a super-cell instead to a primitive unit-cell. The super-cell system applied to line-defect PhC waveguides models an infinite array of identical line-defects separated by a specific number $m$ of photonic crystal rows and by an air layer. A continuation of the super-cell for a substrate-type W1 PhC waveguide of a hexagonal lattice by 3 periods in all directions is shown in Fig. 3.3. An alternative approach is to replace the finite PhC with a lateral periodicity by two

Figure 3.1: Three possible of choices for the primitive unit-cell and the lattice vectors $a_1$ and $a_2$ for the hexagonal lattice.

Figure 3.2: Left: Scanning electron microscope (SEM) picture showing the top view of a PhC W1 waveguide fabricated by etching deep holes in a InP/InGaAsP/InP layer structure. Right: 3D sketch of a super-cell including the vertical layer structure.
semi-infinite PhCs. For the resulting infinite system, the existence and properties of guided modes have already been studied for the TE [143] and the TM case [6]. In Fig. 3.2, left) an SEM micrograph of a fabricated W1 PhC waveguide is shown. The waveguide is laterally terminated by a homogeneous dielectric region. Therefore, the super-cell approach and the approach of using two semi-infinite PhCs cause a modeling error with respect to the fabricated device.

Similar to the primitive unit-cell, the choice of the super-cell is not unique. In Fig. 3.4 two possible super-cells for a PhC waveguide based on the hexagonal lattice are shown. Note that the reciprocal lattice and the irreducible Brillouin zone depend on the choice of the super-cell, as opposed to the primitive unit-cell. This is illustrated in Fig. 3.4. The lattice vectors of the first super-cell are

$$a_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} a, \quad a_2 = \left( \frac{1}{2} \cdot \frac{m+1}{\sqrt{3}/2 \cdot (m+1)} \right) a.$$  \hspace{1cm} (3.1)

where \(m = 7\) is the number of separating layers of holes. The reciprocal lattice vectors can be obtained using Eq. A.29 and Eq. A.30

$$b_1 = \frac{2\pi}{a} \begin{pmatrix} 1 \\ -1/\sqrt{3} \end{pmatrix} \quad b_2 = \frac{4\pi}{\sqrt{3}a \cdot (m+1)} \begin{pmatrix} 0 \\ -1 \end{pmatrix}. \hspace{1cm} (3.2)$$
Figure 3.4: Two different super-cells for a W1 PhC waveguide based on the hexagonal lattice. The reciprocal lattice of the two super-cells are shown on the right. The obtained mode solutions are identical for both super-cells. But the corresponding Bloch index  \( \hat{k}_x \) expressed in reciprocal lattice vectors \( \mathbf{b}_i \) is different, since the reciprocal lattice vectors are different for the two super-cells.
The reciprocal lattice vectors lead to a rhombic reciprocal lattice. The lattice vectors for the second super-cell are
\[
\mathbf{a}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} a, \quad \mathbf{a}_2 = \begin{pmatrix} 0 \\ \sqrt{3}/2 \cdot (m + 1) \end{pmatrix} a,
\]
and the corresponding reciprocal lattice vectors are
\[
\mathbf{b}_1 = \frac{2\pi}{\mathbf{a}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{b}_2 = \frac{4\pi}{\sqrt{3}a \cdot (m + 1)} \begin{pmatrix} 0 \\ -1 \end{pmatrix}.
\]
For the second super-cell a rectangular reciprocal lattice is obtained. The first Brillouin zone is indicated by a red line and the irreducible Brillouin zone is colored in orange for both super-cells in Fig. 3.4. The reciprocal lattice and the Brillouin zone further depend on the choice of \(m\): The more lateral holes are included in the super-cell, the longer becomes \(\mathbf{a}_2\) and the smaller becomes \(\mathbf{b}_2\). For infinitely many lateral numbers of holes, the irreducible Brillouin zone is a line given by \(k_x \in [-\pi/a, \pi/a]\) – the Brillouin zone of a strictly 1D system. A small number of lateral layers of holes \(m\) results in a numerical coupling between the neighboring PhC waveguides modes. Practically, already a modest number \(m\) of lateral layers of holes \(m\) depends on the frequency \(\omega\) prevents coupling between the line-defect PhC waveguides for the case of cylindrical air holes in InP.

In summary, the super-cell approach approximates the modes of the line-defect PhC waveguides. The quality of the approximation depends on the choice of the super-cell: the size of the super-cell should be large enough to completely decouple the line-defect PhC waveguide modes. The choice of the lattice vectors determine the irreducible Brillouin zone. The Brillouin zone determines the irreducible wave vector space to be sampled numerically.

### 3.2.2 3D MPB Simulations of Slab PhC Waveguides

For the computation of the band diagram for a 3D super-cell a two-folded procedure is employed: First the modes of the primitive unit-cell (defect-free PhC) with periodic boundary conditions in all directions are computed to determine the photonic band gap. Then the photonic bands of the line-defect PhC waveguide are computed to determine the dispersion of the line-defect PhC waveguide mode within the photonic band gap.

The unit-cell as used for the 3D MPB simulation is shown in Fig. 3.5 (A). The simulation of a 3D super-cell results in a large number of modes. One reason is that a strict distinction between TE and TM modes is not possible in slab PhC waveguides (cf. 2.3.1) and both TE-like and TM-like modes are obtained by MPB. Furthermore, there are a large number of super-cell modes in the system. The band diagram is thus overloaded with irrelevant modes of the super-cell [184, pp. 52]. Examples of such super-cell modes are shown in Fig. 3.3. A mode is represented by a dot in Fig. 3.5 and Fig. 3.6. An efficient filtering technique is required to extract the relevant information of the photonic band gap and the dispersion of the line-defect PhC waveguide modes from the band diagram. Therefore, we compute the \(z\)-parity – the parity inversion symmetry with respect to the \(x-y\)-plane going
Computation of Dispersion Diagram of PhCs

Figure 3.5: MPB simulation of a periodically continued 3D unit-cell containing a hole with \( r = 0.34 \cdot a \) penetrating through a InP/InGaAsP/InP layer stack as shown in A. By scaling the solutions (B) of the eigenvalue equation with the energy in the core layer (C) and by selecting only the TE modes \((\sigma_z > 0)\) (D), the TE photonic band gap is obtained.

through \( z = 0 \) (cf. Sec. 2.3.1) – and the energy confined to the core layer of the PhC \((\sim \int_{-d_{\text{core}}/2}^{d_{\text{core}}/2} |E|^2 dz)\). Since MPB computes the parties for the symmetry planes going through the origin, the core layer of the slab PhC is centered to \( z = 0 \). By selecting only the modes that have a \( z \)-parity \( \sigma_z > 0 \) the TE-like modes can be separated from the TM-like modes (as shown in Fig. 3.5 (D) and Fig. 3.6 (C-F)). Furthermore the band diagram appears more clearly if the radius of the dots (mode) are scaled proportional to the energy that is confined in the core layer with thickness \( d_{\text{core}} \) \([90]\). The procedure is shown step by step in Fig. 3.5, where the band diagram is shown with (B) equally-sized dots representing the modes, with (C) dots scaled proportional to the percentage of the energy in the core layer \( d_{\text{core}} \) and (D) with colored dots according to \( \sigma_z > 0 \) (blue) and \( \sigma_z < 0 \) (red).

The procedure to determine the dispersion of the line-defect PhC modes is similar to the procedure to determine the photonic band gap for the unit-cell. One difference is that there is a clear mirror symmetry with respect to the \( x \cdot z \)-plane going through the center of the line-defect waveguide \((y = 0)\). The \( y \)-parity \( \sigma_y \) characterizes the mode with respect to this lateral symmetry. A rectangular super-cell as shown in Fig. 3.4 B) is required for the correct computation of the \( y \)-parity with
Figure 3.6: 3D MPB simulation of a 1x15 super-cell for a W1 PhC waveguide implemented in the InP/InGaAsP/InP layer stack (G). The figure illustrate the data processing (A)-(F): only the dispersion data (A), additional scaling of the data proportional to the confinement factor (B) (percentage of the energy confined the the core volume (blue)) and the mode separated by their $\sigma_z$ and $\sigma_y$ symmetry (C)-(F).
Computation of Dispersion Diagram of PhCs

MPB. If tilted basis vectors would be used – i.e., a rhomboidic super-cell – then the \( \sigma_y \)-symmetry cannot be determined with MPB. A further difference compared to the unit-cell simulations is that we compute the confinement factor by computing the percentage of the energy that is located in the core of the PhC waveguide\(^1\). Figure 3.6 shows the 3D super-cell (G) and illustrates the procedure: (A) shows the obtained modes, (B) shows the dispersion diagram with dots that are scaled proportionally to the confinement factor, (C)-(F) show the modes separated by their \( y \)-parity and \( z \)-parity. In other words, if a W1 PhC waveguide is excited with an even \( H_z \)-field distribution, then the relevant modes are expected to be the ones from Fig. 3.6 (C).

3.3 Mode-Maps for Tailoring the Dispersion Relation of Line-Defect PhC Waveguides

PhCs have attracted much attention due to their exceptional ability to engineer the properties of light propagation. Light is guided efficiently in waveguides that are formed by omitting one or a few rows of holes in an otherwise perfectly PhC of finite size. In the field of integrated optics, the ability to tailor the dispersion of guided line-defect PhC waveguide modes is of particular interest, due to the fact that those modes may exhibit narrow stop bands [4] or regions of flat bands (slow light modes). The tailoring of the dispersion of guided modes to obtain slow light modes with low group velocity dispersion by slightly modifying the PhC waveguide has been demonstrated by Li et al. [156] and Kubo et al. [142]. The parameters that can be used for the tailoring of the dispersions are numerous: the radius and the position of any hole can in principle be used for an optimization. Because of the many possible design parameters, it is challenging to find the PhC design with the best approximation of the desired dispersion curve. Rules of thumb are helpful to design an optimization routine for the engineering of the desired dispersion relation. For instance, Frandsen et al. [73] showed that almost any desired dispersion relation of line-defect PhC waveguides can be achieved by only modifying the radius of the first and second row of holes adjacent to the waveguide core. With this information the search-space of possible PhC designs is already reduced considerably. To reduce the search-space even further, we introduce a mode-map plot that can be used to i) identify a suitable design parameter (e.g., the radius of the first hole) and ii) identify the search direction (e.g., increase the radius of the first hole).

3.3.1 Method for Computing the Mode-Maps of Line-Defect PhC Waveguides

Gap-maps as introduced in Sec. 2.2.1.5 have simplified the PhC design process considerably. Dependent on the application and on technology constraints, the best approximation of the desired dispersion curve. Rules of thumb are helpful to design an optimization routine for the engineering of the desired dispersion relation. For instance, Frandsen et al. [73] showed that almost any desired dispersion relation of line-defect PhC waveguides can be achieved by only modifying the radius of the first and second row of holes adjacent to the waveguide core. With this information the search-space of possible PhC designs is already reduced considerably. To reduce the search-space even further, we introduce a mode-map plot that can be used to i) identify a suitable design parameter (e.g., the radius of the first hole) and ii) identify the search direction (e.g., increase the radius of the first hole).

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\(^1\)The core waveguide volume is defined by the thickness of the core layer \( d_{\text{core}} \), the lattice constant \( a \) in \( x \)-direction, and the width of the W1 PhC waveguide \( w_{W1} = (\sqrt{3} - 2 \cdot r) \cdot a \). The energy confined to the core layer is thus \( \sim \int_{-d_{\text{core}}/2}^{d_{\text{core}}/2} \int_{-w_{W1}/2}^{w_{W1}/2} \int_{-a/2}^{a/2} |E|^2 \, dx \, dy \, dz \).
Figure 3.7: Computed TE band diagrams for a PhC W1 waveguide and its corresponding number of states.

PhC design can be chosen without the need of numerical computations. For instance, large TE band gaps are obtained for a hexagonal lattice of air holes, whereas large TM band gaps are obtained for both a square lattice and a hexagonal lattice of dielectric rods. If the gap-map is available for the material system of interest, e.g., InP, then even specific numbers for the basic design parameters – the lattice constant \( a \) and the radius \( r \) – can directly be deduced from the gap-map plots. In this section, we investigate, if a similar design instrument can be developed for line-defect PhC waveguides.

Figure 3.8: In analogy to [104], we computed a sweep of the radius \( r \) over lattice constant \( a \) for a defect-free hexagonal PhC (left) and the corresponding PhC W1 waveguide (right). Instead of plotting the photonic band gap as proposed in [104], the density of states is mapped to a color scheme that is then plotted versus radius \( r \). The calculations have been made with MPB [110] using \( \varepsilon = 10.3 \) and a wave vector resolution of \( \Delta k = 2\pi/(800 \cdot a) \). The computed density of states has a resolution of \( \Delta \omega a/(2\pi c) = 1/2000 \) and was computed over the first 50 TE-bands.
In a first step we analyze the dispersion diagram of a W1 PhC waveguide with air holes of radius $r = 0.31a$ as shown in Fig. 3.7. The characteristic features of interest are the mode cutoff and mode stop-band, the single mode regime, the photonic band gap of the defect-free PhC cladding and multi-mode regimes. The dispersion diagram of the shown W1 PhC waveguide is characterized by two single mode regimes from $\omega a/(2\pi c) = 0.228$ to $\omega a/(2\pi c) = 0.25$ and from $\omega a/(2\pi c) = 0.263$ to $\omega a/(2\pi c) = 0.295$ and a small mode stop-band from $\omega a/(2\pi c) = 0.22$ to $\omega a/(2\pi c) = 0.228$. Outside this frequency range, more than one mode can propagate, e.g., there are many modes propagating in the defect-free PhC cladding.

The number of states (modes) is shown in the right plot of Fig. 3.7. The number is obtained by discretizing the frequency axis into equally sized frequency intervals $\Delta \omega_i$ followed by a subsequent counting of all obtained modes of the super-cell within the frequency interval $\Delta \omega_i$. This count – the number of states (NOS) – is approximately proportional to the photonic density of states within the photonic band gap of the defect-free PhC. The absolute value of the NOS depends mainly on the discretization: Larger counts for the NOS are obtained for a lower discretization of $\omega$. We are thus only interested in the relative values of the NOS. First note that the NOS exhibits many peaks for the frequency range outside the photonic band gap of the defect-free PhC due to the super-cell modes in the PhC claddings. Despite of this strongly varying behavior of the NOS, the average value for these frequency regions is generally larger than for the frequency range of the photonic band gap of the defect-free PhC cladding. As opposed to that, the NOS for a single-mode PhC waveguide mode is characterized by a smooth curve with a low average value. For the W1 PhC waveguide mode, whose wave vector $k_x$ is close to the edge of the first Brillouin zone, a peak is observed in the NOS due to the flat band. A flat dispersion curve manifests itself in a peak in the NOS because of the many similar eigenfrequencies for a wide range of Bloch indices. Generally, a high NOS arises a) from a multimode frequency regime or b) from a mode with a flat dispersion curve.

From the NOS curve (Fig. 3.7, right), we can thus identify the following:

- the frequency regime of mode stop bands (NOS=0)
- the frequency regime of modes of the defect-free PhC cladding (larger average of the NOS value and characterized with irregular peaks in the NOS curve)
- the single mode regime of the PhC waveguide mode (smooth, low NOS value)
- the cut-off frequency of the PhC waveguide mode (the low group velocity at the edge of the first Brillouin zone resulting in a high peak value)

We observe that the NOS is able to map most of the characteristic features of a line-defect PhC waveguide to a single curve. Therefore, we propose to plot the NOS as a function of a certain design parameter of the line-defect PhC waveguide mode.

In the traditional gap-map plots for defect-free PhCs, only the edges of the photonic band gaps are plotted. As opposed to that, the NOS information of the PhC design is added to the maps via a color scheme. Figure 3.8 depicts the proposed mode-map plots for a defect-free PhC (left) and for a W1 PhC waveguide. The band gap information of the defect-free PhC is clearly contained in the mode-map plot.
of the line-defect PhC waveguide as well: the blue lines in Fig. 3.8 (right) are determined from the gap-map plot of the defect free PhC (i.e., the white area of the left plot of Fig. 3.8) and overlaid with the mode-map plot of the W1 PhC waveguide.

Some remarks about the interpretation of the color scheme: the colors are scaled from 0 to 75 – a value that is above the average of the NOS values outside the photonic band gap for our particular example. Note that the color scale is a relative scale only. Our choice of the color scheme allows to make the following interpretation:

- A white area corresponds to a mode stop-band.
- A constant bright (yellow) area denotes a single-mode regime. A frequency range with a constant color signifies a constant slope of the dispersion.
- Dark colors – usually lines – represent either flat bands (slow light modes) or band-edges. Note that the edges of the photonic band gap in Fig. 3.8 (left) are bound by a strong black line. Therefore a large NOS is expected at the band-edge. Typically, PhC lasers operate at the band-edge due to the high density of states [220, 225].

The used colorbar is shown in Fig. 3.9.

In the following, we investigate if the new mode-map representation can be used to analyze the influence of a certain design parameter on the dispersion of the line-defect PhC waveguide mode.

### 3.3.2 Sensitivity Analysis of the W1 PhC Waveguide Mode Using Mode-Map Plots

Five different PhC design parameters are considered for a sensitivity analysis as it is sketched in Fig. 3.10: the radius of all holes of the PhC (A), the radius of the first (B) and the second row (C), the separation distance $w$ of the PhC claddings (width of the line-defect waveguide) (E) and the relative displacement $d$ of the PhC claddings.
with respect to the propagation direction (D). For these parameters, the mode-map plots are computed and shown in Fig. 3.11.

The investigated design parameters constitute only a small modification of the defect-free PhC claddings. Therefore, the considered design parameters almost exclusively influence the dispersion of the W1 PhC waveguide modes. A consultation of the band diagram of the W1 PhC waveguide plot is useful for an initial identification of the different regions. The blue line in Fig. 3.11 marks the initial position, i.e., the W1 PhC waveguide without a modification. Along this line, we can identify single-mode regions, stop-band regions and multimode regions from the band diagram of the W1 PhC waveguide (cf. Fig. 3.7). Thereafter, tracing the regions (e.g., the stop-band region) as a function of the varied parameter is possible.

The following trends can be deduced:

- A larger radius \(r\) of all holes of the W1 PhC waveguide design shifts the frequencies of the line-defect mode towards higher frequencies.
- Separating the PhC claddings (increasing the width \(w\) of the line-defect core) results in a shift of the frequencies of the line-defect modes towards lower frequencies.
- A larger radius in the first \(r_1\) and the second row \(r_2\) of the PhC results in a shift of frequencies of the line-defect modes towards higher frequencies.
- The shifting \(d\) of the PhC claddings relative to each others with respect to the propagation direction yields a frequency shift for the even line-defect modes. In Fig. 3.11 D) it can be seen that the frequencies of the even mode of the line-defect located below the odd mode are shifted towards lower frequencies, whereas frequencies of the even mode located above the odd mode are shifted towards higher frequencies.

Similar to the gap-map plots of the defect-free PhCs that are valid for a specific design (i.e., hexagonal lattice of circular holes), the mode-map plots are only valid

![Figure 3.10: Additionally to the radius \(r\) (A), the following parameters of the W1 PhC waveguide with \(r = 0.3a\) have been investigated: the radius of the first (B) and the second (C) row, a relative shift of the two PhC claddings with respect to the propagation direction (D) and the separation distance \(w\) of the PhC claddings (E).](image)
Figure 3.11: The gap-map plots for the following design parameters: radius of first row \( r_1 \) (B), radius of second row \( r_2 \) (C), waveguide width \( w \) (E) and relative displacement \( d \) with respect to the propagation direction (D). All computations have been performed for \( \varepsilon = 10.63 \) and TE-polarization.

for a specific line-defect PhC waveguide design. In the following, we list two examples to illustrate the usage of the mode-map plots. For instance, let us assume that we want to increase the single mode regime from \( \omega a/(2\pi c) = 0.228 \) to \( \omega a/(2\pi c) = 0.25 \) (below the odd mode). By consulting the new mode-map plots for the \( W_1 \) PhC waveguide in Fig. 3.11, we find that adding a shift \( d \approx 0.25 \cdot a \) maximizes the frequency range of the single-mode regime below the odd mode. Furthermore, the group velocity of this single-mode regime is rather constant, since the color in the mode-map plot stays constant within this frequency range. Or to add another example, in chapter 8 we need a PhC waveguide that lowers the frequencies of the dispersion of the line-defect PhC waveguide. This can be achieved by reducing the radius of all holes of the PhC waveguide design from \( r = 0.31a \) to \( r = 0.26a \) (cf. Figure 3.8 (right)). Furthermore, reducing the radius of the first hole from \( r = 0.3a \) to \( r = 0.23 \) reduces the stop-band regime in exchange for lower frequencies of the dispersion of the line-defect PhC waveguide mode.

We conclude that the new mode-map plots for line-defect PhC waveguides can...
quickly deliver a concrete number for a design parameter that improves the PhC waveguide design according to the needs.

### 3.4 Photonic Band Computation Using hp-FEM Including Dispersive Material

So far we only used MPB for the computation of the photonic bands. Unfortunately, MPB is rather inefficient and allows only strictly periodic boundary conditions. Radiation phenomena and propagation losses cannot thus not be simulated with MPB. For instance, in Fig. 3.5 and Fig. 3.6 it can be seen that a large number of super-cell modes are computed, even though, only a few are modes of the line-defect PhC waveguide. Furthermore, the systematic engineering of the dispersion of line-defect PhC waveguides requires an extensive parameter optimization and efficient numerical methods for the accurate computation of photonic bands are prerequisite. The motivation to develop a more efficient method is thus manifold:

- The engineering of the dispersion of line-defect PhC waveguides requires fast and efficient 2D PhC mode solvers. Furthermore, accurate and efficient 2D PhC mode solvers are highly valuable for mode analysis purposes such as the presented sensitivity analysis by means of mode map plots (Fig. 3.8 and Fig. 3.11).

- The standard procedure to obtain the photonic bands of a PhC is to solve an eigenvalue problem with eigenvalue $\omega(\hat{k}_i)$ in the unit cell for a discrete set of Bloch indices $\hat{k}_i$ within the irreducible Brillouin zone. Subsequently, the frequencies $\omega(\hat{k}_i)$ for each Bloch index sample $\hat{k}_i$ are computed for the unit cell (see [104, 35, 58, 25, 234] and the references therein). But, devices for telecommunications are typically operated only within finite frequency bands. Fabricated PhC waveguides are excited experimentally in the $\omega$-domain by a monochromatic light source with a frequency $\omega_0$ or by pulses with a carrier frequency $\omega_0$ and not by imposing a specific Bloch index $\hat{k}_0$. The question is hence ‘how does the wave propagate when excited with light of frequency $\omega_0$’? This real world situation motivates the computation of Bloch indices $\hat{k}(\omega_0)$ for a given frequency $\omega_0$. Furthermore, this approach would allow us to compute only the modes within a given frequency range, e.g., the photonic band gap, and thus the computation of super-cell modes with frequencies outside the photonic band gap is avoided (cf. Fig. 3.5 and Fig. 3.6). Smajic et al. [247, 37] already proposed in 2004 to tackle the problem by computing the complex wave vector $\hat{k}$ of a mode for a given frequency $\omega_0$. Generally, they studied structures with small material absorption and used an iterative approach, which requires scanning of a large area of the complex wave vector plane to find the mode solutions.

- The restriction to periodic boundary conditions as given by MPB leads to real Bloch indices $\hat{k}$ exclusively. As a consequence, radiation phenomena and lossy materials cannot be investigated with MPB. A method that is more flexible is desired.
MPB is based on a uniform rectangular grid, which makes it difficult to resolve curved dielectric interfaces and interfaces not aligned to the grid. Furthermore, the permittivity is expanded in terms of plane waves in MPB (cf. 2.2.3). Discontinuities in the permittivity as abrupt interfaces typically require many expansion coefficients. This results in a low algebraic convergence (cf. Eq. 3.74).

In this section, we present a new method that naturally includes dispersive and lossy materials by the direct solution of the eigenvalue $\hat{k}$ for a given frequency $\omega_0$ that exhibits an exponential convergence (cf. Eq. 3.75). Hence the method is especially suited for optimization of PhC waveguides of both, dispersive and non-dispersive materials. Compared to the methods based on searching the eigenfrequencies $\omega$ for a given Bloch index $\hat{k}_0$ [131], we are able to directly access the lossy modes by computing the complex Bloch index $\hat{k}$. The computation of the propagation losses of leaky modes of substrate-type PhC waveguides requires appropriate boundary conditions and three-dimensional structures. A two-dimensional system – as implemented so far – is not sufficient to compute the propagation losses. The implementation of the method in three dimension is currently discussed: the implementation requires vector elements and a 3D mesh generator and hence is time-consuming. From a theoretical perspective, the numerical method should behave equally well, e.g., the method should exhibit an exponential convergence rate for 3D simulations as well. The 2D version of the method can already be used to investigate the influence of dispersive material on the frequency features of PhCs.

The following section is organized as follows: First the weak form of the eigenvalue problem in the super-cell for the TE modes is formulated in Sec. 3.4.2. Then Sec. 3.4.3 is dedicated to the numerical solution of the eigenvalue problem which includes the FEM-discretization for triangular elements. This results in a quadratic eigenvalue equation that can be 'linearized'\(^2\). A prototype was programmed in MATLAB. The MATLAB code loads a mesh file that has been generated by COMSOL, assembles the matrices and solves the eigenvalue equation. A verification of the code was performed for a simple example – a rectangular waveguide – that has an analytical solution and for a W1 PhC waveguide. Unfortunately, the MATLAB code is rather inefficient for complicated meshes, such as the mesh of the super-cell for a W1 PhC waveguide. At this stage we decided to use the CONCEPTS libraries. The CONCEPTS C++ libraries already provide a highly efficient framework for FEM analysis. Furthermore, additional features are provided by CONCEPTS such as curved elements and higher order polynomial basis functions. The implementation of the method using the CONCEPTS libraries was accomplished by K. Schmidt [233]. Having now state-of-the-art libraries, a comparison of our method with COMSOL and MPB is made and we can demonstrate an exponential convergence for the method. Finally, we apply our method to investigate the influence of dispersive InP on the photonic band gap and on the mode of the W1 PhC waveguide. This is simpler to investigate by using the $k$-search for given frequencies $\omega_0$.

\(^2\)Here, the term 'linearized' means that the nonlinear quadratic eigenvalue problem is transformed into a linear eigenvalue problem with the same eigenvalues [281].
3.4.1 The Finite Element Formalism

The finite element method delivers an approximate solution of a partial differential equation. The fundamental idea behind the finite element analysis consists of finding an equation that is numerically stable and simultaneously approximates the partial differential equation to be studied. This equivalent equation can be obtained by using variational calculus, where a function $h$ is sought that minimizes the residual. The finite element method is essentially a weighted residual method. Technically, the residual of the partial differential equation is multiplied by a weighting function $g$ followed by an integration over the computational domain. This resulting integral from is called the weak formulation. Thereafter, the approximate solution $h$ is discretized by piecewise linear basis functions (i.e., a linear basis function for each finite element). CONCEPTS uses polynomial basis functions of degree $p$ instead of linear basis functions. By using the discretization on finite elements, the eigenvalue equation in the weak form can be written in matrices, such that a numerical solver can be applied.

3.4.2 Weak Formulation for TE Modes for Systems with a 1D-Periodicity of the Permittivity

We consider a 2D dielectric system with a 1D periodicity of the permittivity along the $x$-axis with a periodicity length $a$. The computational area $\Omega$ is given by the super-cell as shown in Fig. 3.12. Periodic boundary conditions are applied in propagation direction. We further assume time-harmonic fields in a linear, isotropic, non-magnetic and dispersive material. We start with the master equation (cf. A.9)

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

(3.5)

The TE mode of the PhC waveguide is characterized by only a $z$-component of the magnetic field

$$H(r, \omega) = (0, 0, h(x, y, \omega))$$

(3.6)

A scalar equation for $h(x, y, \omega)$ is obtained by inserting $H$ into the master equation.

![Figure 3.12: Illustration of the (super-cell) computational domain $\Omega$ with boundary $\partial \Omega$ for a line-defect PhC waveguide.](image-url)
Photonic Band Computation Using hp-FEM

\[
- \frac{\partial}{\partial x} \frac{1}{\varepsilon(x,y,\omega)} \frac{\partial}{\partial x} h(x,y,\omega) - \frac{\partial}{\partial y} \frac{1}{\varepsilon(x,y,\omega)} \frac{\partial}{\partial y} h(x,y,\omega) = \frac{\omega^2}{c^2} h(x,y,\omega). \quad (3.7)
\]

The complete problem including the periodic boundary conditions can be summarized by

\[
\begin{cases}
- \nabla \cdot \left( \frac{1}{\varepsilon} \nabla h \right) - \left( \frac{\omega}{c} \right)^2 h = 0 \\
\left. h \right|_{x + a} = \left. h \right|_x 
\end{cases}
\]

(3.8)

The boundary conditions for the horizontal boundaries (\(h(x, 0)\) and \(h(x, L)\)) are not included in the formulation yet. But we will use two different boundary conditions for the horizontal boundaries in the following:

- periodic boundary conditions \(h(x, 0) = h(x, L) e^{i \hat{k}_y L}\) with the Bloch index component \(\hat{k}_y\) along the \(y\)-axis and
- Dirichlet boundary condition \(h(x, 0) = \alpha(x), h(x, L) = \beta(x)\), where \(\alpha\) and \(\beta\) are functions on the boundaries.

We seek an approximate solution \(h\) of Eq. 3.8, for which the remaining non-zero residual \(R(x, y) = -\nabla \cdot \left( \frac{1}{\varepsilon} \nabla h \right) - \left( \frac{\omega}{c} \right)^2 h\) is minimum. As mentioned above, the finite element method is based on the idea to minimize this residual \(R(x, y)\). However, first the Bloch theorem is used: The solution \(h\) has the form

\[
h = u_{k_x} e^{i k_x x}, \quad (3.9)
\]

where \(u_{k_x}\) is strictly periodic function with periodicity \(a\). Equation 3.9 is inserted in Eq. 3.8 and is then multiplied by an unknown weight function \(g\) of the form \(g = \overline{v_{k_x} e^{i k_x x}}\) where the overbar signifies the complex conjugate. The complex conjugate form is useful since then the \(e^{i k_x x}\) terms cancel as can be seen in the following. Thereafter, the product is integrated by parts (Gauss theorem). For the first term of Eq. 3.8 we get

\[
\int_{\Omega} - \nabla \cdot \left( \frac{1}{\varepsilon} \nabla u_{k_x} e^{i k_x x} \right) \overline{v_{k_x} e^{i k_x x}} \, dxdy =
\]

\[
\int_{\partial \Omega} - \frac{1}{\varepsilon} \left( \nabla u_{k_x} e^{i k_x x} \right) \overline{v_{k_x} e^{i k_x x}} dS + \int_{\Omega} \frac{1}{\varepsilon} \nabla u_{k_x} e^{i k_x x} \overline{\nabla v_{k_x} e^{i k_x x}} dxdy \quad (3.10)
\]

where \(dS = n \, dS\) is the boundary element and \(n\) is the normal vector to the boundary \(\partial \Omega\). Because of the periodic boundaries, the integration over the boundary \(\partial \Omega\) vanishes. The residual (Eq. 3.8) with all terms writes
\[ \int_{\Omega} \frac{1}{\varepsilon} \nabla (u_{k_x} e^{ik_x x}) \cdot \nabla (v_{k_x} e^{ik_x x}) \, dx \, dy \]
\[ - \left( \frac{\omega}{c} \right)^2 \int_{\Omega} u_{k_x} e^{ik_x x} \overline{v_{k_x}} \, dx \, dy = 0, \quad (3.11) \]

\[ \int_{\Omega} \frac{1}{\varepsilon} \left( \left( \frac{\partial}{\partial x} + i\hat{k}_x \right) u_{k_x} \cdot \left( \frac{\partial}{\partial x} + i\hat{k}_x \right) v_{k_x} + \frac{\partial}{\partial y} u_{k_x} \frac{\partial}{\partial y} \overline{v_{k_x}} \right) \, dx \, dy \]
\[ - \left( \frac{\omega}{c} \right)^2 \int_{\Omega} u_{k_x} \overline{v_{k_x}} \, dx \, dy = 0. \quad (3.12) \]

Thus the weak formulation for the transformed problem is: Seek \( u_{k_x} \in V_{\text{per}} \) such that

\[ \int_{\Omega} \frac{1}{\varepsilon} \nabla u_{k_x} \cdot \nabla v_{k_x} - \left( \frac{\omega}{c} \right)^2 u_{k_x} \overline{v_{k_x}} \, dx \, dy + \]
\[ i\hat{k}_x \int_{\Omega} \frac{1}{\varepsilon} \left( u_{k_x} \cdot \frac{\partial}{\partial x} \overline{v_{k_x}} - \frac{\partial}{\partial x} u_{k_x} \overline{v_{k_x}} \right) \, dx \, dy + \hat{k}_x^2 \int_{\Omega} \frac{1}{\varepsilon} u_{k_x} \cdot \overline{v_{k_x}} \, dx \, dy = 0. \quad (3.13) \]

\( V_{\text{per}} \) is a subspace of all functions that are strictly periodic with periodicity \( a \). Alternatively, the weak formulation can be written as

\[ a(u_{k_x}, v_{k_x}) - \left( \frac{\omega}{c} \right)^2 b_0(u_{k_x}, v_{k_x}) + i\hat{k}_x c(u_{k_x}, v_{k_x}) + \hat{k}_x^2 b_\varepsilon(u_{k_x}, v_{k_x}) = 0. \quad (3.14) \]

where

\[ a(u, v) = \int_{\Omega} \frac{1}{\varepsilon} \nabla u \cdot \nabla v \, dx \, dy, \quad b_0(u, v) = \int_{\Omega} u \overline{v} \, dx \, dy, \quad (3.15) \]
\[ b_\varepsilon(u, v) = \int_{\Omega} \frac{1}{\varepsilon} u \overline{v} \, dx \, dy, \quad c(u, v) = \int_{\Omega} \frac{1}{\varepsilon} \left( u \cdot \frac{\partial}{\partial x} \overline{v} - \frac{\partial}{\partial x} u \cdot \overline{v} \right) \, dx \, dy \quad (3.16) \]

are the bilinear forms of the four different terms of Eq. 3.14. A quadratic eigenvalue equation with strictly periodic eigenfunctions \( u_{k_x} \) with the corresponding eigenvalues \( \omega \) or \( \hat{k}_x \) is obtained. We have now an equation that is numerically stable and approximates the partial differential equation given in Eq. 3.8. However, the sought solution \( u_{k_x} \) is still unknown. Therefore, we assume that the solution can be approximated by a set of piecewise linear functions. The computational domain is discretized in a finite number of triangular or quadrilateral elements. On every element \( e \) the solution is approximated by a different linear function.
3.4.3 Discretization by Means of Finite Elements

The following paragraph represents the standard procedure of a finite element discretization for triangular elements and follows closely Smaïjic [245]. First, the space $V_{\text{per}}$ is discretized into triangular sub-domains called elements. In every element a linear approximation function of the form

$$u^e_{kx} (x, y) = a + bx + cy$$  \hspace{1cm} (3.17)

is defined. The superscript $^e$ denotes the local approximation of the solution within an element $e$. Let $(x^e_j, y^e_j)$ be the coordinates of the node $j \in \{1, 2, 3\}$ of the triangular element $e$. The value of the function $u^e_{kx,j}$ at the node $N_j$ is obtained if the coordinates are inserted into Eq. 3.17

$$\begin{pmatrix} u^e_{kx,1} \\ u^e_{kx,2} \\ u^e_{kx,3} \end{pmatrix} = \begin{pmatrix} x^e_1 & y^e_1 & 1 \\ x^e_2 & y^e_2 & 1 \\ x^e_3 & y^e_3 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$ \hspace{1cm} (3.18)

The parameters $a, b$ and $c$ of the linear approximation function $u^e_{kx}$ are obtained if the matrix $\{S\}^e$ is inverted

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \left[\{S\}^e\right]^{-1} \begin{pmatrix} u^e_{kx,1} \\ u^e_{kx,2} \\ u^e_{kx,3} \end{pmatrix}$$ \hspace{1cm} (3.19)

The approximation function $u^e_{kx}$ can be written in matrix notation

$$u^e_{kx}(x, y) = \begin{pmatrix} 1 & x & y \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 1 & x & y \end{pmatrix} \left[\{S\}^e\right]^{-1} \begin{pmatrix} u^e_{kx,1} \\ u^e_{kx,2} \\ u^e_{kx,3} \end{pmatrix}$$ \hspace{1cm} (3.20)

The $3x3$ matrix $\{S\}^e$ can be inverted analytically for a triangle\(^3\) and we find

$$\left[\{S\}^e\right]^{-1} = \frac{1}{\det(\{S\}^e)} \begin{bmatrix} x_2^e \cdot y_3^e - x_3^e \cdot y_2^e & x_3^e \cdot y_1^e - x_1^e \cdot y_3^e & x_1^e \cdot y_2^e - x_2^e \cdot y_1^e \\ y_2^e - y_3^e & y_3^e - y_1^e & y_1^e - y_2^e \\ x_3^e - x_2^e & x_1^e - x_3^e & x_2^e - x_1^e \end{bmatrix}$$ \hspace{1cm} (3.21)

It is convenient to introduce the following notation

$$u^e_{kx}(x, y) = \sum_{i=1}^{3} \alpha^e_j(x, y) \cdot u^e_{kx,j}$$ \hspace{1cm} (3.22)

where $\alpha^e_j$ are the so called shape functions. In other words, the linear approxima-

\(^3\)Let $A = [x_0, x_1, x_2]$ (consisting of three column vectors, $x_0, x_1,$ and $x_2$), then the inverse of $A^{-1} = \frac{1}{\det(A)} \begin{bmatrix} (x_1 \times x_2)^T \\ (x_2 \times x_0)^T \\ (x_0 \times x_1)^T \end{bmatrix}$
Computation of Dispersion Diagram of PhCs

It can be easily verified that the shape functions \( \alpha_j^e \) have the mentioned important property

\[
\alpha_j^e(x_l, y_l) = \begin{cases} 
0 & \text{if } j \neq l \\
1 & \text{if } j = l
\end{cases}
\]

and

\[
\sum_{j=1}^{3} \alpha_j^e(x, y) = 1
\]

for every point \( (x, y) \) in the triangular element \( e \). Each shape function \( \alpha_j^e \) represents a plane that is one for the node \( N_j(x_j, y_j) \) and zero for the two other nodes \( N_l, l \neq j \).

Now, we switch from a local (one single element) to a global notation. Note that the nodes are shared by the adjacent elements and hence the value at the nodes \( u_{ka}^e \) of the triangular element is the same for all neighboring elements. Therefore, the solution \( u_{ka}^e \) for the complete computation domain \( \Omega \) is obtained by putting together all approximation functions \( u_{ka}^e \) on the individual elements \( e \)

\[
u_{ka}^e(x, y) = \sum_{j=1}^{3} \alpha_j^e(x, y) \cdot u_{ka}^e_{x,j} \quad \rightarrow \quad u_{ka}^e(x, y) = \sum_{l=1}^{N_n} \alpha_l(x, y) \cdot u_{ka}^e_{y,l} \quad (3.28)
\]

where \( N_n \) is the total number of nodes in the system. We have now discretized the solution \( u_{ka}^e \) in piecewise linear approximation functions \( \alpha_l \). In order that we can solve for the coefficients, we need to apply the eigenvalue equation. Therefore we insert the shape functions into the bilinear forms (Eq. 3.15, Eq. 3.16) and compute the integrals.

### 3.4.3.1 Bilinear Forms for Triangular Elements

The computation of the integral form over an arbitrary integral can be simplified by performing a coordinate transformation as illustrated in Fig. 3.13. The node \( a_1 = (x_1, y_1) \) shall be transformed onto \( \hat{a}_1 = (\hat{x}_1, \hat{y}_1) = (0, 0) \), node \( a_2 = (x_1, y_1) \) shall be transformed onto \( \hat{a}_2 = (\hat{x}_2, \hat{y}_2) = (1, 0) \) and \( a_3 = (x_3, y_3) \) shall be transformed onto \( \hat{a}_3 = (\hat{x}_3, \hat{y}_3) = (0, 1) \). The computation of the integrals of the bilinear forms are straight forward on the reference cell \( \hat{K} \) – the unit triangle.
The mapping from the unit-triangle $\hat{K}$ in the $(\hat{x}, \hat{y})$ coordinate system to a particular triangle $K$ in the $(x, y)$-coordinate system is $F_K$. For the triangular element $K$ with corners $a_1, a_2, a_3$ the mapping from the reference cell $\hat{K}$ is

$$F_K \begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix} = a_1 (1 - \hat{x} - \hat{y}) + a_2 \hat{x} + a_3 \hat{y} \quad (3.29)$$

where $a_i = (x_j, y_j)$ are the coordinates of the nodes from the original system. The hat denote the reference system, e.g., $\hat{x}$ and $\hat{y}$ define the coordinate system of the reference system. The transformation $\hat{K} \mapsto K$ is given by:

- transformation of the coordinates:
  $$\begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix} \mapsto F_K (\hat{x}, \hat{y}) \quad (3.30)$$

- transformation of the functions:
  $$\hat{f}(\hat{x}, \hat{y}) := f(F_K(\hat{x}, \hat{y})) \quad (3.31)$$

- transformation of the integrals:
  $$\int_K f(x, y) dx dy = \int_{\hat{K}} f(F_K(\hat{x}, \hat{y})) |J(\hat{x}, \hat{y})| d\hat{x} d\hat{y} \quad (3.32)$$

where $J$ is the Jacobian matrix

$$J = ((a_2 - a_1)(a_3 - a_1)) \quad (3.33)$$

- transformation of the gradients:
  $$\nabla f = J^{-T} \nabla \hat{f} \quad (3.34)$$
where $\hat{\nabla} \hat{f} = \left( \frac{\partial \hat{x}}{\partial f}, \frac{\partial \hat{y}}{\partial f} \right) \nabla f = J^T \nabla f$ and $\nabla^T f = \hat{\nabla}^T \hat{f} J^{-1}$

Having defined the coordinate transformation, we can compute the bilinear forms given in Eq. 3.15 and Eq. 3.16 for triangular elements. We start with transforming the shape functions $\alpha_i^e$ (Eq. 3.23 - Eq. 3.25) to the new coordinate system

$$\alpha_1^e \rightarrow \hat{\alpha}_1^e = 1 - \hat{x} - \hat{y}, \quad \alpha_2^e \rightarrow \hat{\alpha}_2^e = \hat{x}, \quad \alpha_3^e \rightarrow \hat{\alpha}_3^e = \hat{y}. \quad (3.35)$$

Furthermore, the area of the reference triangle $K$ is given by half of the determinant of the Jacobian matrix

$$K = \frac{1}{2} \det J = \frac{1}{2}(x_1 y_2 - x_1 y_3 + x_2 y_3 - x_2 y_1 + x_3 y_1 - x_3 y_2). \quad (3.36)$$

Then, the bilinear forms $a(\alpha_i, \alpha_j)$, $b_0(\alpha_i, \alpha_j)$, $b_e(\alpha_i, \alpha_j)$ and $c(\alpha_i, \alpha_j)$ are transformed to the reference element $\hat{K}$. We start with $a(\alpha_i, \alpha_j)$ (Eq. 3.15)

$$a(\alpha_i, \alpha_j) = \int_{K} \frac{1}{\varepsilon} \hat{\nabla}^T \hat{\alpha}_i \hat{\nabla} \alpha_j dx dy \quad (3.37)$$

$$= \int_{\hat{K}} \frac{1}{\varepsilon} \hat{\nabla}^T \hat{\alpha}_i J^{-1} J^{-\top} \hat{\nabla} \alpha_j \det J \hat{d}x \hat{d}y \quad (3.38)$$

$$= \int_{\hat{K}} \frac{1}{\varepsilon} \hat{\nabla}^T \hat{\alpha}_i \adj(J) \adj(J)^\top \hat{\nabla} \alpha_j \frac{1}{\det J} \hat{d}x \hat{d}y \quad (3.39)$$

where the adjoint Jacobian matrix is

$$\adj(J) = \begin{pmatrix} J_{22} & -J_{12} \\ -J_{21} & J_{11} \end{pmatrix}. \quad (3.40)$$

For the case of a piecewise constant permittivity $\varepsilon$ (constant permittivity $\varepsilon^e$ within element $e$), the bilinear form $a(\alpha_i, \alpha_j)$ can be simplified to

$$a(\alpha_i, \alpha_j) = \frac{1}{2\varepsilon |K|} \int_{K} \hat{\nabla}^T \hat{\alpha}_i \adj(J) \adj(J)^\top \hat{\nabla} \alpha_j d\hat{x} d\hat{y}. \quad (3.41)$$

Because the gradient of a linear function is a constant, the expression to be integrated is constant, thus

$$a(\alpha_i, \alpha_j) = \frac{1}{2\varepsilon |K|} \int_{K} \hat{\nabla}^T \hat{\alpha}_i \adj(J) \adj(J)^\top \hat{\nabla} \alpha_j \int_{0}^{1} d\hat{x} d\hat{y}. \quad (3.42)$$

The remaining integral is $\int_{0}^{1} \int_{0}^{1-x} 1 d\hat{y} d\hat{x} = \frac{1}{2}$, i.e., we finally obtain

$$a(\alpha_i, \alpha_j) = \frac{1}{4\varepsilon |K|} \hat{\nabla}^T \hat{\alpha}_i \adj(J) \adj(J)^\top \hat{\nabla} \alpha_j. \quad (3.43)$$

The integral contributions of the three shape functions $\alpha_j$ are obtained by insertion of transformed shape functions $\hat{\alpha}_j$ (Eq. 3.35), the Jacobian matrix (Eq. 3.33) and the adjoint Jacobian matrix (Eq. 3.40) into the bilinear forms (Eq. 3.43). These contributions can be written in matrix form – the so called matrix element $A$. $A$ is found by inserting all possible combinations of the
shape functions $\hat{\alpha}^e_i$ (i.e., $A_{ij}$ is obtained for $\hat{\alpha}_i = \hat{\alpha}^e_i$ and $\hat{\alpha}_j = \hat{\alpha}^e_j$ in Eq. 3.43)

$$A = \frac{1}{4\varepsilon |K|} \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{pmatrix}, \quad (3.44)$$

where

$$a_{11} = (y_3 - y_2)^2 + (x_3 - x_2)^2 \quad (3.45)$$

$$a_{12} = a_{21} = -(y_3 - y_1)(y_3 - y_2) - (x_3 - x_1)(x_3 - x_2) \quad (3.46)$$

$$a_{13} = a_{31} = -(y_2 - y_1)(y_2 - y_3) - (x_2 - x_1)(x_2 - x_3) \quad (3.47)$$

$$a_{22} = (y_3 - y_1)^2 + (x_3 - x_1)^2 \quad (3.48)$$

$$a_{23} = a_{32} = -(y_1 - y_2)(y_1 - y_3) - (x_1 - x_2)(x_1 - x_3) \quad (3.49)$$

$$a_{33} = (y_2 - y_1)^2 + (x_2 - x_1)^2 \quad (3.50)$$

The procedure is the same for the other bilinear forms. Next we compute $b_0(\alpha_i, \alpha_j)$ (Eq. 3.15)

$$b_0(\alpha_i, \alpha_j) = \int_K \hat{\alpha}_i \hat{\alpha}_j \det J \, d\hat{x}d\hat{y} \quad (3.51)$$

$$b_0(\alpha_i, \alpha_j) = 2 |\hat{K}| \int_K \hat{\alpha}_i \hat{\alpha}_j d\hat{x}d\hat{y}, \quad (3.52)$$

The corresponding matrix element form is

$$B_0 = \frac{|\hat{K}|}{12} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}. \quad (3.54)$$

A constant matrix element for $B_0$ is found. The matrix element for the bilinear form of $b_\varepsilon$ is similar to the one in Eq. 3.54, except for an additional factor $1/\varepsilon$

$$B_\varepsilon = \frac{|\hat{K}|}{12\varepsilon} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}. \quad (3.55)$$

To compute the bilinear form of $c(\alpha_i, \alpha_j)$, the two terms in the integral of Eq. 3.16 are written as

$$c(\alpha_i, \alpha_j) = \int_\Omega \frac{1}{\varepsilon} \left( \alpha_i \cdot \frac{\partial}{\partial x} \alpha_j - \frac{\partial}{\partial x} \alpha_i \cdot \alpha_j \right) \, dxdy \quad (3.56)$$

$$= c_1(\alpha_i, \alpha_j) - c_1(\alpha_j, \alpha_i) \quad (3.57)$$

such that only one of the terms ($c_1(\alpha_i, \alpha_j)$) has to be computed
Computation of Dispersion Diagram of PhCs

\[
c_1(\alpha_i, \alpha_j) = \int_K \frac{1}{\varepsilon} \frac{\partial}{\partial x} \alpha_j \, dx \, dy \tag{3.58}
\]

\[
= \int_K \frac{1}{\varepsilon} (\alpha_i, 0) \nabla \alpha_j \, dx \, dy \tag{3.59}
\]

\[
= \int_K \frac{1}{\varepsilon} (\hat{\alpha}_i, 0) J^{-\top} \nabla \hat{\alpha}_j \det J \, dx \, dy \tag{3.60}
\]

\[
= \int_K \frac{1}{\varepsilon} (\hat{\alpha}_i, 0) \text{adj}(J)^\top \nabla \hat{\alpha}_j \, dx \, dy. \tag{3.61}
\]

Note that the integration of every shape function results in \( \frac{1}{6} \) \( \int_0^1 \int_{-\hat{x}}^{\hat{x}} \hat{x} \, d\hat{x} \, d\hat{y} = \int_0^1 \int_{-\hat{x}}^{\hat{x}} \hat{y} \, d\hat{x} \, d\hat{y} = \int_0^1 \int_{-\hat{x}}^{\hat{x}} \hat{x} \, d\hat{x} = \frac{1}{6} \). Thus we obtain

\[
c(\alpha_i, \alpha_j) = \frac{1}{6\varepsilon} (1, 0) \text{adj}(J)^\top \nabla \hat{\alpha}_j \tag{3.62}
\]

with the corresponding matrix element \( C_1 \)

\[
C_1 = \frac{1}{6\varepsilon} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} -y_3 - y_1 + (y_2 - y_1) \\ y_3 - y_1 \\ -(y_2 - y_1) \end{pmatrix}^\top
\]

\[
= \frac{1}{6\varepsilon} \begin{pmatrix} -y_3 - y_1 + (y_2 - y_1) & y_3 - y_1 & -(y_2 - y_1) \\ -(y_3 - y_1) + (y_2 - y_1) & y_3 - y_1 & -(y_2 - y_1) \\ -(y_3 - y_1) + (y_2 - y_1) & y_3 - y_1 & -(y_2 - y_1) \end{pmatrix}. \tag{3.63}
\]

The matrix element \( C \) can now be assembled according to Eq. 3.57

\[
C = C_1 - C_1^\top = \frac{1}{6\varepsilon} \begin{pmatrix} 0 & 2y_3 - y_1 - y_2 & -2y_2 + y_1 + y_3 \\ -2y_3 + y_1 + y_2 & 0 & 2y_1 - y_2 - y_3 \\ 2y_2 - y_1 - y_3 & -2y_1 + y_2 + y_3 & 0 \end{pmatrix}. \tag{3.64}
\]

We have now a matrix formulation for the bilinear form for an element \( e \). The matrices describing the global system have the size \( N_n \times N_n \), where \( N_n \) is the number of nodes. The matrix elements are computed for every element and its integral contributions for each node of the element are added to the node in the global matrix. The number of unknowns is thus \( N_n \times N_n \) and is referred to the degree of freedom.

### 3.4.4 Matrix Eigenvalue Problem

Finally, we obtained a matrix formulation of the eigenvalue equation for the global system. The weak formulation of Eq. 3.14 writes in the matrix formulation as
\[
\left( A - \frac{\omega^2}{c^2} B_0 + i \hat{k}_x C + \hat{k}_x^2 B_\varepsilon \right) \vec{x} = 0,
\]

where \( \vec{x} \) is the eigenvector, i.e., the solution \( u_{\hat{k}_x} \) for the nodes \( n \). There are two possibilities to solve this eigenvalue equation:

- search for eigenfrequencies \( \omega \) for a given value of \( \hat{k}_x \) which we call the \( \omega \)-formulation.
- search for eigen Bloch index \( \hat{k}_x \) for a given frequency \( \omega \) which we call the \( k \)-formulation.

The \( \omega \)-formulation can only be used for non-dispersive permittivities. The \( \omega \)-formulation is quadratic in \( \omega \), but the problem can be reduced to a linear eigenproblem in \( \lambda = \omega^2 \). The \( k \)-formulation is also quadratic in \( \hat{k}_x \). But for the \( k \)-formulation, the problem cannot be reduced to a linear eigenvalue equation. Opposed to the \( \omega \)-formulation, the \( k \)-formulation allows the usage of dispersive materials \( \varepsilon(x, \omega) \).

### 3.4.4.1 The \( \omega \)-Formulation

For a given Bloch index \( \hat{k}_x \), the linear matrix eigenvalue problem is: Seek for a pair \((\lambda = \omega^2, \vec{x})\) such that

\[
\left( A + i \hat{k}_x C + \hat{k}_x^2 B_\varepsilon \right) \vec{x} = \lambda \left( \frac{1}{c^2} B_0 \right) \vec{x}.
\]

This linear eigenvalue equation can be solved numerically by a standard eigenvalue solver such as ARPACK.

### 3.4.4.2 The \( k \)-Formulation

We have the quadratic matrix eigenvalue problem: Seek for pair \((\hat{k}_x, \vec{x})\) such that

\[
\left( -\hat{k}_x^2 B_\varepsilon - i \hat{k}_x C - A + \left( \frac{\omega}{c} \right)^2 B_0 \right) \vec{x} = 0.
\]  \hspace{1cm} (3.65)

According to Tisseur and Meerbergen [281, Case P7] a quadratic eigenvalue equation can be transformed into a linear eigenvalue equation with the same eigenvalues as follows

\[
\begin{pmatrix}
-\left( A - \left( \frac{\omega}{c} \right)^2 B_0 \right) & 0 \\
C & -\left( A - \left( \frac{\omega}{c} \right)^2 B_0 \right)
\end{pmatrix}
\begin{pmatrix}
\vec{x} \\
\vec{y}
\end{pmatrix}
= \hat{k}_x
\begin{pmatrix}
0 & i \left( A - \left( \frac{\omega}{c} \right)^2 B_0 \right) \\
i B_\varepsilon & 0
\end{pmatrix}
\begin{pmatrix}
\vec{x} \\
\vec{y}
\end{pmatrix}.
\]  \hspace{1cm} (3.66)

Again a linear eigenvalue equation is obtained, but with new matrices of size \( 2N_n \times 2N_n \). Eq. 3.66 has the same discrete eigenspectrum as Eq. 3.65.
Hence, we benefit from two advantages of the $k$-formulation: the sampling scheme over a limited frequency range and a linear eigenvalue problem also for frequency-dependent materials.

3.4.5 Verification for a Test Structure with a Analytical Solution

The algorithm is first tested for a simple example – a rectangular waveguide, for which an analytical solution exists. Therefore we consider the test structure as shown in Fig. 3.14. The rectangular waveguide consists of a rectangular unit cell with Dirichlet boundary conditions ($H(x,0) = H(x,L) = 0$) for the horizontal boundaries. A homogeneous material with permittivity $\varepsilon$ is used. Maxwell’s equation can be solved analytically for the test structure. The master equation (Eq. A.9) is

$$-\Delta H - \varepsilon \frac{\omega^2}{c^2} H = 0$$

Following the approach of separation of variables, we assume that $H(x,y)$ can be written as a product of a function $X(x)$ (only dependent on $x$) and a function $Y(y)$ (only dependent on $y$)

$$H(x,y) = X(x)Y(y).$$

Inserting the separation ansatz into Eq. 3.67 results in

$$-\frac{\partial^2}{\partial x^2} X(x) - \varepsilon \frac{\omega^2}{c^2} X(x) = \frac{\partial^2}{\partial y^2} Y(y) = \mu^2.$$  

This equation can be solved by solving the $X$ and $Y$ problem separately. After some mathematical steps and by applying the boundary conditions, the general analytical solution of the system is found

$$H(x,y) = H_0 e^{ik_n x} B_n \sin\left(\frac{n\pi}{L} y\right).$$

Figure 3.14: A rectangular waveguide is used as a test structure.
By Inserting the solution Eq. 3.70 in Eq. 3.67 the dispersion relation \( k_n(\omega) \) of the system is obtained

\[
-k_n^2 + \left( \varepsilon \frac{\omega^2}{c^2} - \frac{n^2 \pi^2}{a^2} \right) = 0,
\]

which can be solved for \( \omega \) and \( k_n \), respectively

\[
k_n = \sqrt{\varepsilon \frac{\omega^2}{c^2} - \frac{n^2 \pi^2}{a^2}} \quad \text{(3.72)}
\]

\[
\omega_n = \sqrt{\left( k_n^2 + \frac{n^2 \pi^2}{a^2} \right)} \frac{c^2}{\varepsilon}.
\]

These analytical formulae are used in the following for a verification of the developed finite element method.

For the numerical verification, we chose the following parameters: \( \varepsilon = 1, c = 1, a = 1 \) and \( L = 1 \). A mesh with triangular elements is generated with COMSOL and is shown in Fig. 3.15 A).

A prototype code was established with MATLAB. The MATLAB-script loads the mesh file generated by COMSOL, computes the matrix elements, assembles the matrices and finally solves the eigenvalue equation. Fig. 3.15 E) shows the real part of the obtained eigenfrequencies \( \omega \) for a given real wave vector \( k \). It can be seen that the \( \omega \)-formulation produces additional solutions \( \omega \) for the same \( k \) that are periodic with \( k = 2\pi \). This is a direct consequence from the used Bloch ansatz (cf. Eq. 3.9).

Only real eigenfrequencies are found, as it is expected for a closed, loss-less system. Fig. 3.15 shows the real (G) and imaginary part (H) of the obtained eigen wave vectors \( k \) for a given frequency \( \omega \). Note that the plot (G) showing the real part of the eigen wave vectors \( k \) is identical to the plot (E) showing the real part of the eigenfrequencies – only the axis are interchanged. As opposed to the eigenfrequency search \( \omega(k) \), the wave vector \( k_n(\omega) \) does have an imaginary part for some frequencies \( \omega \). For these frequencies the rectangular waveguide is cutoff, i.e., evanescent waves are obtained.

Figure 3.16 shows the convergence of the \( k \)-formulation by plotting the absolute error \( \text{error} = k_{\text{sim}} - k_{\text{analytic}} \) as a function of the degree of freedom (left) and the runtime (right). Note that the run-times are already rather long for small degrees of freedoms. This is due to the fact that our MATLAB code is not optimized. Especially the for-loop required for the assembly of the global matrices is rather slow for larger numbers of nodes.

### 3.4.6 Realistic Test Case: W1 PhC Waveguide

In the next example, we compute the photonic bands of a W1 PhC waveguide. The W1 PhC waveguide consists of a core with a \( \varepsilon = 11.09 \) and a hexagonal lattice of air holes with radius \( r = 0.3a \). The test structure can be seen in Fig 3.17 B). Figure 3.17 B) additionally shows the used mesh that has been generated by COMSOL. The band diagram is shown in Fig. 3.17 A). The periodic function \( u_{k_x} \) corresponding to the even and odd TE W1 PhC waveguide mode is shown for \( \hat{k}_x a/(2\pi) = 0.5 \)
Figure 3.15: Results obtained by our MATLAB-code: A) the mesh used in the simulation, the magnetic field of the periodic function $\tilde{h}$ for the first two eigen wave vectors B) and C) and for a higher order wave-vector D). The eigenfrequencies obtained by using the $\omega$-formulation are shown in E) and F) and the eigen wave vectors obtained by using the $k$-formulation are shown in G) and H).
Figure 3.16: Convergence plot for a given $\omega_0 = 2$. The absolute error was determined by computing the difference of the numerically obtained value $k_n(\omega_0)$ with the analytical solution (Eq. 3.72). The error is plotted as a function of degree of freedoms (left) and as a function of simulation runtime. A linear convergence rate is obtained as expected for linear basis functions.

and for $\hat{k}_x a/(2\pi) = 0.25$. Whereas the computation of the eigenfrequencies for a single Bloch index $\hat{k}_x$ using the $\omega$-formulation requires less than 1s runtime, the computation of the eigen wave vectors for a single $\omega$ requires about 110s in average for the shown mesh in Fig. 3.17. The limiting factor is eigen-mode solver. We will reconsider a similar test structure in Sec. 3.4.8.1.

3.4.7 Implementation in Concepts

The MATLAB code could be optimized to perform better. However, instead of optimizing the MATLAB code that served as a prototype and as a proof of principles instrument, we decided to use the already optimized CONCEPTS C++ libraries. CONCEPTS additionally supports higher order polynomial basis functions and curved elements. Curved elements are particularly interesting, since they allow to perfectly model the circular hole shape of our line-defect PhC waveguides as shown in Fig. 3.18 (right). In Sec. 3.4.3 we used linear shape functions, i.e., a polynomial of degree 1. A higher degree of the polynomial basis function improves the convergence rate considerably. For instance, for the computation of the PhC band structure it was shown that the finite element method (FEM) with polynomial degree 2 already achieves double the convergence rate of MPB [290]. For material interfaces having continuous contours (continuous also in their derivatives such as e.g., circles) the FEM with higher polynomial degree and with curved cells leads to an exponential convergence, i.e., the convergence rate increases continuously (cf. Eq. 3.75). And a limited, but high convergence rate (algebraic convergence, cf. Eq. 3.74) can be achieved for the ‘worst case’ scenario, i.e., geometries with contours with sharp corners [234].

A FEM that reduces the error by refining the mesh is called h-FEM. A FEM with
the possibility to reduce the error by increasing the polynomial degree of the basis function is called $p$-FEM. The CONCEPTS-libraries provide both, mesh ($h$-)refinement and ($p$-)refinement of the polynomial degree of the basis function. A FEM that supports both refinement methods is called a $hp$-FEM.

The mentioned refinement methods have different efficiencies, i.e., the achieved accuracy of the solution using a particular number $N$ of basis functions. The $h$-version of the FEM achieves an algebraic convergence, i.e., the convergence rate is proportional to

$$N^{-\alpha},$$  

(3.74)

where the convergence rate $\alpha$ is restricted by the polynomial degree $p$ and by singular points in the material contours. By doubling the number of basis functions the error decreases by a factor $2^\alpha$, e.g., by 4 for a method of order 2.

The $p$-version of the FEM can approximate eigenmodes with exponential convergence, i.e., the convergence rate follows

$$\exp(-\beta N^{1/3}) = B^{\frac{3}{\sqrt{N}}},$$  

(3.75)

where $N$ is the degree of freedom and $\beta$ and $B$ are fitting parameters ($\beta > 0$ and $B := \exp(-\beta)$). For non-smooth contours the $p$-FEM would achieve only algebraic convergence where, however, the convergence rate would be still larger than for $h$-FEM. For this ‘worst case scenario’ a proper combination of mesh refinement and polynomial degree enhancement [237, 234] can retrieve the exponential convergence. For smooth surfaces, such as our circular holes, we expect thus as high convergence rate for the $p$-FEM and therefore $p$-FEM is our method of choice. The $h$-FEM is only used for comparison.

K.Schmidt implemented the $\omega$- and the $k$-formulation in the numerical C++
library CONCEPTS [42] using a quadrilateral mesh with curved cells. In the following we apply to this code to perform an efficiency analysis.

3.4.8 Efficiency Analysis

In this section we will study numerically the efficiency of the new method, i.e., the focus lies on the $k$-formulation. Nevertheless, we start with the convergence analysis of the $\omega$-formulation for non-dispersive material (in Sec. 3.4.8.2), because it allows a direct comparison of the efficiency of our $hp$-FEM code to MPB and COMSOL. Then, in Sec. 3.4.8.3 we study the convergence behavior of the $k$-formulation with the $p$-FEM and the $h$-FEM implementation, which is very similar to the one of the $\omega$-formulation.

3.4.8.1 The Test Structure: W1 PhC Waveguide

The TE modes of a PhC W1 waveguide based on a hexagonal lattice structure with five lateral rows of air holes in an otherwise homogeneous and isotropic dielectric media with $\epsilon = 11.4$ are studied. The used mesh is the one of Fig. 3.18(D) and some modes are depicted in Fig. 3.18(A)–(C) that have been obtained with the $k$-formulation using a polynomial degree of $p = 8$. Our simple in-house 2D mesher for PhC waveguides allows to generate super-cells by translating a unit-cell. Therefore we used a rhomboidic super-cell. A band calculation example is shown in Fig. 3.19(A) for the $\omega$-formulation and Fig. 3.19(B) for the $k$-formulation. Both formulations result in the same band structure. But, for the $\omega$-formulation, we obtain

A) Even mode at $\frac{\omega a}{2\pi} = 0.25$, $\frac{k_x a}{2\pi} = 0.23854$

B) Even mode at $\frac{\omega a}{2\pi} = 0.221$, $\frac{k_x a}{2\pi} = 0.46957$

C) Odd mode at $\frac{\omega a}{2\pi} = 0.25$, $\frac{k_x a}{2\pi} = 0.38600$

D) Computational mesh with curved cells.

Figure 3.18: In the sub-figures (A)–(C) the real part of the magnetic field component for three typical guided PhC waveguides modes at different frequencies are shown: (A) an even TE mode where the slope of the dispersion is relatively steep, (B) another even TE mode where the slope is flat and (C) a typical odd TE mode. In sub-figure (D) the mesh of the super-cell is illustrated.
A) Band diagram with equally spaced Bloch indices ($\omega$-formulation).

B) Band diagram with equally spaced frequencies ($k$-formulation).

Figure 3.19: The same band diagram, once computed with the $\omega$-formulation and uniformly distributed Bloch indices $\hat{k}_x$ shown in (A), and once with the $k$-formulation and uniformly distributed frequencies $\omega_i$ (B). The PhC configuration is shown in Fig. 3.18.

equally spaced Bloch indices $\hat{k}$, whereas for the $k$-formulation the frequency intervals are equally spaced. It can be seen that flat bands are poorly resolved by the $k$-formulation. If a large frequency range has to be analyzed to locate regions of flat bands, then the $\omega$-formalism is clearly superior to the $k$-formalism.

3.4.8.2 Comparison of the $p$-FEM With Other Methods for the $\omega$-Formulation

The exponential convergence behavior of the best-approximation to a solution of a partial differential equation by means of $p$-FEM discretization is proven in [237] and can be transferred to the FEM solution of many equations. This has recently been verified for the computation of the PhC band structure and the $\omega$-formulation [234]. We investigate the efficiency of the $p$-FEM implemented with the CONCEPTS-libraries for the computation of the dispersion of the waveguide modes of the test structure presented in Sec. 3.4.8.1. The convergence rate of our method is compared to the convergence rates of MPB, of COMSOL and of the $h$-FEM version of our code.

The mesh of the used super-cell in CONCEPTS is presented in Fig. 3.18(D). For the mesh refinement experiment ($h$-FEM) with CONCEPTS the shown mesh is successively refined. For the refinement of the degree of the polynomial basis function experiment ($p$-FEM), the mesh remains at the coarsest, initial level. Our COMSOL simulation uses triangular meshes and polynomial degree 2. MPB uses rectangular meshes. For all methods the same one-dimensional Brillouin zone is sampled at $#\hat{k}_{x,i} = 51$ equally spaced values. For every Bloch index $\hat{k}_{x,i}$ the 30 smallest eigenvalues $\omega(\hat{k}_{x,i})$ are computed. Subsequently, only the two guided modes in the PhC band gap are selected for the convergence analysis. These eigenvalues are compared to those of the reference solution (CONCEPTS with polynomial degree $p = 19$) by evaluating the average error. This error is obtained by summing
Figure 3.20: A comparison of the convergence for various codes, each using an \( \omega \)-formulation. We plot the average error of all eigenfrequency values that are part of the dispersion of the guided PhC modes versus the degree of freedom (left) and computing time (right). MPB (red) shows a algebraic convergence, COMSOL (blue) and CONCEPTS with \( h \)-refinement (green) converge quadratically. The best convergence is achieved with CONCEPTS and refinement of the polynomial degree of the basis functions (black curve). The gray dotted lines are the fits that have been used to determine the convergence rates.

The error is calculated up the differences between the approximated and the exact eigenfrequency solutions. The number is then divided by the total number of compared values

\[
\text{error} = \frac{1}{\text{#modes} \cdot \#k} \sum_{j=1}^{\text{#modes}} \sum_{i=1}^{\#k} \omega_{test,i,j} - \omega_{ref,i,j},
\]

(3.76)

where \( \omega_{ref} \) is the frequency obtained from the reference solution, \( \omega_{test} \) is the frequency obtained for a particular experiment. The first summation represents the \#modes = 2 guided PhC waveguide modes (even and odd TE mode). The second summation takes all frequencies for the 51 predefined Bloch indices \( \hat{k}_{x,i} \) into account. The error is plotted in Fig. 3.20 once versus the degree of freedom \( N \) (left) and once versus the computing time (right). All simulations have been performed on a Debian GNU/Linux SMP system running on a Sun Fire V40z with 4 Dual Core AMD Opteron Processors at a clock of 2591 MHz and equipped with 32GB RAM. The specified time in Fig. 3.20 (right) correspond to the time required by the software on a single CPU core to complete the program.

Figure 3.20 shows a quadratic convergence of COMSOL and CONCEPTS with \( h \)-refinement (uniformly \( p = 2 \)), and an almost quadratic convergence for MPB up to an relative error of \( 10^{-3} \). For a further refinement, MPB achieves an approximately linear convergence. Even if the slope of the convergence of COMSOL and CONCEPTS with \( h \)-refinement is similar, it is interesting that the convergence curve of COMSOL
has an offset of roughly one order of magnitude to CONCEPTS. We attribute that offset to a higher quality of the mesh used by COMSOL. However, for p-refinement the mesh quality does not contribute a lot and a high convergence rate of about 7.5 is achieved. Hence, it is the most efficient method of the presented ones for all relative error levels below $10^{-4}$. MPB is the best program if larger errors ($\text{error} > 10^{-3}$) are tolerated. With $p = 15$ the averaged relative error of the dispersion of the guided modes is about $10^{-8}$. Note that the exponential convergence of the p-refinement is difficult to distinguish from a high algebraic one (cf. [234]) at this refinement level.

Similar behaviors of the convergence curves are observed for the error versus time: MPB is converging linearly, COMSOL and CONCEPTS with $h$-refinement and $p = 2$ have roughly a quadratic convergence rate and CONCEPTS with $p$-refinement converges with order 4. For the $p$-refinement the computational effort increases faster with increasing number of degrees of freedom $N$ due to our current implementation of the curved cells. These results may be improved.

We conclude that MPB is the most efficient program to compute photonic bands for errors up to $10^{-3}$ for the presented example. Our method based on $p$-FEM using the CONCEPTS-libraries is superior for errors below $10^{-3}$.

### 3.4.8.3 Convergence Analysis for the $k$-Formulation

The second convergence analysis is performed with the $k$-formulation proposed in this work. We show in Fig. 3.21 a similar convergence plot as in the previous section. The band structure of the same test PhC waveguide was computed using the $k$-formulation. Hence, the frequency axis $\omega$ was sampled at $\#\omega_i = 51$ equally spaced samples from $\omega a/(2\pi c) = 0$ to $\omega a/(2\pi c) = 0.5$, and similar to the previous experiment, we computed the 30 eigenvalues with the lowest magnitude. The band diagram – i.e., the Bloch indices $\hat{k}_i$ – can be found by selecting the eigenvalues having a negligible imaginary part (we used $\Im(\lambda) < 10^{-7}$) and simultaneously having a positive real part $\Re(\lambda) \geq 0$). Analogous to the previous convergence experiment (cf. Fig. 3.20), the error was computed according to

$$\text{error} = \frac{1}{51} \sum_{i=1}^{\#\omega_i} k_{\text{test},i,j} - k_{\text{ref},i,j}.$$

The averaged sum of the difference between the approximated and the reference Bloch index is plotted in Fig. 3.21. The convergence plots in Fig. 3.21 cannot directly be compared to those in Fig. 3.20 because Fig. 3.20 shows the frequency-error and Fig. 3.21 shows the Bloch index-error. Nevertheless, the posed problems are comparable in terms of computational resources and also in behavior of the slope of the convergence curve. We observe a quadratic convergence for $h$-refinement with $p = 2$ and a convergence rate of about $\alpha = 7.2$ for the $p$-refinement.

The dash-dotted line above the $p$-refinement curve in Fig. 3.21 (left) is the exponential fit according to Eq. 3.75 with parameters $\beta = 1.08$ and $B = 0.34$. The results shown in this section demonstrates the superiority of the $p$-FEM for the computation of line-defect PhC waveguide modes for given frequencies $\omega$ with the $k$-formulation. As already mentioned, the $k$-formulation is especially suited for dis-
3.5 PhC Band Diagram Computations Using Dispersive Material Models

The material dispersion of semiconductors in the transparent (non-absorptive) frequency region is commonly neglected in integrated optics, because of two reasons: first the propagation distances on a chip are short and secondly the material dispersion is small for typical frequency ranges of communication bands (a few GHz). As long as a PhC device is operated in a narrow band within the transparency region of a semiconductor material, one may use a constant permittivity for the center wavelength $\omega_0$. However, it is not clear that the material dispersion can be neglected for a photonic band gap calculation. The photonic band gap for PhC based on a hexagonal lattice of air holes in InP with $r = 0.34a$ and $a = 435$ nm extends over a large frequency range of about $\Delta f \approx 70$ THz for $\lambda = 1550$ nm.

The simulation can no longer be performed in reduced frequency units
Computation of Dispersion Diagram of PhCs

ωa/(2πc) since the permittivity depends on the frequency in Hz. Therefore, we have to restrict the computation to a specific lattice constant a₀. As a consequence, the scaling property of PhCs [104] is lost in the case of a dispersive permittivity ε(ω). The scaling law is the main motivation to use frequency units that are normalized to the lattice constant a. The dispersion relation given in normalized frequency units transforms to any frequency by simply scaling the lattice constant a. For example, the operation regime can be transformed to the doubled frequency ω' = 2ω by adjusting the lattice constant to a' = a/2. But, for dispersive materials the permittivity for the doubled frequency ω' is not the same and we cannot simply transform the results.

3.5.1 Influence of a Dispersive InP Material Models on the PhC properties

We apply the k-formalism of our method to answer the question 'Is it justified to neglect the dispersive behavior of the semiconductor material for passive devices?' Therefore we consider an example: We investigate the influence of a dispersive InP model on both, the photonic bands and the dispersion relation of the line-defect modes of a W1 PhC waveguide.

3.5.1.1 The Material Model For InP

We use the model of S. Adachi [2] to describe the frequency dependent permittivity of undoped InP. The model of S. Adachi [2] agrees accurately with measurements by spectroscopic ellipsometry in the near infra-red regime. The model approximates the permittivity of InP by the sum of three different interband transitions for three different critical points of the InP crystal

ε(ω) = ∑₃ᵢ₌₁ εᵢ(ω).

(3.78)

Table 3.1: Parameters as used by S. Adachi [2]. The intra-band gap energies range from the visible to the ultra-violet wavelength range. Even so, the tails of all spectra of the transitions are required to model the permittivity in the near infra-red.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>E₀</td>
<td>1.35</td>
<td>eV</td>
<td>band gap energy</td>
</tr>
<tr>
<td>E₀ + Δ₀</td>
<td>1.466</td>
<td>eV</td>
<td>+ splitting energy Δ₀</td>
</tr>
<tr>
<td>E₁</td>
<td>3.163</td>
<td>eV</td>
<td>band gap energy (L-points)</td>
</tr>
<tr>
<td>E₁ + Δ₁</td>
<td>3.296</td>
<td>eV</td>
<td>+ splitting energy Δ₁</td>
</tr>
<tr>
<td>E₀'</td>
<td>4.72</td>
<td>eV</td>
<td>band gap energy (Γ-point)</td>
</tr>
<tr>
<td>A</td>
<td>5.4</td>
<td>eV¹.₅</td>
<td>fitting parameter</td>
</tr>
<tr>
<td>B₁</td>
<td>4.91</td>
<td>-</td>
<td>fitting parameter</td>
</tr>
<tr>
<td>B₂</td>
<td>0.09</td>
<td>-</td>
<td>fitting parameter</td>
</tr>
<tr>
<td>C</td>
<td>1.3</td>
<td>-</td>
<td>fitting parameter</td>
</tr>
<tr>
<td>γ</td>
<td>0.093</td>
<td>-</td>
<td>fitting parameter</td>
</tr>
</tbody>
</table>
Transition 1 (center of the Brillouin zone):

\[ \varepsilon_1(\omega) = AE_0^{-1.5} \left[ f \left( \frac{\hbar \omega}{E_0} \right) + \frac{1}{2} \left( \frac{E_0}{E_0 + \Delta_0} \right)^{1.5} f \left( \frac{\hbar \omega}{E_0 + \Delta_0} \right) \right], \]

where

\[ f(x) = \frac{1}{x^2} \left( 2 - \sqrt{1 + x} - \sqrt{1 - x} \cdot H(1 - x) \right) \]

and \( H \) is the Heavyside function defined as

\[ H(z) = \begin{cases} 1 & \text{for } z \geq 0 \\ 0 & \text{for } z < 0 \end{cases}. \]

Transition 2 (along the (111) directions or at L points in the Brillouin zone):

\[ \varepsilon_2(\omega) = -\frac{B_1 E_1^2}{\hbar^2 \omega^2} \ln \left( 1 - \left( \frac{\hbar \omega}{E_1} \right)^2 \right) - \frac{B_1 (E_1 + \Delta_1)^2}{\hbar^2 \omega^2} \ln \left( 1 - \left( \frac{\hbar \omega}{E_1 + \Delta_1} \right)^2 \right) \]

Transition 3 (Γ-point of the zinc blende structure):

\[ \varepsilon_3(\omega) = \frac{C(1 - \left( \frac{\hbar \omega}{E_0} \right)^2)}{(1 - \left( \frac{\hbar \omega}{E_0} \right)^2 + \left( \frac{\hbar \omega}{E_0} \right)^2 \gamma^2} \]

The energy levels \( E_0, E_0 + \Delta_0, E_1, E_1 + \Delta_1 \) and \( E_0' \) correspond to the different interband transitions. In the following, we investigate the influence of the dispersive InP-model \( \varepsilon(\omega) \) on the band-edges of the photonic band gap and the dispersion curve of the guided TE mode of the W1 PhC waveguide. For that purpose, the imaginary part of permittivity can be neglected. Note that the complexity of the used permittivity model is irrelevant for the \( k \)-formulation, i.e., the permittivity \( \varepsilon(\omega_i) \) is first evaluated for a given frequency \( \omega_i \) and then both parameters \( (\varepsilon(\omega_i) \) and \( \omega_i \)) are used to assemble the matrices.

### 3.5.1.2 Influence of the Dispersive InP Model on the Gap-Map

Typically, the photonic band gap of a PhC extends over a rather broad frequency range. The broad frequency range of the photonic band gap may enable considerable shifts of the photonic band gap due to a dispersive permittivity. In this investigation we compute the lower and upper band-edges for a triangular lattice of air holes in InP for a lattice constant \( a = 400 \) nm. In Fig. 3.22 (left) the frequency boundaries of the photonic band gap for both a constant permittivity for InP \( \varepsilon = 10^4 \) (blue area) and with the dispersive model according to Eq. 3.78 (red area) is shown. On the right of Fig. 3.22 the error due to a frequency shift is plotted for the lower and upper edge of the band gap as well as the change of the frequency range of the band gap. A maximum frequency shift of about 50 GHz is observed for \( r = 0.41 a \). The orange area in Fig. 3.22 (left) is the overlap of both band gaps, i.e., propagation of light is not permitted in this area regardless of the

\(^4\varepsilon = 10 \) is fixed for the frequency \( \omega a / (2\pi c) = 0.26 \), which is represented by a black line
two material models. The desired frequency features of PhC devices are usually designed such that they are located in the center of the photonic band gap. Therefore we conclude that the influence of the shift of the photonic band gap due to the frequency dependence of the permittivity can be considered to be a second-order effect.

3.5.1.3 Influence of the Dispersive InP Model on the Guided Modes of a W1 PhC Waveguide

We have seen in Sec. 3.5.1.2 that the frequency error can be in the order of 50 GHz – roughly the frequency range for a single transmission channel of a WDM system. However, if narrow frequency features in the dispersion are investigated, e.g., flat dispersion curves for slow light, resonances, etc, a noticeable deviation of the frequency behavior may result. Therefore, we investigate the influence on the frequency features of the TE modes of a PhC W1 waveguide. The waveguide is based on a hexagonal lattice structure with lattice constant $a = 400$ nm and five lateral rows of air holes in InP, the substrate material for our devices. Apart from the fixed lattice constant $a$, the geometrical settings are identical to the test PhC waveguide in Fig. 3.18.

Fig. 3.23 shows both the band diagram of the dispersive InP (red) and the one with a constant permittivity $\varepsilon = \varepsilon(\omega_0)$, where $\omega_0 = 2\pi \cdot 195$ THz. The corresponding wavelength is $\lambda_0 = 1538$ nm. On the right side of the plot $\varepsilon(\omega)$, the used real part of the permittivity model according to [2], is shown. First, a ‘red’ shift of the higher band gap frequency from $\omega a/(2\pi c) = 0.304$ to $\omega a/(2\pi c) = 0.302$ and a small ‘blue’ shift of the lower band gap frequency from $\omega a/(2\pi c) = 0.2252$ to $\omega a/(2\pi c) = 0.2264$ can be deduced from the PhC modes from Fig. 3.23 – a reduction of the band gap of about 4%. As already discussed above, the deviation of the band-edges of the photonic band gap for InP based PhC devices is rather small. The frequency error of the PhC waveguide mode is very small too, particularly for the slow light frequency regime. To further quantify the error of the Bloch
Figure 3.23: On the left side, a comparison of the band diagrams for the case of W1 PhC waveguide with a constant dielectric constant (blue) and for the case of a dispersive permittivity (red) are shown. Both have been computed using the \( k \)-formulation. Despite their non-scalability we labeled the frequency and the wave vector for comparison purpose in dimensionless units. The absolute wave-length is labeled on the right axis. On the right side the real part of the permittivity model of Adachi [2] for InP is plotted.

For the \( \hat{k}_x \) we performed an example: we vary the permittivity by \( \Delta \varepsilon \in [0, 0.5] \) for a given frequency \( \omega = \omega_0 \) and compute the Bloch index \( \hat{k}_x \). A linear relation \( (\Delta \hat{k}_x = 0.0486\Delta \varepsilon) \) between \( \Delta \varepsilon \) and the deviation in the Bloch index \( \Delta \hat{k}_x \) is obtained and depicted in Fig. 3.24.

### 3.5.2 Outlook

The main motivation for the development of a new numerical method was the direct computation of propagation losses of substrate-type PhC waveguides from

Figure 3.24: The error \( \Delta \hat{k}_x \) in the Bloch index \( \hat{k}_x \) for a given frequency \( \omega_0 \) (\( \omega_0/(2\pi c) = 0.26 \) and \( a = 400 \) nm) as a function of the deviation \( \Delta \varepsilon \) of the permittivity \( \varepsilon(\omega_0) = 10.007 \). The frequency is kept to \( \omega_0 \). For the \( k \)-formulation for each frequency the right permittivity value can be used directly (corresponding to \( \Delta \varepsilon = 0 \)) whereas with the \( \omega \)-formulation an iteration procedure has to be used.
the complex Bloch index $\hat{k}_{x,i}$. However, as we will see in the following chapters, the main loss contribution of the propagation losses of substrate-type PhC waveguides are out-of-plane radiation losses. Therefore, strictly 3D super-cells are required to compute the propagation losses. Nevertheless, the idea to compute the periodic function $u_{\hat{k}}$ (cf. Eq. 3.9) equally applies to 3D super-cells.

The computation of the eigen-modes for a given frequency $\omega_i$ results in guided and leaky modes as described in Sec. 2.1.2.5. We reconsider the imposed periodic boundary condition Eq. 3.8

$$H(x + a, y) = H(x, y) \cdot e^{i\hat{k}_x x}.$$  

A complex Bloch index $\hat{k}_x = k' + ik''$ is obtained for lossy materials or for absorbing boundary conditions and the boundary conditions would read as

$$H(x + a, y) = H(x, y) \cdot e^{i(k' + ik'')x}.$$  

This approach is commonly used to compute leaky modes of PhC waveguides [157, 247, 233, 131, 140]. The obtained eigen-modes maintain their shape on the cross section of the waveguide along the propagation direction $x$. Potentially, many leaky modes are obtained for a given frequency $\omega_0$ by the super-cell method. In a real experiment the dielectric waveguide is excited at the input. It is not necessarily clear i) which eigen-mode is excited and ii) how many eigen-modes are excited. This information would be required to compute the experimentally measured propagation losses from the individual loss values from the leaky modes. The excitation of a waveguide is a different problem. Therefore, we decided to pursue the approach to compute the propagation losses by solving the excitation problem in the time domain as it is presented in chapter 5.

### 3.6 Conclusion

In summary, we described the procedure to obtain the dispersion curves and the photonic band gaps for substrate-type PhCs from 3D super-cell simulations performed with MPB. Those band diagrams are shown in various parts of this thesis (cf. chapter 5 and chapter 8). Furthermore, we introduced mode-map plots for line-defect PhC waveguides. These plots can be used to identify the design parameters that can be used to modify the dispersion of the line-defect PhC waveguide mode according to the desired specification. In the third part of this chapter, we reported on a mode solver based on the finite element method that allows to directly compute the Bloch index $\hat{k}$ for a given frequency $\omega$. In order that the method can be used to compute the losses of substrate-type PhC waveguide modes, the code has to be extended to three dimensions. Even so, we could demonstrate that the proposed approach is very efficient: The implementation of the code using the numerical C++ library CONCEPTS achieves a exponential convergence for $p$-FEM and curved elements. Furthermore, dispersive permittivities can naturally be included in the simulation.
Nowadays, most planar PhC devices are implemented in a vertical layer structure of strong refractive index contrast (membrane-type), mainly because of the low propagation losses that are obtained experimentally in these structures. On the other hand, for electrically pumped active devices, it is interesting to use epitaxially grown heterostructures for the vertical light confinement (substrate-type). These layer stacks typically offer only small refractive index contrasts, and the fabricated waveguides suffer from high optical losses. For a single line defect waveguide (W1), losses in the order of 1000 dB/cm are measured [295, 117] which are high in comparison to less than 10 dB/cm for the corresponding membrane-type devices [203, 173, 60]. Why is that? We get to the bottom of this question in this chapter.

We start with an article by Krauss [137], which summarizes the state-of-the-art knowledge about the loss mechanism in substrate-type PhC waveguides. We start the chapter by two citations from this article, describing the origin of the losses and the countermeasures to prevent propagation losses:

- «Out-of-plane leakage is the dominant loss mechanism for heterostructure waveguides. As all waveguide modes are situated above the light-line, there is always the possibility of coupling to radiation modes. In simple terms, the origin of these losses is a) the lack of waveguiding in the holes, with resulting diffraction loss and b) the fact that the holes are not etched sufficiently deeply, so the tail of the mode radiates into the substrate.»

- «All of the models conclude, that low-loss propagation above the light-line is indeed possible and that current waveguide designs are not yet optimized. The key parameters to improve are diffractive loss at the holes (reduced by smaller hole size), scattering into the substrate (reduced by deeper holes) and improvement of the waveguide geometry, away from the current asymmetric surface waveguides.»

In this chapter, we will critically discuss the statements above and present a more
rigorous analysis about the loss mechanism in slab PhC waveguides. We start
the chapter by listing the fundamental physical processes and with a definition
of the waveguide losses in Sec. 4.1. Then, we formulate a theory of loss mecha-
nism in substrate-type PhC waveguides consisting of five hypotheses in Sec. 4.2.
To numerically prove the hypotheses, we first review two perturbation approaches
with relation to periodic structures: i) Marcuse (cf. 4.3.1) developed a model for the
radiation losses for small periodic wall distortion functions for slab waveguides.
ii) Benisty et al. (cf. 4.3.2) developed an empirical model for substrate-type PhCs
that is based on identifying scatterers (imperfections) giving rise to scattering loss.
The model is still considered to be state-of-the-art for computing the out-of-plane
losses in substrate-type PhC waveguides. We conclude this section by demonstrat-
ing that scattering disturbances do not necessarily cause radiation if they are ar-
ranged periodically. Thus, the main assumptions that would be required for a con-
ventional theory based on incoherent scatterers are not valid for PhCs.

Since an expansion in terms of modes of the slab waveguide is not appropri-
ate for strong periodic modulations, we derive the modes for a slab PhC waveguide
with a strongly modulated permittivity in the core in Sec. 4.4. We find that guided
Bloch waves only exist if all spatial Fourier components are located outside the do-
main of radiation modes. Similar to the slab waveguide, we find a discrete set of
guided Bloch waves and a continuum of radiative Bloch waves.

Then we shift our attention away from a periodically modulated permittivity
in the waveguide core to a periodically modulated permittivity in the claddings
and find that the ‘light-line’ i.e., the separatrix between confined and unconfined
modes has to be generalized to the fundamental mode of the dielectric system at
infinity. It is further observed that the slab waveguide mode propagating in the ho-
mogeneous core layer exhibits small photonic band gaps at the Brillouin zone edge
of the periodic system of the cladding. Finally, we leave the domain of simplifying
2D models and investigate the field solutions of a membrane-type PhC waveguide
in 3D. Those results indicate that the hypothesis also applies to slab PhCs with a
2D periodic pattern. Finally, we address the question if the radiation losses can
be approximated by a simple ray model. We find the correct order of magnitude
for the propagation losses and the same trends in the propagation loss spectrum.
The chapter is closed by a summary and a discussion of the statements made by
Krauss [137] on the preceding page.

4.1 Waveguide Losses

The fundamental physical processes that can result in losses in a dielectric wave-
guide are [97, pp. 107] i) absorption losses and ii) scattering losses. There are three
different types of scattering processes: volume scattering, surface scattering, and
leaky waves. The term leaky waves is introduced in Sec. 4.1.2.4. We explain the
three different scattering processes for an asymmetric slab waveguide in the fol-
lowing. We will see by the end of this chapter that leaky waves are responsible for
the large propagation losses observed in substrate-type PhC waveguides. There-
fore, the emphasis of this section lies on leaky waves. The other loss mechanisms
are introduced for the sake of completeness.
4.1.1 Absorption Losses

Absorption is the process in which a photon is annihilated by transferring its energy to particles of the material, such as electrons. The loss in optical intensity $\Delta I = I_{in} - I_{out}$ per unit length $\Delta x$ due to absorption is proportional to intensity of optical signal $I$

$$\frac{\Delta I}{\Delta x} = -\alpha_{abs} I$$  \hspace{1cm} (4.1)

$$\Rightarrow I(x) = I_0 e^{-\alpha_{abs} x}. \hspace{1cm} (4.2)$$

The absorption coefficient $\alpha_{abs}$ is a material property and $I_0$ is the initial intensity at $x = 0$. We obtain an exponential decay of the optical intensity $I(x)$ along the propagation direction $x$ for $\alpha_{abs} = const$. Usually, the assumption of a constant absorption coefficient is valid for the operation of dielectric waveguides with modest light intensities. There are a many different physical processes in semiconductors that result in an absorption coefficient $\alpha_{abs}$ [304, chapter 6 u. 7], such as free-carrier absorption, interband absorption, intraband absorption etc.

4.1.2 Scattering Losses

4.1.2.1 The Scattering Process

Scattering is the physical process describing the change of the trajectory of a particle/wave by an object. Scattering in optics occurs, if the propagation of light is disturbed by an object, such that a part of the light changes its propagation direction. Although not different from a physical point of view, the mathematical treatments of scattering tends to be separated according to the relative size of the scatterer with relation to the wavelength [100, pp. 456]. For example, scattering at large objects $\gg \lambda$ can be treated by geometrical optics (cf. 2.1.1.1). On the other hand, scattering at small objects $\ll \lambda$ is treated by approximating the scattered fields by the radiating fields of a dipole. Scattering is the fundamental physical process of many optical phenomena, such as diffraction, interference, reflection, transmission, Rayleigh scattering, etc.

4.1.2.2 Volume Scattering Losses

A material consists of a number of imperfections, such as voids, contaminant atoms and crystalline defects [97, p. 107]. Those volume defects are able to scatter the light. If the imperfections are incoherently distributed in the material, then the scattering loss per unit length $\Delta x$ is proportional to the number of imperfections (summarized by a scattering constant $\alpha_{VS}$) per unit length and the light intensity $I$

$$\frac{\Delta I}{\Delta x} = -\alpha_{VS} I$$  \hspace{1cm} (4.3)

$$\Rightarrow I(x) = I_0 e^{-\alpha_{VS} x}. \hspace{1cm} (4.4)$$
Volume scattering results in an exponential decay of the optical intensity $I(x)$ along the propagation direction. Because of the small sizes of the imperfections compared to the wavelength $\lambda$ and because of the purity of state-of-the-art semiconductor materials, volume scattering usually results in negligible scattering losses.

### 4.1.2.3 Surface Scattering Losses

![Figure 4.1: Illustration of surface scattering losses using the ray optics model.](image)

Usually, irregularities at the surfaces are responsible for the dominant loss contribution of passive dielectric waveguides. The treatment of surface scattering losses is different from the treatment of volume scattering loss. This is best explained by the visualization given in Fig. 4.1. As opposed to volume scattering, where a ray may scatter at every scatterer along its path, the ray scatters only at the rough surface. The scattering at the surface is also proportional to the intensity of the propagating light. Thus, an exponential attenuation process is used [97, 166, 280, p. 108] to describe the magnitude of the optical intensity $I(x)$

$$I(x) = I_0 e^{-\alpha_{SS} x}. \quad (4.5)$$

### 4.1.2.4 Leaky Waves

![Figure 4.2: Illustration of leaky waves using the ray optics model.](image)

In Sec. 2.1.1 we established a connection between guided modes and rays launched into a slab waveguide. We have seen that the ray is guided by means of total in-
ternal reflection if the incident angle $\theta$ of the ray with respect to the interface (cf. Fig. 2.2) is larger than the critical angle $\theta_c = \arcsin\left(\frac{\max(n_2, n_3)}{n_1}\right)$. However, it is possible to launch a ray with an incident angle $\theta < \arcsin\left(\frac{\max(n_2, n_3)}{n_1}\right)$. Then, every time the ray interacts with the dielectric interface, the ray is partially reflected and partially transmitted as illustrated in Fig. 4.2. The launched wave propagates in the slab waveguide but continuously loses a part of its energy. The slab waveguide is operated ‘beyond’ the cutoff condition ($\theta < \theta_c = \arcsin\left(\frac{\max(n_2, n_3)}{n_1}\right)$).

A dielectric waveguide is operated ‘beyond’ cutoff, if the waveguide is excited with a frequency, for which no guided mode exists. A more detailed mathematical description of this phenomenon in terms of ray optics can be found in Sec. 4.7, where we compute the waveguide losses of an asymmetric slab waveguide using ray optics.

This nearly guided traveling wave is called a **leaky wave** [275, 170, p. 33]. Other names for leaky waves are leaky rays [253, 251, 252, 250], resonant modes [163, p.190], tunneling modes [249], nearly guided modes [94] and ‘guided modes’ beyond cutoff [172, p.42]. But, we distinguish between leaky waves and leaky modes as introduced in Sec. 2.1.2.5. Leaky waves differ fundamentally from leaky modes. A leaky mode is a solution of the eigenvalue equation Eq. 2.17, i.e., an eigenmode (state) of the system. Being a eigenmode, a leaky mode always maintains its shape on the cross section of the waveguide for any propagation distance except for a phase change and an attenuation factor of the form $e^{-\alpha x}$ (cf. Marcuse [170, p.33]). On the other hand, a leaky wave is associated with the **excitation of waveguide beyond the cutoff**. Leaky waves are transient solutions in the sense that their transverse ‘mode profiles’ depend on propagation distance $x$ as opposed to eigenmodes. Hu and Menyuk [94] distinguish between three different phases: in the injection phase a portion of the energy rapidly diffracts and quickly a quasi-mode [231] is established in the core of the waveguide. The next phase is mostly dominated by this quasi-mode that slowly decays along the propagation direction. The last phase basically consists of long-term diffractions, i.e., the mode in the waveguide core has disappeared and only radiative field components in the cladding are remaining.

The example used by Marcuse [170, p.33] describes best the leaky wave phenomenon in terms of modes. In his example two different dielectric waveguides are connected in series. The second waveguide is designed such that it is cutoff for the given frequency $\omega$ and for the field distributions traveling in the first waveguide. At the waveguide interface, the propagating light in the first waveguide excites a field distribution in the second waveguide, whose energy is concentrated in the waveguide core, but which decays along the propagation direction. In Fig. 4.3 we simulated two different slab waveguides that are connected with 2D FEM (COMSOL). The first (left) slab waveguide is symmetric ($n_1 = 3.5, n_2 = n_3 = 1$) and hence supports a guided mode for any excitation frequency. The second (right) slab waveguide is asymmetric ($n_1 = 3.5, n_2 = 2.8, n_3 = 1$) and exhibits frequency regions, where no guided mode exists – but a continuum of radiation modes and leaky modes. The inset (top-right) in Fig. 4.3 informs about the cutoff frequency of the structure: The red line represents the substrate line $\omega = c \cdot \beta_x / n_3$ and the blue line is the difference between the dispersion curve of the asymmetric slab and the substrate line. The left panel of Fig. 4.3 shows the electric field distribution $E_y$ for an excitation frequency $\omega a / (2\pi c) = 0.2$ and the right panel shows the electric
Figure 4.3: A symmetric and an asymmetric slab waveguide are connected. In the first experiment, the symmetric waveguide is excited with a frequency $\omega a/(2\pi c) = 0.2$. For this frequency, only the symmetric slab waveguides supports a guided mode. The asymmetric slab waveguide supports only radiation modes and leaky modes. The asymmetric slab waveguide is thus excited beyond cutoff and a leaky wave is established. In the second experiment, the symmetric waveguide is excited with frequency $\omega a/(2\pi c) = 0.5$. Both slab waveguides support a guided mode for this frequency.
field distribution $E_y$ for an excitation frequency $\omega a/(2\pi c) = 0.5$, i.e., on either side of the substrate light-line. A radiation pattern in the substrate can be observed for both excitation frequencies and is due to the mode mismatch between the guided mode in the first waveguide and the modes of the second waveguide. The electric field $E_y$ in the center of the slab waveguide is shown in Fig. 4.3 (bottom) and reveals that the wave propagating in the second, asymmetric slab waveguide only decays along the propagation direction if it is excited beyond the cutoff. This is not surprising in any way. It is shown here, because we have reasons to believe that operation beyond cutoff is the main mechanism behind propagation losses in substrate-type PhC waveguides.

The shown example of exciting an asymmetric planar slab wave beyond the cutoff exhibits very large propagation losses (also refer to Sec. 4.7). Because of the large losses, leaky waves may appear irrelevant in practice. However, already in 1974 Snyder et al. [250, 253, 251, 252] discussed the existence and behavior of leaky waves in circular optical fibers and they showed that many leaky waves persist over an enormous (km-scale) distance [253]. Leaky waveguides are also relevant in integrated optics. Kaspar et al. [121] presented a buried rectangular waveguide design, which theoretically only supports leaky waves for low frequencies. In this article, it was demonstrated that the losses of the propagating leaky waves can be reduced to an arbitrarily low value. A fabricated waveguide will always have a finite loss (fabrication imperfections, material absorption, etc.), even if the waveguide design would theoretically allow for loss-free guided modes. If the losses of the leaky waves are so small that they are not limiting the performance of the waveguide, then the fact that they are not truly guided modes loses its relevance.

### 4.1.3 Waveguide Losses

Finally, we define the waveguide losses: Consider a dielectric waveguide of length $L$ with a cross-section $\Omega$ as shown in Fig. 4.4.

$$P_{\text{abs}} + P_{\text{rad}} = \int_{\Omega} S_{\text{in}} \, dy \, dz - \int_{\Omega} S_{\text{out}} \, dy \, dz, \quad (4.6)$$

where $S$ is the electromagnetic power flux density. The electromagnetic power...
Loss Mechanism in Substrate-Type Photonic Crystal Waveguides

flux through an area is given by the Poynting vector \( \mathbf{S} = \mathbf{E} \times \mathbf{H} \). The total radiated power \( P_{\text{rad}} \) the absorbed power \( P_{\text{abs}} \) is

\[
P_{\text{abs}} + P_{\text{rad}} = \frac{1}{2} \hat{n} \Re \left( \int_{\Omega} \mathbf{E}(0) \times \mathbf{H}(0) \, dy \, dz \right) - \frac{1}{2} \hat{n} \Re \left( \int_{\Omega} \mathbf{E}(L) \times \mathbf{H}(L) \, dy \, dz \right)
\]

(4.7)

where \( \hat{n} \) is the normal (propagation) direction to the cross-section \( \Omega \). We can define a relative loss number according to

\[
\text{Loss} = \frac{P_{\text{rad}} + P_{\text{abs}}}{P_{\text{in}}} = \frac{P_{\text{out}} - P_{\text{in}}}{P_{\text{in}}},
\]

(4.8)

where \( \text{Loss} \) is the ratio between the radiated and absorbed power for a propagation by a distance \( L \) and the input power. In case of an exponential dependence of the power with the propagation distance \( x \) for the waveguide cross-section \( \Omega \), i.e.,

\[
P(x) = P_{\text{in}} e^{-\alpha x},
\]

(4.9)

we can define a propagation loss \( \alpha \)

\[
\alpha = -\frac{1}{x} \ln \left( \frac{P(x)}{P_{\text{in}}} \right)
\]

(4.10)

that can be expressed in a dB scale according to

\[
\alpha_{\text{dB}} = 10 \log_{10} \left( \frac{P(x)}{P_{\text{in}}} \right) \frac{1}{x} = -\frac{10}{\ln(10)} \alpha \approx -4.34 \alpha.
\]

(4.11)

It is more convenient to determine a propagation loss \( \alpha \), since it allows to easily compute the \( \text{Loss} \) for any propagation distance \( x \).

### 4.1.3.1 The Loss Mechanism for Volume and Surface Scattering Losses

Volume and surface scattering losses represent small imperfections of an otherwise perfect slab waveguide. Those small imperfections are able to couple light from the desired guided mode of the slab waveguide to other guided modes and to radiation modes of the slab waveguide. Mode conversion is the mechanism that results in a scattering loss for the desired guided mode. Those scattering losses can be computed by using perturbation theory, which is applicable for the case of small disturbances of the slab waveguide (cf. D. Marcuse [166]). We have already seen in Fig. 2.8 that a sum of radiation modes results in a radiation in lateral direction.

### 4.1.3.2 The Loss Mechanism for Leaky Waves in Terms of Mode Solutions

As opposed to the volume and surface scattering processes, where a disturbance results in a coupling of the energy carried by a (confined) guided mode to (unconfined) radiation modes [166], there are no imperfections and thus no coupling processes involved for leaky waves. We need another explanation for the waveguide loss for leaky waves. First, let’s recall that a leaky wave is obtained in a perfect slab
waveguide if it is excited beyond cutoff, i.e., it is excited with a frequency for which no guided mode exist (cf. Fig. 4.5,B). For the example of an asymmetric slab waveguide this is the case for $\theta < \theta_c = \arcsin((\text{max}(n_2,n_3))/n_1)$. The condition for the propagation constant $\beta_x$ reads $\beta_x < k_0 \cdot \text{max}(n_2,n_3)$. Because it is possible to express any field distribution of a perfect slab waveguide by means of radiation modes and guided modes [170], it is possible to express a leaky wave by means of radiation modes $E(\rho)$ only [94]

$$E_y = \int_{-\infty}^{\infty} g(\rho,x)E(\rho) d\rho,$$

where $\rho$ is the transverse wave number in the bottom cladding. Because the leaky wave can be expressed in terms of radiation modes only, the energy is theoretically already completely contained in terms of (unconfined) radiation modes at any time $t$ and position $x$ along the propagation direction. We consider an asymmetric slab waveguide as shown in Fig. 4.5. The excitation shall be given by $E_y(x=0,t=0) = A_0(z)$, such that the energy is completely confined in the core of the waveguide. Let us consider an excitation with $\omega = c/\lambda_0 = 1550 \text{ nm}$ of the asymmetric slab $n_1 = 3.5$, $n_2 = 2.8$ and $n_3 = 1$ with thickness $d = 130 \text{ nm}$ given by an initial transverse mode profile

$$E_{y,0}(x=0,z) = \begin{cases} A_0 & -d < z < 0 \\ 0 & \text{otherwise} \end{cases} \quad (4.12)$$

The guided and radiation modes form a complete basis set for the asymmetric slab waveguide. Since for the excitation frequency $\omega_0$ no guide mode exist, the mode profile can be expanded in terms of radiation modes only

$$E_{y,0}(x=0,z) = \int_{-\infty}^{\infty} g(\rho)E(\rho, x=0, z) d\rho. \quad (4.13)$$

Because the waveguide is free of defects, the weight of the radiation mode $g(\rho)$ is
not a function of propagation distance $x$. The power at the input of our waveguide $(x = 0)$ is thus

$$P_{\text{in}} = -\frac{1}{2} \int_{-d}^{0} \int_{-\infty}^{\infty} g(\rho) E_y(\rho, x = 0, z) g(\rho) H_z(\rho, x = 0, z) \, d\rho \, dz$$

$$= \int_{-d}^{0} \int_{-\infty}^{\infty} \frac{\beta_x(\rho)}{2\omega \mu_0} g(\rho)^2 E_y(\rho, x = 0, z)^2 \, d\rho \, dz. \quad (4.14)$$

Since the power is confined completely to the core of the slab waveguide the power at the input is

$$P(x = 0) = P_{\text{in}} \propto d \cdot A_0^2. \quad (4.15)$$

The initial condition represents thus a very particular field solution, namely all fields of the radiation modes add up in such a way that the rectangular mode profile ($A_0$ in the waveguide core and 0 otherwise) is produced. After the excitation, all radiation modes $E(\rho, x)$ propagate with a different propagation constant $\beta_x(\rho)$ such that the particular initial field distribution is "slowly" dispersed as soon as $x > 0$.

We define the cross-section $\Omega$ of the slab waveguide as the core of the slab waveguide, i.e., the measured power as a function of the position $x$ is

$$P_{\text{out}}(x) = \int_{-d}^{0} \int_{-\infty}^{\infty} \frac{\beta_x(\rho)}{2\omega \mu_0} g(\rho)^2 E_y(\rho, x, z)^2 \, d\rho \, dz. \quad (4.16)$$

And thus the waveguide loss is

$$\text{Loss} = 1 - \frac{\int_{-d}^{0} \int_{-\infty}^{\infty} \frac{\beta_x(\rho)}{2\omega \mu_0} g(\rho)^2 E_y(\rho, x, z)^2 \, d\rho d\rho dz}{\int_{-d}^{0} \int_{-\infty}^{\infty} \frac{\beta_x(\rho)}{2\omega \mu_0} g(\rho)^2 E_y(\rho, x = 0, z)^2 \, d\rho d\rho dz}. \quad (4.17)$$

Here, a numerical treatment would be appropriate to compute the waveguide losses at position $x$ for the given example and is performed in cf. Fig. 4.6. But first, it is stated that a waveguide loss is obtained if

$$P_{\text{out}}(x) < P_{\text{in}} \quad (4.18)$$

Now, we numerically compute the losses according to Eq. 4.17 for a propagation length of $x = L = 40 \cdot a$. We excite an asymmetric slab waveguide of thickness $d$ with a plane wave with frequency $\omega a/(2\pi c) = 0.28$ (corresponds to $\lambda = 1550\,\text{nm}$ for $a = 435\,\text{nm}$) as shown in Fig. 4.6 A). The waveguide losses are computed for various refractive indices of the substrate $n_{\text{substrate}}$ and are shown in Fig. 4.6 C). A loss is obtained for any $n_{\text{substrate}} = 1$ to $n_{\text{substrate}} = 3.5$ and hence Eq. 4.18 holds for the chosen experiment.

Let us discuss the results in more detail. For $n_{\text{substrate}} = n_1 = 3.5$, the slab waveguide disappears and the light can freely diffract into the lower sub-plane. No guided mode exists in this system, hence the loss is approximately 1, i.e., the maximum value. On the other hand, a symmetric slab waveguide that supports

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1slowly, because we expect a smooth transition while increasing $x$
guided modes is obtained for $n_{\text{substrate}} = n_1 = 1$. For a particular excitation frequency, we can numerically determine the cutoff condition of the slab waveguide, i.e., the refractive index of the substrate $n_{\text{substrate}}$ for which a slab waveguide makes the transition from ‘no guided modes’ to ‘one guided mode’. First, the cutoff frequency is calculated as a function of the substrate refractive index. Therefore the dispersion relation of the slab waveguide is computed for various $n_{\text{substrate}}$ with MPB. Then the cutoff frequency is determined by intersecting the dispersion curves with the substrate lines. This results in a cutoff frequency vs. $n_{\text{substrate}}$ plot, which is shown in Fig. 4.6 B). From this plot Fig. 4.6 B), the cutoff ($n_{\text{cutoff}} = 2.945$) can graphically be deduced for the used excitation frequency $\omega a/(2\pi c) = 0.28$. The cutoff condition $n_{\text{cutoff}} = 2.945$ is drawn into the Loss vs. $n_{\text{substrate}}$ plot (Fig.4.6 C)) and clearly marks the transition from very high losses to lower losses. For slab waveguides with $n_{\text{substrate}} > n_{\text{cutoff}}$ (excited beyond cutoff), the losses are almost maximum ($\text{Loss} \approx 1$) as it can be seen in Fig. 4.6 C). However, for slab waveguides with $n_{\text{substrate}} < n_{\text{cutoff}}$, guided modes exist and may be excited in the experiment, which is manifested in a $\text{Loss} < 1$. Even so,

Figure 4.6: Computation of the Loss for an asymmetric slab waveguide. A) shows a sketch of the performed experiment. We excite an asymmetric slab waveguide with thickness $d = 0.3a$ by a plane wave with frequency $\omega a/(2\pi c) = 0.28$. To model the excitation as given in Eq. 4.12 an aperture with a slit of size $d$ is inserted at the input of the slab waveguide. The Loss is computed for a propagation length $L = 40a$ and various refractive indices of the substrate $n_{\text{substrate}}$ as shown in C). The plot shown in B) was obtained by MPB simulations of the slab waveguide aiming to determine the cutoff condition for the waveguide design shown in A) for the excitation frequency $\omega a/(2\pi c) = 0.28$. 
the losses are never zero, since there is always a mismatch between the field distribution of the plane wave at the input and the transverse field distribution of the guided mode(s).

We intentionally designed the experiment with a strong resemblance to a wave interference experiment, because the excitation of a slab waveguide beyond the cutoff can also be viewed as a diffraction experiment.

### 4.1.3.3 Conclusion

There are two different loss mechanism in slab waveguides that result in a waveguide losses. The first loss mechanism is based on mode conversion due to small imperfections of the waveguide. A guided mode propagates along the waveguide and at every imperfection a small portion of the energy of the guide mode is coupled to other guided modes and radiation modes. The second loss mechanism that results in waveguide losses originates from the excitation of a dielectric waveguide that does not support a guided mode.

### 4.2 The Loss Mechanism in Line-Defect Slab PhC Waveguides

So far, we have only discussed the loss mechanisms in slab waveguides and not for PhCs. The described loss mechanisms in the previous paragraphs are not sufficient to explain the radiation losses observed in periodic structures. The reasons are the following:

- PhCs are characterized by a strong periodic modulation of the permittivity. The periodic modulation does not represent a small disturbance of the slab waveguide. Therefore, the guided modes and the radiation modes of the slab waveguide are not adequate to describe the observed propagation phenomena.

- The appropriate basis set that would allow to apply perturbation theory to compute the scattering losses due to imperfections is not known analytically.

Figure 4.7: Substrate-type line-defect PhC waveguide.
• The modulation of the permittivity is periodic, i.e., strongly coherent.

The system of interest is a substrate-type PhC waveguide as shown in Fig. 4.7. This line-defect slab PhC waveguide cannot be solved analytically and hence, it is not possible to analytically compute the waveguide losses. Quantitative numbers for the propagation losses can only be obtained by numerical simulations. Even though we cannot give a simple analytical equation to quantitatively determine the radiation losses for a PhC structure, we can nevertheless improve the physical understanding of the loss mechanism. Therefore, we formulate five hypotheses describing the loss mechanism of a line-defect slab PhC waveguide.

When radiation losses have to be expected

I.) A Bloch mode $E_B$ is only a truly guided (loss-free) mode, if the wave vectors $k_n$ of all spatial Fourier components $n$ are larger than the largest wave vector $k_{clad}$ of the oscillatory modes of the cladding (discussed in Sec. 4.3.1, in Sec. 4.4 and in Sec. 4.5.2).

II.) If one of the spatial Fourier components of the Bloch mode is located within the domain of radiation modes (oscillatory fields solutions in the cladding), then the Bloch mode as a whole becomes a mode with (an) oscillation(s) in the cladding, i.e., a ‘radiation mode’. We call this a radiative Bloch mode (discussed in Sec. 4.4 and in Sec. 4.3.1).

III.) The domain of radiation modes in the cladding is bounded by the dispersion curve of the fundamental mode of the dielectric system at infinity (discussed in Sec. 4.5).

How the light is lost

IV.) If a PhC waveguide is excited at the input with an excitation frequency $\omega$, for which no guided Bloch mode exists, then the propagation in the PhC waveguide can be expressed in terms of radiative Bloch modes. The propagating wave is a leaky wave and is inherently lossy (as introduced in Sec. 4.1.2.4 and Sec. 4.1.3.2). For all following numerical investigations, the excitation problem is solved.

How much of the light is lost

V.) The radiation losses of an excited leaky Bloch wave – i.e., the ensemble of radiative Bloch modes – is approximately proportional to its normalized spatial Fourier components of the power spectrum of the leaky Bloch wave above the background-line (addressed in Sec. 4.3.1 and Sec. 4.7).

An analytical proof of the hypotheses is not feasible. However, for some simple examples (cf. Sec. 4.4), we can analytically verify some of the made claims. But mostly, numerical examples are performed. The purpose of the following chapters is to test the hypotheses.
4.3 Existing Loss Theories Based on Perturbation Theory

This section discusses two models that have been developed by Marcuse [166] and by Benisty et al. [18]. Both models are based on a perturbation approach. The goal of this section is not the to re-derive already performed work by Marcuse and Benisty, but to introduce the state-of-the-art of the loss theory for slab PhC waveguides. Furthermore, the postulated hypotheses about the loss mechanism in slab PhC waveguides should also hold for simpler systems, such as a small periodic wall distortion function.

4.3.1 Perturbation by a Small Wall Distortion Function

Marcuse discussed a perturbation theory based on the expansion in terms of the complete set of guided and radiation modes of a symmetric planar slab waveguide to describe the radiation losses suffered by a guided mode due to the imperfections of the waveguide wall [166]. In a follow-up article, Marcuse discussed the case of a periodic wall distortion function $f(x)$ [167] as shown in Fig. 4.8. Finally, the analysis was applied also to asymmetric planar slab waveguides in [168] and his book [170, pp. 134-147]. Even though the theory holds only for small disturbances of the dielectric interfaces of the slab, the results are very important, since all relevant dependences of the radiation loss on the periodic disturbances are obtained.

The observed radiation pattern in terms of guided and radiation modes writes as

$$E_y(x, z, t) = \sum_m C_m(x)E_m(x, z, t) + \int_0^\infty g(\rho, x)E(\rho, x, z, t)d\rho. \quad (4.19)$$

The first term represents the summation of all guided modes $E_n$ weighted by a coefficient $C_n$. The second term takes the continuum of all radiation modes $E(\rho)$ weighted by a factor $g(\rho, x)$ into account. $m$ and $\rho$ label a guided and a radiation mode, respectively. The resulting electric field $E_y$ (Eq. 4.19) has to obey the wave equation

$$\frac{d^2 E_y}{dz^2} + \frac{d^2 E_y}{dx^2} + (n_0^2 + \Delta n^2(x))\frac{\omega^2}{c^2} E_y = 0. \quad (4.20)$$

Figure 4.8: Slab waveguide with a periodic wall distortion function $f(x)$. 
where \( f(x) = \Delta n^2(x) \) is the wall distortion function. If Eq. 4.19 is inserted into Eq. 4.20, followed by a multiplication by the magnetic field of a guided mode \( H_z = \beta_{x,p}/(2\omega \mu) \overline{E_p} \) (the overbar denotes the complex conjugate) and integrated over \( z \) from \(-\infty\) to \(\infty\), then all integrals over two distinct guided modes and radiation modes are zero \((E_p \neq E_m \neq \mathcal{E}(\rho))\). A differential equation for the coefficients \( C_p \) results

\[
\frac{d^2 C_p}{dx^2} - 2i\beta_{x,p} \frac{dC_p}{dx} = F_p(x) \tag{4.21}
\]

with

\[
F_p(x) = -\frac{\beta_{x,p}\omega}{2\mu Pe^2} \left[ \sum_p C_p(x) \int_{-\infty}^{\infty} \overline{\mathcal{E}_m} \Delta n^2 \mathcal{E}_m dx + \sum \int_0^{\infty} g(\rho, x) d\rho \int_{-\infty}^{\infty} \overline{\mathcal{E}_p} \Delta n^2 \mathcal{E}(\rho) dx \right] \tag{4.22}
\]

The coefficients \( g(\rho, x) \) for the expansion in radiation modes are obtained in an analogous procedure: instead of multiplying with the magnetic field of a guided mode, it is multiplied by the magnetic field of a radiation mode \( H_z = \beta'_x/(2\omega \mu) \mathcal{E}(\rho') \) followed by an integration over \( z \) from \(-\infty\) to \(\infty\) and one obtains

\[
\frac{d^2 g(\rho')}{dx^2} - 2i\beta'_x \frac{dg(\rho')}{dx} = G_p(\rho', x) \tag{4.23}
\]

with

\[
G_p(\rho', z) = -\frac{\beta_{x,p}\omega}{2\mu Pe^2} \left[ \sum_m C_m(x) \int_{-\infty}^{\infty} \overline{\mathcal{E}_p(\rho')} \Delta n^2 \mathcal{E}_m dx + \sum \int_0^{\infty} g(\rho, x) d\rho \int_{-\infty}^{\infty} \overline{\mathcal{E}_p(\rho')} \Delta n^2 \mathcal{E}(\rho) dx \right] \tag{4.24}
\]

\( F_p(x) \) and \( G_p(\rho', x) \) are distortion terms, i.e., they become zero for \( \Delta n^2 = 0 \). If the used modes have all the same amount of power, then the power carried by a mode can be expressed in terms of \( C_m \) and \( g \) coefficients only. We skip here the detailed derivation of the determination of the coefficients, since it can be found detailed in [166] and we focus on the result instead.

The relevant quantity is the ratio of scattered power to incident guided mode power. We assume a single guided mode at the input of a slab waveguide with a wall distortion function \( f(x) \). The ratio between the scattered power \( \Delta P \) and the power \( P \) of the incident guided mode is [166, Eq. 48]

\[
\frac{\Delta P}{P} = \sum_{n=1}^{\infty} \left[ |C_n^+(L)|^2 + |C_n^-(0)|^2 \right] + \sum \int_0^{\infty} \left[ |g^+(\rho, L)|^2 + |g^-(\rho, 0)|^2 \right] d\rho, \tag{4.25}
\]

where the first sum runs over all forward-propagating guided modes \( ^{(+)} \) at
the output \( x = L \) and backward-propagating modes \((-)\) at the input \( x = 0 \) and the second sum runs over the corresponding radiation modes at the same positions. By using initial conditions and after some mathematical calculations the scattered power ratio for a periodic distortion function is obtained (according to Marcuse [167, Eq. 14a u. Eq. 14b])

\[
\frac{\Delta P}{P} = \int_{-k}^{k} \frac{1}{d^2} L |\varphi(\beta_0 - \beta_x)|^2 I(\beta_x) d\beta_x
\]  

(4.26)

where \( d \) is the thickness of the core layer of the slab, \( \beta_x \) the component of the propagation constant of the radiation mode in \( x \)-direction, \( \beta_0 \) the propagation constant of the guided mode, \( k \) the propagation constant in free space, \( L \) the length of the waveguide section with the wall distortion function \( f(x) \) and \( I(\beta_x) = \left( \frac{4 \omega^2}{c^2} \right)^2 \left( n_g^2 - 1 \right) \cos^2(\kappa_0 d) \beta_0 d + \frac{\beta_0}{\gamma_0} \left( \frac{\cos^2(\sigma d)}{(pd)^2 \cos^2(\sigma d) + (\sigma d)^2 \sin^2(\sigma d)} + \frac{\sin^2(\sigma d)}{(pd)^2 \sin^2(\sigma d) + (\sigma d)^2 \cos^2(\sigma d)} \right) \) \( \right) \) (4.27)

\( n_g \) is the refractive index of the core of the slab waveguide and \( \kappa_0 = \sqrt{n_g^2 \omega^2/c^2 - \beta_0^2} \), \( \sigma = \sqrt{n_g^2 \omega^2/c^2 - \beta_x^2} \), \( \gamma_0 = \sqrt{\beta_0^2 - \omega^2/c^2} \). Furthermore,

\[
\varphi(\beta_0 - \beta_x) = \frac{1}{L} \int_0^L [f(x) - d] e^{-i(\beta_0 - \beta_x)x} dx
\]  

(4.28)

are the spatial Fourier coefficients of the wall distortion function \( [f(x) - d] \) expanded in the domain \( 0 \leq x \leq L \). The relative scattering loss \( \Delta P/P \) thus directly depends on the Fourier components \( \varphi(\beta_0 - \beta_x) \) of the wall distortion function \( f(x) \), i.e., its absolute square value

\[
|\varphi(\beta_0 - \beta_x)|^2
\]  

(4.29)

that is the power spectral density of \( f(x) \). The integral of Eq. 4.26 extends from \(-k\) to \( k \), the range of radiation modes. This is an important result, since only those parts of the power spectrum that have a \( \beta_x \) within the range of \(-k < \beta_x < k\) can contribute to radiation loss. Note that this model complies with the hypotheses I)-III) and is identical to hypothesis V) as stated in Sec. 4.2 and affirms our theory. But opposed to hypothesis IV), the loss mechanism here is based on mode conversion due to small geometrical disturbances of the slab waveguide.

Unfortunately, this perturbation approach formalism cannot be applied to PhC waveguides, because the etched holes represent a strong periodic modulation of the refractive index. Expanding the solution in terms of modes of the unperforated slab waveguide is therefore not appropriate.

### 4.3.2 \( \varepsilon'' \)-Model

A major effort was made by Benisty and Ferrini [18, 19, 72, 70, 71] to approximate the propagation losses for substrate-type PhCs. Benisty et al. [18] started to view a part
of the holes as a perturbation. They realized the following: If the permittivity can be separated into a horizontal function $\varepsilon^h(x, y)$ and a vertical function $\varepsilon^v(z)$ such that $\varepsilon(x, y, z) = \varepsilon^h(x, y) + \varepsilon^v(z)$, then the scalar wave equation can be solved instead of the vector wave equation. Thus, if $\varepsilon(x, y, z) = \varepsilon^h(x, y) + \varepsilon^v(z)$ holds, then the electric field $E^S$ solution of the scalar wave equation can be formulated as a product of functions of separated variables $E^S(x, y, z) = \psi(x, y)\zeta(z)$, where $\psi(x, y)$ is the solution of the 2D PhC. The approach of the separation of variables was justified in the appendix of Ref. [18]. In case of a slab PhC with a weak vertical refractive index contrast the permittivity is almost given by $\varepsilon(x, y, z) = \varepsilon^h(x, y) + \varepsilon^v(z)$, it only differs by $\Delta\varepsilon(r)$, a periodic pattern of cylindrical rods in the waveguide core of the PhC with $\Delta\varepsilon = \varepsilon_2 - \varepsilon_1$ as schematically shown in Fig. 4.9. Benisty et al. considered these periodic rods as the scatterers responsible for the out-of-plane losses observed in slab PhCs. The notion that the light is not vertically guided anymore in the holes – as it is commonly argued (cf. citation) – may originate from this concept. The radiation losses are approximated by employing the First Born Approximation, i.e., the radiating field of a single rod is approximated by the radiating field of an electric dipole

$$p = \varepsilon_0 \Delta\varepsilon \langle E^s \rangle V \cdot V,$$

where $V = \pi r^2 w$ is the volume of a perturbation rod, $w$ is the height of the rod, $\langle E^s \rangle V$ is the averaged electric field in volume $V$ and $r$ is the radius of the rod. Using this approximation, the radiation losses per hole can be derived and are given by [18]

$$W_{RL} = \frac{\langle E^s \rangle^2 \Delta\varepsilon^2}{n_2^3} \frac{V^2}{(\lambda/2n_2)^4} \frac{\pi^3 \varepsilon_0}{12 \eta},$$

where $\eta$ is the extraction efficiency, i.e., the fraction $\eta$ of the total energy of a guided mode that couples into radiation modes. The dissipated energy of a 2D PhC field $\psi(x, y)$ with an imaginary part of the permittivity $\varepsilon''$

$$W_{diss} = \frac{1}{2} \varepsilon_0 \varepsilon'' \langle |\psi|^2 \rangle V \frac{V \pi c}{n_2(\lambda/2n_2)}.$$

can be related to the radiation loss per hole $W_{RL}$ by equating $W_{RL} = W_{diss}$. 

![Figure 4.9: The definition of the perturbation for the empirical model for the out-of-plane losses by Benisty et al. [18].](image)
It follows
\[
\varepsilon'' = \frac{\pi^2}{6} \frac{V}{(\lambda/2n_2)^2} \frac{(\Delta\varepsilon)^2}{n_2^2} \eta \Gamma_1, \tag{4.33}
\]
where \(\Gamma_1\) is the confinement factor with respect to the out-of-plane axis \(z\) of the guided mode. Note that \(\varepsilon''\) is proportional to both, the volume of the rod \(V\) and the vertical confinement factor \(\Gamma_1\). Thus, this model suggests that, reducing the volume (e.g., the radius) of the holes reduces the radiation losses (cf. citation). Finally, they compared the transmission of optically measured PhCs and the transmission obtained by their model and they find a fairly good agreement for a \(\varepsilon'' = 0.18\) for frequencies outside the band gap, where \(\varepsilon''\) is used as a fitting parameter.

Benisty et al. [18] correctly noted that in case of a membrane PhC, the perturbation \(\Delta\varepsilon\) becomes large and the approximation of a small perturbation is not valid any longer. Notwithstanding, they concluded that “... with sufficient etch depth, high-index claddings are superior to low-index ones to form high Q-cavities”.

Thereafter the model was extended to compute the radiation losses originating from a finite-etch depth [19] and any other kind of imperfections of the hole shape [72, 70, 69, 71]. In those publications, the scatterer is defined by the difference of the imperfect hole shape to the ideal cylindrical hole shape as illustrated in Fig. 4.10. The volume of this difference is considered to give rise to dipole radiation according to the First Born Approximation.

The model does not take coherent radiation effects into account and thus the hypotheses I)-III) cannot be confirmed by this model. Furthermore, according to this model, the radiation losses are proportional to the volume \(V\) of the holes and to \(\lambda^{-4}\) according to Rayleigh scattering, i.e., the radiation losses increase for higher frequencies. We will further discuss the model developed by Benisty et al. [18] and Ferrini et al. [72, 70, 69, 71] in the following section.

![Figure 4.10](image-url): Illustration of procedure behind the \(\varepsilon''\)-model: The voluminous difference between the perfect cylindrical hole and the realistic hole is conceived as a perturbation, which act as a scattering source giving rise to dipole radiation into a homogeneous medium (cf. [72], Fig.1).
4.3.3 Concluding Remarks on the Scattering Process in Strongly Modulated Periodic Structures

The empirical model developed by Benisty and Ferrini assumes that the scattering resulting in out-of-plane loss can be assigned to a localized scatterer. We want to eradicate this misconception, because it does not reflect the situation in periodic structures. If the approach were correct, we would expect that a stronger scattering source always yields a stronger radiation loss. This assumption is reasonable for randomly localized disturbances. In Fig. 4.11 (A) the electric field $E_y$ is shown for a symmetric planar slab waveguide with air claddings and core refractive index $n_{\text{core}} = 3.3296$ excited with a frequency $\omega_a/(2\pi c) = 0.3$. In panel B) and C), a disturbance consisting of a rectangular notch with a depth $d$ is inserted into the slab waveguide. Two different depths $d_1 = 0.1 \cdot a$ and $d_2 = 0.6 \cdot a = d_{\text{slab}}$ are investigated to represent the weak and the strong disturbance, respectively. Comparing Fig. 4.11 A) and B) and C) reveals that a single inserted disturbance results in a radiation pattern that is stronger for the deeper disturbance.

Next, we investigate the influence of the periodicity. Therefore, the slab waveguide is periodically modulated by the same weak and strong disturbances. The detailed description of the investigated dielectric systems is given in Fig. 4.11 D). In Fig. 4.11 E) and F) the field plots are shown for the periodically modulated disturbances for an excitation with the same frequency $\omega_a/(2\pi c) = 0.3$. Whereas the periodic modulation with the weak disturbance (Bragg grating) results in a rather strong radiation pattern, the periodic modulation with the strong disturbance (PhC) does not radiate at all. This simple example shows that the assumption (as used by Benisty et al. [18]) that the total radiated field can be obtained by summing the radiated fields of isolated scatters, is not justified for periodic structures.

Instead, the examples demonstrate the importance of the relative locations of the spatial Fourier components of the Bloch mode with respect to the light-line. Therefore, the dispersion diagram is computed for the undisturbed slab waveguide (blue), the Bragg grating (red) and the PhC (violet) and plotted in a plane wave vectors $k_x$ basis in Fig. 4.11. It can be seen that for the used excitation frequency of $\omega_a/(2\pi c) = 0.3$, one spatial Fourier component of the plane wave expansion of the Bloch wave of the Bragg grating is located within the air light cone. On the other hand, all spatial Fourier components of the Bloch wave for the PhC waveguide are located outside of the air light cone. This confirms hypothesis I) and II).

Let us verify our understanding of the importance of the relative location of Fourier components of the Bloch mode. According to the dispersion diagram, all spatial Fourier components of the Bloch mode of the Bragg grating would be located outside the domain of radiation modes (cf. red curve in Fig. 4.11) for a slightly lower frequency, e.g., $\omega_a/(2\pi c) = 0.25$. Then the Bragg grating should not radiate anymore. Figure 4.12 A) confirms that no radiation occurs for the described situation. A slight change of the excitation frequency can thus have a dramatic influence on the existence of radiation losses. On the other hand, for a slightly higher frequency, e.g., $\omega_a/(2\pi c) = 0.35$, one Fourier component of the Bloch mode of the 1D PhC (strong periodic modulation) would be located inside the light cone, i.e., within the domain of radiation modes (cf. violet curve in Fig. 4.11). And indeed,
Figure 4.11: Left: Radiation pattern of a undisturbed slab waveguide (A) and of a small (B) and a large (C) geometrical imperfection. Right: Periodic pattern of a small (E) and large (F) geometrical imperfection. The radiation patterns are computed with 2D FEM (Comsol) by exciting the slab waveguides from the left. Bottom (G): the dispersion diagram of the slab waveguide mode (A), of the Bragg grating (E) and of a PhC (F) computed with 2D MPB.
We conclude that the hypotheses I)-II) of Sec. 4.2 strictly hold for weak and strong 1D periodic systems.

4.4 Plane Wave Expansion for a Slab with 1D Periodicity

We stated above that the complete set of guided modes and radiation modes of the perfect slab waveguide cannot be used for slab PhCs, because of their strong periodic modulation of the permittivity. Thus, the complete basis set for the PhC would be highly valuable, since it would allow us to perform perturbation theory to analyze the radiation losses induced by small deviations such as surface roughness. But a rigorous analytical solution of a line-defect slab PhC waveguide
is not possible to the best of our knowledge. One reason is that a separation into TE and TM modes is not possible for a planar slab PhC structure (cf. Sec. 2.3.1). As a consequence, the full vectorial wave equation has to be solved and the boundary condition has to be applied for each of the six field components. Usually, numerical methods are applied for such complicated systems.

Nevertheless, a separation into two distinct polarizations can be made for any 2D system. Therefore, we consider a simplified system as depicted in Fig. 4.13. Note that this simplified dielectric system is similar to a line defect PhC waveguide: both have a 1D periodicity of the permittivity in propagation direction and a slab structure in transverse direction. The new, simplified system is invariant in \( y \)-direction and thus there are two distinct polarizations: \( H_y, E_x, E_z \) and \( E_y, H_x, H_z \). Furthermore, non-absorbing (\( \sigma = 0 \)) and source free materials (\( J = 0, \varrho = 0, \nabla \cdot D = 0, \nabla \cdot H = 0 \)) with a magnetic permeability \( \mu_r (r) = 1 \) are assumed. Encouraged by the possibility to solve periodic system with a plane wave expansion technique (cf. Sec. 2.2.3) all fields are expanded in terms of plane waves. These expressions are inserted into the wave equation for the core and the cladding separately. Finally, the boundary conditions are applied. Analogous to the procedure for the planar slab waveguide (cf. Sec. 2.1) we seek the eigenvalues \( \omega \) and the corresponding eigenfunctions. The goal of this section is to derive the guided modes and the radiation modes for the simplified system.

4.4.1 Description of the Mode Solutions

We investigate only the polarization that is defined by a magnetic field \( H_y \)

\[
H(x, z) = H(x, z)e_y = H_y e_y.
\]  

(4.34)

The discussion of the other polarization given by an electric field \( E_y \) is analogous. Even though the periodicity is given only for the permittivity of the core of the planar slab, the total system – consisting of the periodic core and the claddings – as a whole is strictly periodic in the \( x \)-direction. As a consequence the Bloch theorem
holds for the $x-$dependence for all layers

$$H_{y,k_x}(x,z) = u_{k_x}(x,z)e^{i k_x x} \quad (4.35)$$

From the Bloch theorem, we know that $u_{k_x}(x,z)$ is a periodic function in $x$ with periodicity $a$. For the moment, the Bloch index $k_x$ is assumed to be real quantity (analogous to the derivation of the guided modes and radiation modes of a slab waveguide). A periodic function can always be expanded in a discrete series of harmonic functions according to

$$H_{y,k_x}(x,z) = \sum_m A_{m,k_x}(z)e^{i(k_x+mK)x}, \quad (4.36)$$

where $K = \frac{2\pi}{a}$. The dependence of the magnetic field $H_{y,k_x}(z)$ in transverse direction can also be represented by a series of harmonic functions, i.e., analogous to the slab waveguide we make the following ansatz

$$A_{m,k_x}(z) = \begin{cases} A_{m,k_x,3}e^{ik_xz,mz} & z > 0 \\ \sum_q A_{m,q,k_x,1}e^{iq2\pi z} & 0 > z > -d. \\ A_{m,k_x,2}e^{ik_xz,m(z+d)} & z < -d \end{cases} \quad (4.37)$$

In the following we solve the wave equation in every layer separately. All possible transverse functions can be represented by the made ansatz. Alternatively, it would be possible to assume a single plane wave expansion to describe the transverse function in all layers simultaneously. But then, the permittivity would have to be expanded in two dimensions. The made ansatz (Eq. 4.37) allows us to write

$$\varepsilon_r(x,z) = \varepsilon_r(x+a,z) = \begin{cases} \varepsilon_3 & z > 0 \\ \varepsilon_{core}(x) = 1/\sum_l v_l e^{ilKx} & 0 > z > -d. \\ \varepsilon_2 & z < -d \end{cases} \quad (4.38)$$

Note that the inverse of the permittivity $\varepsilon(x)$ is expanded in plane waves, since the inverse of the permittivity is needed in the master equation Eq. A.9.

In the next step, the wave equation is solved in the cladding and the core layer separately. Then the partial solutions in the separate layers have to be combined by applying the boundary conditions.

### 4.4.2 Solving the Helmholtz Equation in the Cladding Layer

We first solve the master equation Eq. A.9 for time harmonic magnetic fields $H_{y,k_x}$

$$-\nabla \times \left( \frac{1}{\varepsilon(x)} \nabla \times \left( H_{y,k_x}(x,z) \right) \right) + \frac{\varepsilon^2}{c^2} \left( H_{y,k_x}(x,z) \right) (x,z) = 0 \quad (4.39)$$

for each cladding layer. Since the permittivity is constant in the cladding (e.g.,
\( \varepsilon_r(x, y) = \varepsilon_3 \) the Helmholtz equation can be used

\[
\Delta H_{y,k_z}(x,z) + \varepsilon_3 \frac{\omega^2}{c^2} H_{y,k_z}(x,z) = 0. \tag{4.40}
\]

By inserting \( H_{y,k_z}(x,z) \) from Eq. 4.36 into the Helmholtz equation Eq. 4.40 we arrive at

\[
-\sum_m A_{m,k_z,3} e^{ik_{z,m,3}z} \cdot (\hat{k} + mK)^2 e^{i(\hat{k}x + mK)x} - \sum_m k_{z,m,3}^2 A_{m,k_z,3} e^{ik_{z,m,3}z} \cdot e^{i(\hat{k}x + mK)x} + \frac{\omega^2}{c^2} \varepsilon_3 \sum_m A_{m,k_z,3} e^{ik_{z,m,3}z} \cdot e^{i(\hat{k}x + mK)x} = 0 \tag{4.41}
\]

By multiplying with a function \( e^{-i(\hat{k}x + pK)x}, p \in \mathbb{Z} \) (the function is orthogonal to the function \( e^{i(\hat{k}x + mK)x} \) if \( m \neq p \)) followed by an integration over a period \( \frac{1}{a} \int_{-a/2}^{a/2} dx \), one obtains \( p \)-equations for \( p \in \mathbb{Z} \)

\[
- A_{p,k_z,3} e^{ik_{z,p,3}z} \cdot (\hat{k}_x + pK)^2 - k_{z,p,3}^2 A_{p,k_z,3} e^{ik_{z,p,3}z} + \frac{\omega^2}{c^2} \varepsilon_3 A_{p,k_z,3} e^{ik_{z,p,3}z} = 0 \tag{4.42}
\]

Eq. 4.42 can be simplified to

\[
A_{p,k_z,3} e^{ik_{z,p,3}z} \left( \frac{\omega^2}{c^2} \varepsilon_3 - k_{z,p,3}^2 - (\hat{k}_x + p \frac{2\pi}{a})^2 \right) = 0. \tag{4.43}
\]

In order for this equation to be fulfilled for all \( z \), either \( A_{p,k_z,3} \) must be zero (trivial solution) or

\[
k_{z,p,3} = \sqrt{\frac{\omega^2}{c^2} \varepsilon_3 - (\hat{k}_x + p \frac{2\pi}{a})^2} \tag{4.44}
\]

has to hold. Hence, we obtained for every equation \( p \in \mathbb{Z} \) a condition for \( k_{z,p,3} \).

Two distinct cases for the form of the transverse function in the cladding can be identified:

- \((\hat{k}_x + pK)^2 < \varepsilon_3 \omega^2 / c^2\):
  \( k_{z,p,3} \) is a real quantity. Therefore, an oscillating solution of the form \( A_{p,k_z,3} e^{ik_{z,p,3}z} \) is expected in the cladding for a Fourier component with a wave vector \( k_{z,p,3} = (\hat{k}_x + pK) < \sqrt{\varepsilon_3} \omega / c \).

- \((\hat{k}_x + pK)^2 > \varepsilon_3 \omega^2 / c^2\):
  \( k_{z,p,3} \) is a purely imaginary quantity \( k_{z,p,3} = i \sqrt{(\hat{k}_x + pK)^2 - \frac{\omega^2}{c^2} \varepsilon_3} \). Thus an exponentially decaying or exponentially increasing function is found in the cladding for a Fourier component with a wave vector \( k_{z,p,3} = (\hat{k}_x + \)
plane wave expansion for a slab with 1d periodicity

\[ pK > \sqrt{\varepsilon_3} \omega/c. \] Further note that the \( k_{z,p,3} \) depends directly on the difference of \( (\hat{k}_x + pK)^2 - \frac{\omega^2}{c^2} \varepsilon_3 \), hence the fields decay/increase faster for larger values of \( p \).

Finally, the total magnetic field in the cladding layer \( n_3 \) has the following form

\[
H_{y,k_x,3}(x, z) = \sum_m A_{m,k_x,3} e^{i\sqrt{\varepsilon_3} \omega^2/c^2 - (k_x + mK)^2 z} \cdot e^{i(k_x + mK)x}. \quad (4.45)
\]

Analogous, the magnetic field in the cladding layer \( n_2 \) is

\[
H_{y,k_x,2}(x, z) = \sum_m A_{m,k_x,2} e^{i\sqrt{\varepsilon_2} \omega^2/c^2 - (k_x + mK)^2 z} \cdot e^{i(k_x + mK)x}. \quad (4.46)
\]

### 4.4.3 Solving the Wave Equation in the Core Layer

Now the master equation (Eq. A.9)

\[
-\nabla \times \left( \frac{1}{\varepsilon(x)} \nabla \times \begin{pmatrix} 0 & H_{y,k_x}(x, z) \\ 0 & 0 \end{pmatrix} \right) + \frac{\omega^2}{c^2} \begin{pmatrix} 0 & H_{y,k_x}(x, z) \\ 0 & 0 \end{pmatrix} = 0 \quad (4.47)
\]

is solved for the core layer. We follow closely the calculation in Appendix A.4. For the polarization of a magnetic field \( H_{y,k_x} \), Eq. 4.47 simplifies to the scalar equation

\[
\frac{1}{\varepsilon_{\text{core}}(x)} \frac{\partial^2}{\partial z^2} H_{y,k_x}(x, z) - \frac{1}{\varepsilon_{\text{core}}(x)} \frac{\partial}{\partial x} \frac{1}{\varepsilon_{\text{core}}(x)} \frac{\partial}{\partial x} H_{y,k_x}(x, z) + \frac{\omega^2}{c^2} H_{y,k_x}(x, z) = 0. \quad (4.48)
\]

By using Eq. 4.36, Eq. 4.38 and Eq.4.37 in the Eq. 4.47 the following equation is obtained

\[
- \sum_l v_l e^{ilKx} \sum_m \sum_q \left( q \frac{2\pi}{d} \right)^2 A_{m,q,k_x,1} e^{i\frac{2\pi}{d}z} \cdot e^{i(k_x + mK)x} \\
+ \sum_l lK_l e^{ilKx} \sum_m \sum_q A_{m,q,k_x,1} e^{i\frac{2\pi}{d}z} \cdot (\hat{k}_x + mK) e^{i(k_x + mK)x} \\
+ \sum_l v_l e^{ilKx} \sum_m \sum_q A_{m,q,k_x,1} e^{i\frac{2\pi}{d}z} \cdot (\hat{k}_x + mK)^2 e^{i(k_x + mK)x} \\
+ \frac{\omega^2}{c^2} \sum_m \sum_{q} A_{m,q,k_x,1} e^{i\frac{2\pi}{d}z} \cdot e^{i(k_x + mK)x} = 0 \quad (4.49)
\]

after some mathematical manipulations and by finally multiplying with \( e^{i(k+pK)x} \) and integrating over one period \( \int_{-a/2}^{a/2} dx \), \( l \)-equations are obtained
\[
\sum_l v_l \left[ \sum_q A_{p-l,q,\hat{k}_x,1} e^{iq\frac{2\pi}{d}z} \left\{ \left( \frac{2\pi}{q} \frac{2\pi}{d} \right)^2 - (\hat{k}_x + pK)(\hat{k}_x + (p-l)K) \right\} \right]
= \frac{\omega^2}{c^2} \sum_q A_{p,q,\hat{k}_x,1} e^{iq\frac{2\pi}{d}z} \quad (4.50)
\]

4.4.4 Boundary conditions

The coefficients \( A_{p,q,\hat{k}_x,1}, A_{p,\hat{k}_x,2} \) and \( A_{p,\hat{k}_x,3} \) are linked to each other via the boundary conditions. Therefore, we require the continuity of the tangential magnetic and electric field at the interfaces at \( z = 0 \) and \( z = -d \). We start by establishing the boundary conditions for the magnetic fields \( H_{y,\hat{k}_x} \) for \( z = 0 \)

\[
\sum_m A_{m,\hat{k}_x,3} e^{i(k_x + m \frac{2\pi}{a})x} = \sum_m \sum_q A_{m,q,\hat{k}_x,1} e^{i(k_x + mK)x} \quad (4.51)
\]

and \( z = -d \)

\[
\sum_m A_{m,\hat{k}_x,2} e^{i(k_x + \frac{2\pi}{a})x} = \sum_m \sum_q A_{m,q,\hat{k}_x,1} e^{i(k_x + mK)x}. \quad (4.52)
\]

The tangential electric field \( E_{x,\hat{k}_x}(x) \) is derived from the magnetic field \( H_{y,\hat{k}_x}(x) \) by using Eq. A.5

\[
E_{x,\hat{k}_x}(x) = \frac{1}{i\omega\varepsilon(x,z)} \frac{\partial}{\partial z} H_{y,\hat{k}_x}(x,z).
\]

This allows us to formulate the boundary condition for the tangential electric field \( E_{x,\hat{k}_x}(x) \) for \( z = 0 \)

\[
\frac{1}{\varepsilon_3} \sum_m k_{z,m,3} A_{m,\hat{k}_x,3} e^{i(k_x + mK)x} = \sum_m \sum_l q \frac{2\pi}{d} A_{m,q,\hat{k}_x,1} \cdot v_l \cdot e^{i(k_x + (m+l)K)x} \quad (4.53)
\]

and \( z = -d \)

\[
\frac{1}{\varepsilon_2} \sum_m k_{z,m,2} A_{m,\hat{k}_x,2} e^{-ik_z \cdot \frac{2\pi}{d}} e^{i(k_x + mK)x} = \sum_m \sum_l q \frac{2\pi}{d} A_{m,q,\hat{k}_x,1} \cdot v_l \cdot e^{i(k_x + (m+l)K)x}. \quad (4.54)
\]

By multiplying with an orthogonal function \( e^{-i(k_x + pK)x} \) and integrating over one period \( \frac{1}{a} \int_{-a/2}^{a/2} dx, p \in \mathbb{Z} \) equations are obtained for all four boundary condi-
Plane Wave Expansion for a Slab with 1D Periodicity

\[ A_{p, k_x, 3} = \sum_q A_{p, q, k_x, 1} \] (4.55)

\[ A_{p, k_x, 2} = \sum_q A_{p, q, k_x, 1} \] (4.56)

\[ A_{p, k_x, 3} = \frac{\varepsilon_3}{k_{z, p, 3}} \sum_l \sum_q q \frac{2\pi}{d} A_{p-l, q, k_x, 1} \cdot v_l \] (4.57)

\[ A_{p, k_x, 2} = \frac{\varepsilon_2}{k_{z, p, 2}} \sum_l \sum_q q \frac{2\pi}{d} A_{p-l, q, k_x, 1} \cdot v_l. \] (4.58)

The terms \( A_{p, k_x, 1} \) and \( A_{p, k_x, 3} \) can be eliminated by equating Eq. 4.55 and Eq. 4.57

\[ \sum_q A_{p, q, k_x, 1} = \frac{\varepsilon_3}{k_{z, p, 3}} \sum_l \sum_q q \frac{2\pi}{d} A_{p-l, q, k_x, 1} \cdot v_l \] (4.59)

and by equating Eq. 4.56 and Eq. 4.58

\[ \sum_q A_{p, q, k_x, 1} = \frac{\varepsilon_2}{k_{z, p, 2}} \sum_l \sum_q q \frac{2\pi}{d} A_{p-l, q, k_x, 1} \cdot v_l. \] (4.60)

Two sets of equations are obtained that can be used to determine \( A_{p, q, k_x, 1} \). Furthermore, Eq. 4.50 has to be fulfilled for any \( z \), also for \( z = 0 \) and \( z = -d \). Therefore, we insert Eq. 4.59 into Eq. 4.50 for \( z = 0 \) and obtain

\[ \sum_l v_l \sum_q \left[ \left( q \frac{2\pi}{d} \right)^2 - \left( q \frac{2\pi}{d} \right)^2 \frac{\omega^2}{c^2} \frac{\varepsilon_3}{k_{z, p, 3}} - (\hat{k}_x + pK)(\hat{k}_x + (p-l)K) \right] A_{p-l, q, k_x, 1} = 0 \]

Analogous, we insert Eq. 4.59 into Eq. 4.50 for \( z = -d \) and obtain

\[ \sum_l v_l \sum_q \left[ \left( q \frac{2\pi}{d} \right)^2 - \left( q \frac{2\pi}{d} \right)^2 \frac{\omega^2}{c^2} \frac{\varepsilon_2}{k_{z, p, 2}} - (\hat{k}_x + pK)(\hat{k}_x + (p-l)K) \right] A_{p-l, q, k_x, 1} = 0 \]

**4.4.5 Conclusion**

Finally, we obtained two equations for the eigenvalue \( \omega \) of the modes of the 1D PhC slab waveguide as shown in Fig. 4.13. No simplifications have been applied so far, such that the equations hold for any kind of periodic modulation of the permittivity in the core, i.e., also for strong periodic modulations of the refractive index in the slab (as opposed to the perturbation model presented in Sec. 4.3.1). In principle, we could now compute the dispersion relation of the system by solving the resulting eigenvalue equation numerically. Instead, we focus on the found solutions and compare them to the familiar guided modes and radiation modes of the slab waveguide. The solutions – i.e., the eigenmodes – of the considered dielectric system can be written as sum of plane waves in propagation...
Figure 4.14: Top: spatial Fourier spectrum of a Bloch mode. Middle: the transverse field distribution associated with each spatial Fourier component for the case of a guided Bloch mode. Bottom: transverse field distribution associated with each spatial Fourier component for the case of a radiative Bloch mode.

Figure 4.15: Transverse field profile associated with A) a guided Bloch mode and with B) a radiative Bloch mode. The transverse mode profile is obtained by a superposition of the transverse mode profiles of each spatial Fourier component as shown in Fig. 4.14.
direction $e_x$ that are multiplied by the transverse function $e(z)$. An important result is that the form of the transverse functions $e(z)$ depends on the location of the spatial Fourier component $k_p = (\hat{k}_x + pK)$ with respect to the line given by $k_{\text{separatrix}}(\omega) = \max(n_2, n_3) \cdot \omega / c$. An oscillating transverse function in the claddings is obtained for $k_p < k_{\text{separatrix}}$. An exponentially decaying function in the claddings is obtained for $k_p > k_{\text{separatrix}}$. Analogous to the slab waveguide, we require for a guided Bloch mode that all transverse functions $e(z)$ decay in the claddings for $z \to \pm \infty$. If for one or more spatial Fourier components holds $k_p > k_{\text{separatrix}}$, then at least one oscillating transverse function is contained in the Bloch mode. In analogy the slab waveguide (cf. 2.1.2.4), we call these modes with oscillatory fields in the claddings radiative Bloch modes. Figure 4.14 shows schematically the spatial Fourier spectrum of a Bloch mode and a drawing of the transverse function for the two different types of modes, i.e., a guided Bloch mode is obtained for frequency $\omega_2$ and a radiative Bloch mode is obtained for frequency $\omega_1$. Figure 4.15 illustrates the resulting transverse mode profile of a guided Bloch mode and a radiative Bloch mode. The transverse mode profiles are obtained by a summation of all transverse mode profiles associated with the different spatial Fourier components. Note that there is a continuum of radiative Bloch modes similar to the radiation modes of a slab waveguide. For instance, we can imagine an impinging plane wave from the bottom cladding with incident angle $\theta$. A part of the incident plane wave is reflected and a part of the incident wave is transmitted. In principle, we can freely choose $\theta$. For every $\theta$ a radiative Bloch mode is found.

This section essentially consists of a mathematical description of hypotheses I) and II) of Sec. 4.2 for a 1D slab PhC waveguide with homogeneous cladding layers. Furthermore, we found the analogon to the ‘light-line’ for the slab waveguide: for a guided Bloch mode in a slab waveguide with a strong periodic modulation, all its spatial Fourier components have to be located below the ‘light-line’. We will further elaborate on this ‘light-line’-concept in the following Sec. 4.5.

### 4.4.6 The Loss Mechanism

The considerations about the loss mechanisms in a slab waveguide were based on guided modes and radiation modes of the slab waveguide. Since we have now the equivalent guided Bloch modes and radiative Bloch modes of the slab with a strong periodic modulation along one direction, we can apply the made considerations for the periodic system. The first loss mechanism consist of coupling energy from a guided Bloch mode to radiative Bloch modes due to geometrical imperfections. The second loss mechanism consists of exciting a slab PhC waveguide with a frequency $\omega$ at the input, for which no guided Bloch mode exists. Then the excitation has to be expanded in terms of radiative Bloch modes only. The loss mechanism is thus expected to be identical to the one of leaky waves as discussed in Sec. 4.1.3.2.

### 4.5 The Background Concept

In the previous sections, all considerations have been made for the example of a slab waveguide with a 1D periodicity in propagation direction $e_x$ and with homo-
geneous cladding layers. It was shown that the light-line of the cladding material separates the band diagram into two frequency regions of ‘no’-loss and loss, respectively. To be more precise, in Sec. 4.4.2 we have seen that oscillatory field components of the propagating Bloch wave exist in the cladding if a spatial Fourier component \( k_{z,p,3} \) exists if \( k_{z,p,3} = (k_x + pK) < \sqrt{\varepsilon_{\text{cladding}} \omega / c} \). This is the light-line condition (cf. Sec. 2.1.2.6) for slab waveguides with a 1D periodic modulation of the permittivity in the core. But for a substrate-type PhC waveguide, the cladding layers consist of nano-structured material as well and not of a constant permittivity \( \varepsilon_{\text{cladding}} \). Thus the light-line given by the constant permittivity is not necessarily the relevant criterion for the design of low-loss substrate-type PhC waveguides. Furthermore, so far we have not considered a lateral confinement as it is the case for line-defect slab PhC waveguides. This raises the question: what is the relevant criterion for substrate-type PhC waveguides?

### 4.5.1 Failure of the Light Line Concept for Substrate-Type PhCs

Guided modes of the asymmetric slab waveguide (cf. Sec. 2.1.2) and guided Bloch modes of 1D periodic slab waveguide are located below the light-line as discussed in Sec. 2.1.2.6 and in Sec. 4.4. The light-line represents the cutoff condition for the guided modes. The cutoff condition of the ‘guided’ eigenmodes \( m \) of a waveguide system can generally be formulated as [172, p.42]

\[
\varepsilon_m = \max(\varepsilon(r_b)),
\]

where \( r_b \) is the boundary located at infinity and \( \varepsilon_m \) is the effective dielectric constant of the eigenmode \( m \). This condition has been proven in [57] for the case of a homogeneous material at infinity. In other words, a truly guided mode can only be obtained, if the waveguide core has the higher refractive index than the homogeneous material at infinity. Even so, two objections can be raised against condition Eq. 4.61 for substrate-type PhC waveguides: First, Eq. 4.61 implicitly assumes that the dielectric constant at the boundary \( r_b \) can be treated as a homogeneous material. This is clearly not the case for inhomogeneous material, such as a periodic modulation of the permittivity in the order of the wavelength. Secondly, from a practical point of view a mode does not need to be truly guided – a small propagation loss is acceptable for certain applications. It was shown by Kaspar et al. [121] that optical waves can exist that violate Eq. 4.61 and despite of that exhibit very low propagation losses. Kaspar et al. [121] showed that the propagation losses of those modes can be reduced to an arbitrarily low number for the example of a buried rectangular waveguide.

### 4.5.2 The Background Line Concept

So far, the light-line has always been the separatrix between guided (confined) and unguided (unconfined) modes for dielectric waveguides with homogeneous claddings. The background concept is the generalization of this notion of separating guided and unguided modes for inhomogeneous claddings. A mode is guided, if it does not oscillate undamped in the cladding. This is only true, if the dielectric
system at infinity does not support oscillating solutions of Maxwell's equation. The dielectric system at infinity is defined as the background according to Kaspar [121]. The line in the dispersion diagram that separates guided from unguided modes is the background-line. The background-line is identical to the dispersion curve of the fundamental mode of the background system. Kaspar et al. [121] validated the background concept by demonstrating numerically the relevance of the background-line for the case of a 2D buried rectangular waveguide.

The generally applicable methodology of the background concept is illustrated in Fig. 4.16.

Figure 4.16: The methodology of the background concept is explained for the example of the dielectric waveguide, whose cross-section is depicted in (A). There are 9 different areas with a constant refractive index. The background-line is given by the fundamental mode of the background. The background consists of 8 different dielectric systems at infinity as shown in (B): regions I), III), VI) and VIII) are homogeneous materials, whose fundamental mode is given by the line $k = n\omega/c$. Regions II), IV) V) and VII) are planar slab waveguides, whose fundamental mode is given by the dispersion of the TE mode of the slab waveguide. The relevant separatrix – the background-line – is given by the ‘lowest’ dispersion curve.

In the following, we will validate the background concept for a planar slab waveguide with a periodic modulation of the cladding layer – a situation very similar to the one of a substrate-type line-defect PhC waveguide.

### 4.5.3 The Background Line Concept for a Slab Waveguide with a 1D Periodic Substrate

In this section, we investigate the influence of a periodically modulated background on the propagation loss of a waveguide mode. Therefore we study a slab waveguide that has an invariance in lateral direction as discussed in Sec. 4.4. But in contrast to Sec. 4.4 where a 1D periodic modulation in the core layer was analyzed, we now consider a periodic modulation of the substrate layer as shown in Fig. 4.17, (A). The aim of the following investigation is the verification of the claim that the slab waveguide mode is loss-less, if its propagation constant $\beta_x$ is located outside the region of modes with oscillatory fields in the cladding. The region of
Figure 4.17: A) A slab waveguide with an air top-cladding and a periodically modu-
lated substrate layer. The fundamental mode of the substrate layer is computed for 
three different $n_{\text{grating}} = \{1, 1.5, 2.6\}$. For $n_{\text{grating}} = 1$, the relevant separatrix is 
the light-line of air (B). There is no cutoff for a symmetric slab. In (C) the case of a 
weak periodic modulation in the substrate is shown. The Bloch mode of the back-
ground system (the 1D PhC as shown in the insets) has spatial Fourier components 
every Brillouin zone. Therefore the separatrix of the background is periodic with 
$2\pi/a$. As a consequence, the dispersion of the slab waveguide mode intersects 
(cutoff-frequency) the background-line in the second Brillouin zone. (D) shows the 
case of a strong periodic modulation of the substrate. Note that the slab wave-
guide mode is influenced by the periodic substrate: a small photonic band gap 
can be observed for $k_z a/(2\pi) = 0.5$. Furthermore, note that there are two intersection 
points of the slab waveguide mode with the background-line. The slab waveguide 
mode thus has both, a low and a high cutoff-frequency.
modes with oscillatory fields in the cladding is bounded by the background-line. The background-line is given by the fundamental mode of the background system – a 1D PhC in our case.

To theoretically determine the cutoff frequency we need to compute the propagation constant $\beta_x(\omega)$ of the slab waveguide mode and the dispersion curve of the fundamental mode of the 1D PhC. MPB was used for the numerical computation of both dispersion curves. Fig. 4.17 shows the numerically computed background-line (blue) and the dispersion of the slab waveguide mode (red) for $n_{\text{grating}} = 1$ (B), $n_{\text{grating}} = 1.5$ (C) and $n_{\text{grating}} = 2.6$ (D). The insets in Fig. 4.17 (B)-(D) show the dielectric background system and the 'complete' system used to determine the background line and the dispersion of the slab waveguide mode. Figure 4.17 (B) shows the well-known symmetric slab waveguide, where the background line is given by the refractive index of the homogeneous cladding layers. Figure 4.17 (C) and (D) show an exemplary situation for a weak and a strong periodic modulation of the substrate layer, respectively.

According to the background-line concept, the slab waveguide modes are guided in the white regions of Fig. 4.17 (B),(C), and (D), whereas the slab waveguide modes have oscillatory fields in the cladding for the gray regions. The intersection between the background-line and the dispersion of the slab waveguide mode determines the cutoff frequency for a particular waveguide structure. In this way, the cutoff frequency can be computed for a large number of $n_{\text{grating}}$. These cutoff frequencies are plotted in Fig. 4.19 (B) as a function of $n_{\text{grating}}$.

In a next step, we verify that the theoretically computed cutoff frequencies correspond to the frequencies that separate regions of lossy propagation of light from loss-free propagation of light in the slab waveguide for the excitation experiment. Therefore, we numerically excite the slab waveguide as shown in Fig. 4.17 (A) with a specific frequency $\omega a/(2\pi c)$ by using COMSOL. An example of the performed COMSOL simulations is shown in Fig. 4.18 for an excitation frequency $\omega a/(2\pi c) = 0.22$. Figure 4.18 shows the electric field $E_y$ that decays along the propagation direction $x$. The normalized time-averaged Poynting vector is also shown and reveals that energy is radiated into the substrate. From these simulations, we can deter-

Figure 4.18: Electric field obtained by exciting the slab waveguide with a frequency $\omega a/(2\pi c) = 0.25$. 
Figure 4.19: A: Computed propagation loss as a function of the refractive index $n_{grating}$. The mode is guided loss-free for $n_{grating} < 1.9343$. B) shows the theoretically predicted cutoff frequency for a certain $n_{grating}$. The cutoff (red dots) determined by the excitation problem agrees fairly well with the theoretically predicted cutoff frequencies (blue).

mine the cutoff condition $n_{cutoff}$ for a given excitation frequency by computing the propagation loss for various refractive indices of $n_{grating}$. For every $n_{grating}$ the propagation loss $\alpha$ is computed by fitting an exponential function to the time-averaged Poynting vector extracted for $z = d/2$. The computed propagation loss $\alpha(n_{grating})$ as a function of the refractive index is shown in Fig. 4.19 A) for an excitation frequency $\omega a/(2\pi c) = 0.22$. For this frequency $\omega a/(2\pi c) = 0.22$ the cutoff condition $n_{grating} = 1.9343 = n_{cutoff}$ is found. The cutoff condition $n_{cutoff}$ (red dot) from the COMSOL excitation experiment with excitation frequencies $\omega a/(2\pi c) = \{0.155, 0.19, 0.22, 0.25\}$ are added to Fig. 4.19 B) for comparison with the theoretically predicted cutoff frequencies from the MPB simulations: The red dots lie rather accurately on the curve of the theoretically predicted cutoff-frequencies. Therefore, the theoretically predicted cutoff frequencies are identical to the cutoff frequencies obtained empirically from the excitation experiment.

In summary, we conclude that

- If we excite a slab waveguide with a frequency $\omega$, a loss-free guided mode is established if the propagation constant $\beta_x$ of the slab waveguide mode for that excitation frequency $\omega$ is below the background-line.

- The background-line of a periodically modulated substrate is given by the fundamental modes of the 1D PhC.

- The slab waveguide mode is influenced by a strongly modulated substrate layer, such that its dispersion exhibits a small photonic band gap (cf. Fig. 4.17, D).

### 4.5.4 Finite Etch Depth - Approximate Background Line

The background-line concept is only exact if the cladding structure extends to infinity. But, for real slab PhC devices, the periodically modulated cladding layers do
not extend to infinity. To investigate the influence of the finite dimension of the periodic cladding layer, we repeat the excitation experiment from the previous section, but for various depth $d_{\text{grating}}$ of the grating. A homogeneous substrate layer with a refractive index $n_{\text{grating}}$ is added below the periodic layer. The structure is excited with an excitation frequency $\omega a/(2\pi c) = 0.155$. The background-line is the substrate line for the limiting case of $d_{\text{grating}} = 0$. For the infinitely extended cladding layer, i.e., $d_{\text{grating}} \to \infty$, the background-line is given by the fundamental mode of the 1D PhC as we have seen in the previous experiment. The refractive index $n_{\text{grating}} = 3.1$ is chosen, such that the slab waveguide mode is truly guided for $d_{\text{grating}} \to \infty$ and it is cutoff for $d_{\text{grating}} = 0$. We thus expect low propagation losses for $d_{\text{grating}} \to \infty$ and high propagation losses for $d_{\text{grating}} = 0$. The aim of this numerical experiment is to determine the critical depth $d_{\text{grating}}$, for which the waveguide becomes lossy. The experiment is depicted in Fig. 4.20 A). Fig. 4.20 B) shows the computed propagation loss $\alpha$ as function of the depth of the periodic cladding layer $d_{\text{grating}}$. It is observed that very low propagation losses are obtained for $d_{\text{grating}} > 3.7a$. Therefore, the fundamental mode of the 1D PhC is the approximately the relevant separatrix for depths of the grating $d_{\text{grating}} > 3.7a$. Figure 4.20
C) and D) depict the electric field $E_y$ for two different depths $d$. Figure 4.20 C) represents a situation, for which the background-line of the 1D PhC is the approximate separatrix. A wave propagates in the core layer. There is continuous radiation in the substrate, however, the majority of the observed radiation into the substrate in Fig. 4.20 C) originates from the mode conversion from the excitation profile at the input and the slab waveguide mode. Fig. 4.20 D) represents a situation, for which the substrate line is the approximate separatrix. The propagating wave in the core layer of Fig. 4.20 D) is decaying in propagation direction.

We conclude that a finite-sized periodically modulated cladding layer connected to the core of the slab waveguide can guide the light if the cladding layer is sufficiently thick.

Figure 4.21: The membrane-type W1 PhC waveguide is shown in the middle. The different background systems are determined for the cross-section of the W1 PhC waveguide and are arranged around the W1 PhC waveguide. We can eliminate the backgrounds IV) and V) from the list of relevant backgrounds if the W1 PhC waveguide is operated within the PhC band gap of the 2D PhC. The relevant separatrix thus given by the light-line of air (background I-III and VI-VIII).
Figure 4.22: The substrate-type W1 PhC waveguide is shown in the middle. The different background systems are determined for the cross-section of the W1 PhC waveguide and are arranged around the W1 PhC waveguide. We can eliminate the backgrounds IV) and V) from the list of relevant backgrounds if the W1 PhC waveguide is operated within the PhC band gap of the 2D PhC. The relevant separatrix is given by background VII).

4.5.5 The Background Line Concept Applied to Line-Defect Slab PhC Waveguides

In this section, we deduce consequences from the above elaborated background line concept for line-defect slab PhC waveguides. We start by considering a membrane-type line-defect PhC waveguide as shown in Fig. 4.21. The background of this system is determined by using the methodology as demonstrated in Fig. 4.16. Therefore, we consider the permittivity at infinity for the cross-section of the W1 PhC waveguide. The background system is shown in Fig. 4.21 I)-VIII). If the membrane-type W1 PhC waveguide is operated within the photonic band gap of the 2D PhC (Fig. 4.21 IV) and V)), then only homogeneous air layers remain at infinity and the background-line is the air light-line. The light-line of air can be used to identify guided modes in the numerically obtained band diagrams of the PhC waveguides: guided modes of the W1 PhC waveguide have to be located below the air light-line.

The background analysis is more complicated for a substrate-type W1 PhC waveguide as shown in Fig. 4.22. The background system is shown in Fig. 4.22 I)-
VIII). If the W1 PhC is operated with a frequency within the photonic band gap of the 2D slab PhC (Fig. 4.21 IV-V), then the background-lines of the backgrounds IV and V) are irrelevant. The background-line is thus either given by the air claddings or the backgrounds VI-VIII). To determine the relevant background-line, we need to numerically compute the eigenfrequencies for all possible wave vectors \( \mathbf{k} = (k_x, k_y, k_z) \) of the infinitely extruded 2D PhC waveguide (the dielectric waveguide shown in VII) in Fig. 4.22) and also for the 2D PhCs (VI) and VIII) in Fig. 4.22). Thereafter, the separatrix from this background is defined by the lowest frequencies \( \omega(k) \).

The sampling of the 3D wave vector space is accomplished as follows. First we sample the ‘in-plane’ wave vector space, since there we can restrict us to the border of the irreducible Brillouin zone for the 2D W1 PhC waveguide. This yields the ‘in-plane’ wave vectors \( k_x \) and \( k_y \). Then we continuously increase the ‘out-of-plane’ wave vector \( k_z \to \infty \). Fig. 4.23 (left) shows the computed eigenfrequencies \( \omega(k) \) for the supercell as shown in the inset. The parameters of the PhC W1 waveguide are: \( n_{\text{hole}} = 1, n_{\text{InP}} = 3.15 \) and \( r = 0.34 \cdot a \). It can be seen that the lowest eigenfrequencies are obtained for \( k_z = 0 \). This reduces the numerical effort substantially: Instead of sampling the 3D wave vector space, the background-line can be obtained by computing only the band diagram for the ‘in-plane’ 2D PhC waveguide (\( k_z = 0 \)).

The background-line has to be compared to the spatial Fourier components \( k_{x,m} \) of the Bloch mode of the slab W1 PhC waveguide. Therefore, we only plot the background-line \( \omega(k_z) \) as a function of the wave vector in propagation direction. Figure 4.23, right) shows the background-line (red) and the light-line of the substrate material and the light-line of the air cladding. The background-line lies below the air light-line and slightly above the light-line of the substrate material. The photonic band gap of our InP/InGaAsP/InP system is indicated by the two horizontal lines in Fig. 4.23 (right). A truly gap-guided PhC waveguide mode has to lie below the background-line and within the photonic band gap. For our material system, the background-line is far away from the photonic band gap. As a consequence, it is not expected that low-loss propagation (truly guided modes) can be obtained for substrate-type line-defect PhC waveguides in our material system.

### 4.6 Full 3D Simulation of a Membrane-Type W1 PhC Waveguide

The aim of this section is to verify the set of hypotheses made in Sec. 4.2 by means of numerical 3D simulations. Full 3D simulations allow to inspect the fields of a realistic PhC waveguide. Note that the presented p-FEM Method in chapter 3 currently supports only 2D systems and thus cannot be employed here. Instead we used the 3D FDTD method, which is derived from first principles - i.e., no questionable assumption or simplifications have been made. The only remaining inaccuracy originates from the discretization of the problem. However, the inaccuracy can be reduced to an arbitrary low number by simply increasing the resolution of the mesh. In the following section we investigate the fields of a membrane-type W1 PhC waveguide by means of full 3D FDTD simulations. The membrane-type W1
Figure 4.23: Left: W1 PhC waveguide modes of the background for $n_{InP}$ and air holes. The lowest frequencies are found for $k_z = 0$. Right: the background-line (red) of a substrate-type W1 PhC waveguide for the material system InP/InGaAsP/InP. The background-line is only slightly above the light-line of the substrate material $n_{InP}$.

PhC waveguide is used as an illustrative example, because the background-line is known – it is the air light-line. The dispersion of the PhC defect mode has frequency regions ‘above’ and ‘below’ the air light-line. Therefore, it is possible to study the behavior of a PhC waveguide above and below the background-line. The waveguide is excited once with an excitation frequency, for which guided Bloch modes exists (below the light-line) and once for an excitation frequency beyond the cutoff (above the light-line).

### 4.6.1 Setup of the Membrane-Type W1 PhC Waveguide Simulation

The membrane-type W1 PhC waveguide is based on a triangular lattice of air holes ($n_{holes} = 1$) with a radius $r = 0.3016 \cdot a$ in a planar Si ($n = 3.4$) slab of thickness $t_{core} = 0.6 \cdot a$ and with lattice constant $a = 435 \text{nm}$. The thickness of the slab supports only one fundamental TE-like PhC waveguide mode in the vertical direction. The waveguide is excited by a continuous wave source with a spatial Gaussian mode profile (cf. Sec. 5.2.2). Two different frequencies $\omega a/(2\pi c) = 0.275$ (below the light-line) and $\omega a/(2\pi c) = 0.305$ (above the light-line) are applied. The photonic wire input access waveguide is $10 \cdot a$ periods long and has a width of $w = \sqrt{3}a - 2 \cdot r$.

Figure 4.24: 3D visualization of the simulated membrane-type W1 PhC waveguide. The PhC waveguide is 30 periods long.
This length of the photonic wires guarantees that a settled guided mode is established in the photonic wire to excite the PhC waveguide (cf. Sec. 5.3.4.3). The computational domain is surrounded by a PML layer of thickness $t_{PML} = a$ except for the propagation direction where the PML layer has a thickness $t_{PML,x} = 3 \cdot a$. The air cladding layers have a thickness of $t_{air} = 2 \cdot a$. The grid resolution is $a/20$. The simulation setup is very similar to the one described in Sec. 5.2.2 and thus the reader is referred to chapter 5 for further details about mode settling and accuracy considerations.

### 4.6.2 Radiating Spatial Fourier Component Above the Light Line

In Sec. 4.4 we derived the modes of a slab waveguide with a periodic modulation of the permittivity in the core. We could show that a guided Bloch mode is obtained, if all spatial Fourier components of the Bloch mode are located below the air light-line. The purpose of this investigation is to verify that this conclusion also holds for a 2D periodic modulation in the core of the slab waveguide. As opposed to the analytical investigation, where we had a direct access to all transverse mode profiles for each spatial Fourier component, we only obtain the summation of all the transverse mode profiles as schematically shown in Fig. 4.15. We cannot decompose the resulting field pattern in guided and radiative Bloch modes, since we do not know the analytical form of the modes for a slab W1 PhC waveguide. Nevertheless, we can access the spatial Fourier decomposition of the resulting field pattern. By computing the 2D Fourier transform for horizontal planes at discrete points $z_i$ along the transverse direction $e_z$, we can follow the behavior of the spatial Fourier component in the cladding layer. If the spatial Fourier component disappears for larger numbers of $z$, then the fields in the cladding for that particular wave vector component is decaying. If the spatial Fourier component stays constant as a function of $z$, then the fields in the cladding are oscillatory.

The wave vector components of the magnetic fields $H_z(x, y, z_i)$ for the hori-

![Figure 4.25](image-url) Even TE-like mode of a silicon membrane PhC W1 waveguide computed with the 3D MPB. We have chosen two sample frequencies ($\omega a/(2\pi c) = 0.275$ and $\omega a/(2\pi c) = 0.305$) to represent the situation above and below the light-line.
Figure 4.26: Comparison between the mode solutions above and below the air light-line. A) shows a vertical cross section of the dielectric constant. The white horizontal lines indicate the horizontal cross sections, which have been taken to compute the 2D Fourier transform. The 2D Fourier transform is shown in B) and C) for the case of above and below the air light-line respectively. The different rows correspond to two different color scaling schemes (1st row: optimum color scaling, 2nd row: fixed color bar). The white circle indicates the location of the light cone. D) shows two different plots of the magnetic fields.
horizontal cross sections $z_i$ for two distinct frequencies are compared: one frequency represents the situation below the air light-line ($\omega_a/(2\pi c) = 0.275$) whereas the other frequency is chosen, such that it shows the situation above the air light-line ($\omega_a/(2\pi c) = 0.305$). The location of the two frequencies in relation to the photonic band of the PhC W1 waveguide is shown in Fig. 4.25. For the comparison, we compute the 2D Fourier transform of four different horizontal cross sections ($z_i = \{0 \cdot a, 0.65 \cdot a, 1.15 \cdot a, 1.95 \cdot a\}$) for a $10 \cdot a$ long waveguide section (ranging from 15 periods after the input interface to 5 periods before the output interface). The heights $z_i$ of the cross sections are indicated by the white horizontal lines in Fig. 4.26 A). Figure 4.26 shows a vertical cross section of the dielectric constant. Figure 4.26 B) shows the Fourier transforms for $\omega_a/(2\pi c) = 0.275$ (i.e., below the light-line) and Fig. 4.26 C) is for $\omega_a/(2\pi c) = 0.305$ – i.e., above the light-line. For each of the two cases, the Fourier transform is plotted using two different color schemes: in the first row the color is scaled to the maximum value of the 2D Fourier component of each cross section to show the relative weights of the Fourier components within a cross section. The second row uses a fixed color scheme (scaled to the maximum value of all cross sections) in order to enable a quantitative comparison between the cross sections. From the fixed color scheme plots, it can be seen that the Fourier components decay quickly if they are located outside the core of the PhC waveguide ($|z| > 0.3 \cdot a$). The plots of the first row additionally reveal that the further away the components are from the air light cone (indicated by a white circle), the faster they decay in the air cladding layer: e.g., the component in B) that is closest to the light-line decays rather slowly compared to the other components. In Fig. 4.26 C) one of the Fourier components is located inside the light cone. This component is so weak that it can hardly be seen in the first two plots of the top row of Fig. 4.26 C). However, because this Fourier component does not decay (note the color bar of the last two plots of the first row of Fig. 4.26 C) the component suddenly becomes visible as the other components vanish with increasing distance from the waveguide core.

Finally, Fig. 4.26 D) shows the magnetic field on the cross-section for the case below the light-line (left) and above the light-line (right). Both vertical mode profiles are similar for both modes: The light is nicely confined to the core of the PhC waveguide. The similarity implies that the radiation above the light-line is still very weak, such that it cannot be seen in a regular field plot. The visualize the difference between ‘above’ and ‘below’ the light-line we compute the isoline plots. Isoline plots are better suited to reveal small differences. The isoline plots show a clear difference between the two field plots. For instance, a unique feature for $\omega_a/(2\pi c) = 0.305$ (rightmost plot in Fig. 4.26D)) is the oval-shaped blue isoline spanning over the whole plot. This line suggests an oscillatory part of the excited mode in the cladding layer.

The numerical experiments confirm a few statements made earlier: firstly, the Fourier component located inside the air light cone is weak (cf. Sec.2.2.3.1) and hence the out-of-plane radiation is weak too. Secondly, the Fourier components decay the faster the further away they are located from the air light cone (cf. Eq. 4.44). The Fourier component located inside the air light cone does not decay (cf. Eq. 4.44). As a conclusion, the prediction of Sec. 4.4.2 that only the spatial Fourier component located above the light-line has an oscillatory solution also holds for the 3D
membrane-type W1 PhC waveguide.

4.6.3 Exponential Decay of the Fourier Components in the Cladding

We obtained exponentially decaying fields in the cladding for the transverse function $e(z)$ for the spatial Fourier components $k_{x,m}$ below the light-line for the simplified slab waveguide of Sec. 4.4. The aim of this experiment is to verify, if the transverse functions $e(z)$ for the spatial Fourier components $k_{x,m}$ below the air light-line also decay exponentially with $z$. In the following the 2D Fourier transform for seven equally spaced cross-section along the out-of-plane direction $e_z$ are computed. The first two plots in Fig. 4.27 show an exemplary wave vector plane in the center of the membrane-type W1 PhC waveguide ($z = 0$) for the two cases of below ($\omega a/(2\pi c) = 0.275$) and above ($\omega a/(2\pi c) = 0.305$) the light-line. For every point in the wave vector plane an exponential fit is performed to determine the decay constant $k_{z,m,2}$. The obtained decay constant $k_{z,m,2}$ is shown in the second

![Figure 4.27: Verification of the exponential decay. Top row: the 2D FFT of the magnetic field $H_z(x, y, z = 0)$ for a horizontal plane ($z = 0$). Center row: transverse wave number $k_{z,m,2}$ obtained by exponential fits. Bottom row: coefficient of determination of the fits (1 denotes a perfect exponential behavior, wheres 0 signifies a non-exponential behavior).](image-url)
row of Fig. 4.27. Note that the decay constant $k_{x,m,2}$ increases for larger wave vectors $k_{x,y,m} = (k_{x,m}, k_{y,m})$. However, an additional pattern of vertical lines can be observed in these plots. These lines originate from the $\sin(x)/x$-shaped spectral artifact of the Fourier transform along the $k_x$-axis that has values close to zero for the same $k_x$-values. This translates into a pattern of lines of zero-values perpendicular to the $k_x$-axis. In order that an exponential decay of the transverse function in the cladding can be diagnosed, a large ($\approx 1$) coefficient of determination of the fit is required. The lowest row shows the coefficient of determination for each of the exponential fits. The dark red area in the coefficient of determination plot are values very close to 1, which signifies an extraordinarily good exponential behavior. Of course, the zero-lines result in a poor coefficient of determination and thus the vertical line pattern is also visible in the coefficient of determination plot. Note that a particularly poor coefficient of determination is obtained for the Fourier component which is located within the air light cone ($k_y \approx 0 - 0.2, k_x \approx 0.25$) for $\omega a/(2\pi c) = 0.305$. This spatial Fourier component of the Bloch wave does not decay exponentially in the cladding but appears to be rather constant along the $z$ direction. This indicates an oscillatory transverse function $e(z)$ in the cladding.

We verified the hypothesis that the form of the transverse function $e(z)$ of spatial Fourier components of the Bloch mode of the W1 PhC waveguide is essentially the same as for the slab waveguide with a 1D periodic modulation of the permittivity in the core (as discussed in Sec. 4.4).

### 4.6.4 Backward Radiation

So far, we only discussed the form of the possible solutions of Maxwell’s equation of the slab PhC waveguide that turned out to be similar to the ones of the simplified problem discussed in Sec. 4.4. Here, we investigate the radiation observed from the membrane-type W1 PhC waveguide if excited beyond the cutoff. In the illustration of Fig. 4.14 and Fig. 2.19, the radiating Fourier component in the first Brillouin zone is drawn in the negative wave vector plane due to two reasons: First, the wave vectors are expected to be equally spaced by $2\pi/a$ because of the 1D periodicity. Secondly, the strongest Fourier component is expected to roughly follow to the light-line of the core index material $\omega = ck_n$ and thus is usually located in the 2nd Brillouin zone (cf. Sec. 2.2.3.1). It follows that actually no noteworthy Fourier component is found in the interval $[0..k_x a/(2\pi)]$ that is usually used for the Bloch diagram plots. Instead, the Fourier component that potentially is located above the light line, is found in the first Brillouin zone in the negative wave vector space (i.e., within the interval $[-k_x a/(2\pi)\ldots0]$). As a consequence, oscillating fields in the cladding should have a negative wave vector and thus should propagate in the backward direction.

We can confirm this behavior by the 3D FDTD simulation. In Fig. 4.28 the Poynting vector is computed for an excitation frequency above the light line ($\omega a/(2\pi c) = 0.305$) for two horizontal planes: one plane is intersecting the center of the membrane PhC waveguide and the other one has a constant $z$-component equal to $z = 2.2 \cdot a$. The lengths of the arrows representing the Poynting vector have been scaled by a constant factor such that they are visible in the plot. Fig. 4.28 (A) shows
that the energy flow is strongly confined to the PhC waveguide core for the plane \( z = 0 \). For the horizontal plane in the cladding \((z = 2.2 \cdot a)\), however, the Poynting vector directs in the \(-x\) direction: a backward radiating wave can be observed. The vertical cross-section going through the center of the W1 PhC waveguide \((y = 0)\) reveals an additional \( z \)-component of the Poynting vector. Note that the periodicity of the wave is longer than the periodicity of the PhC pattern, which implies a wave vector \( k_{\text{wave}} < \pi / a \), i.e., the wave vector component located in the first Brillouin zone \([[-k_x a/(2\pi), k_x a/(2\pi)]\]). This shows again that the spatial Fourier component in the first Brillouin zone is responsible for the radiation losses of the PhC waveguide above the light-line. Note that already the example of a slab waveguide with a periodically modulated substrate layer (shown in Fig. 4.18) reveals an energy flow in the periodic cladding that is directed into the substrate and in backward
As a conclusion, the FDTD simulations are consistent with the observation in Sec. 2.2.3.1 that the Fourier component in the first Brillouin zone is located in the negative wave vector plane and that this component is responsible for the radiation losses of the PhC waveguide above the light-line.

4.7 Simple Loss Model by Means of Ray Optics

So far, we only discussed to question of “How the light is lost” and “When the light is lost”. But we have not yet discussed “How much light is lost”. Numerical simulations are unavoidable to determine a quantitative propagation loss number. Nevertheless, we try to establish a simple ray optics model to estimate the radiation losses of a PhC waveguide. Ray optics could correctly predict the correct order of magnitude of the radiation losses of leaky waves for simple geometries as the asymmetric slab waveguide [280, 170, pp. 31-42] and for fibers [251, 252, 249]. First we revise the concept for the computation of the propagation losses using a ray optics model for a slab waveguide. Thereafter, we develop a very simple approximate model based on the same concept for the computation of the propagation losses of a PhC waveguide with homogeneous claddings.

4.7.1 Propagation Losses of a Leaky Wave of a Slab Waveguide

It is commonly argued that out-of-plane losses in PhC waveguides originate from the loss of total internal reflection of the vertical slab of the substrate-type PhC waveguide. Total internal reflection refers to a ray model. Therefore, we compute the propagation losses of an asymmetric slab waveguide if operated beyond the cutoff, i.e., the propagation loss of a leaky wave as introduced in Sec. 4.1.2.4. The procedure follows the path of the propagating ray shown in Fig. 4.29.

First, the power reflection coefficient at the interfaces for the two polarizations are computed according to Fresnel’s equations

\[
R_{s,2,3} = |r_{s,2,3}^2| = \left| \frac{n_1 \cos \theta - n_{2,3}}{n_1 \cos \theta + n_{2,3}} \sqrt{1 - \left( \frac{n_1}{n_{2,3}} \sin \theta \right)^2} \right|^2
\]  

(4.62)

Figure 4.29: Ray model illustration of a leaky wave.
\[ R_{p,2,3} = |r_{p,2,3}^2| = \left[ \frac{n_1 \sqrt{1 - \left( \frac{n_1}{n_{2,3}} \sin \theta \right)^2 - n_{2,3} \cos \theta}}{n_1 \sqrt{1 - \left( \frac{n_1}{n_{2,3}} \sin \theta \right)^2 + n_{2,3} \cos \theta}} \right]^2. \] (4.63)

\( R_s \) \((R_p, j)\) is the power reflection coefficient at interface \( n_j / n_j \) for the \( s \) \((p)\) polarization. After the propagation of distance \( l = 2 \cdot d \cdot \tan(\theta) \), the ray undergoes one reflection at the top cladding \( R_3 \) and one reflection at the bottom cladding \( R_2 \). For an initial power of \( P_0 = P(x = 0) \), the remaining power in the core after one round trip is \( P_1 = P_0 R_3 R_2 \) and the lost power is \( P_{\text{lost}} = P_0 (1 - R_3) + P_0 R_3 (1 - R_2) \). The waveguide loss is defined according to Eq. 4.7 by

\[ \text{Loss} = \frac{P_0 - P(z = L)}{P_0}, \] (4.64)

where \( P \) is the power in the core of the slab waveguide. We can write \( P \) as a function of propagation distance \( x \) and angle \( \theta \)

\[ P(x, \theta) = P_0 (R_3(\theta) R_2(\theta))^{x/(2 \cdot d \cdot \tan(\theta))}. \] (4.65)

Asymmetric Planar Slab with \( d=522\text{nm}, n_1=3.35, n_2=3.17, n_3=1 \)

Symmetric Planar Slab with \( d=522\text{nm}, n_1=3.35, n_2=n_3=1 \)

Figure 4.30: Results from the propagation loss computation using the ray model for asymmetric (top row) and a symmetric (bottom row) planar slab waveguide. The Brewster angle \((p\text{-polarization})\) translates to a singularity in the propagation loss figure.
This is an exponential function\(^2\)

\[ P(x, \theta) = P_0 e^{-\alpha x} \quad (4.66) \]

and thus we can determine a propagation loss

\[ \alpha(\theta) = \frac{\ln(R_2(\theta)R_3(\theta))}{2 \cdot d \cdot \tan(\theta)}, \quad (4.67) \]

that can be expressed in \(dB/cm\) by using Eq. 4.11

\[ \alpha_{dB}(\theta) = -\frac{10}{\ln(10)} \alpha(\theta) \quad (4.68) \]

The propagation loss \(\alpha_{dB}(\theta)\) according to Eq. 4.68 is numerically evaluated and plotted in Fig. 4.30 (right-hand plots) for both polarizations for a symmetric (bottom row) and an asymmetric (top row) layer structure. The power reflection coefficients for the interfaces are also shown in Fig. 4.30 (left). There is a root point (Brewster angle) for each interface for the \(p\)-polarization (cf. inset of Fig. 4.30 (left)) that are transformed to two singularities in the propagation loss plot on the right. Further note the scale of the propagation loss axis, which ranges from \(-2 \times 10^{6}\) to 0 dB/cm. In other words, as soon as the total internal reflection condition is not met for one of the interfaces, the propagation losses increase dramatically. The losses increase the more the angle deviates from the critical angle. This model – despite of the large propagation losses – is accurate for the case of asymmetric planar slab waveguides [170]. In other words, operating an asymmetric slab waveguide beyond the cutoff is practically useless.

In case of substrate-type planar PhC waveguides, almost exclusively the weak vertical index contrast is put forward to explain the large propagation losses. Actually, the concept of the light-line is based on it. However, the presented estimation of the propagation loss for a planar slab waveguide beyond the cutoff using the ray model predicts extremely high losses (cf. Fig. 4.30 (right)) that we do not observe in our PhC waveguide structures.

The propagation losses of an asymmetric slab waveguide excited beyond the cutoff are enormous. If the loss of total internal reflection would be the only physical mechanism, then the propagation losses of a substrate-type W1 PhC waveguide would be much larger. We will see that the concept of spatial Fourier components is required – i.e., only a weak spatial Fourier component contributes to loss – to achieve a propagation loss in the same order of magnitude.

### 4.7.2 Estimation of the Propagation Losses of a Membrane Type PhC W1 Waveguide

Knowing that the above elaborated ray model is too simple to approximate the propagation losses of planar slab PhC waveguides, we try to improve our estimate of the propagation losses by accounting for the fact that a Bloch wave can be represented by a sum of propagating plane waves.

\[ A^x = (e^{\ln(A)})^x = e^{\ln(A) \cdot x} = e^{\alpha \cdot x} \text{ with } \alpha = \ln(A). \]
Following assumptions and approximations are made

- The Bloch wave is approximated by two propagating rays. In Fig. 4.14 it can be seen that the two strongest spatial Fourier components are located within the range of \(-k_{InP} < k_{x,m} < k_{InP}\). The strongest spatial Fourier component is located in the second Brillouin zone and has a weight \(\varphi_2(\hat{A}_1)\) and a wave vector \(k_{x,2}\). The other one \((\varphi_{-1}, k_{x,-1})\) is located within the domain of radiation modes \(-k_{Air} < k_{x,-1} < k_{Air}\).

- We assume that the power spectrum of the spatial Fourier components of the Bloch wave is constant along the propagation direction. This directly follows from the Bloch theorem that holds for infinite periodic structures. It is thus reasonable to assume that spatial Fourier expansion of the Bloch wave is approximatively constant for a finitely extended PhC waveguide.

- We approximate the magnitude of the spatial Fourier components of the Bloch wave by the ones obtained numerically from a 2D COMSOL simulation of a W1 PhC waveguide as shown in Sec. 2.2.3.1 for \(k_y = 0\).

We consider a symmetric planar slab \((n_1 = 3.4, n_2 = n_3 = 1)\) of thickness \(t_{core} = 261\, nm\), which corresponds to the design used in Sec. 4.6 (cf. Fig. 4.24). The spatial Fourier component \((\varphi_2, k_{x,2})\) in the second Brillouin zone is always located below the light-line, i.e., the angle \(\theta_2\) of the ray that models the dominant Fourier component is larger than the critical angle \(\theta_c\). The wave vector \(k_{x,-1}\) in \(x\)-direction for the spatial Fourier component in the first Brillouin zone is obtained by the COMSOL simulation and shown in Fig. 4.31. The angle \(\theta_{-1}\) is computed using the relation

\[
n_{core}k_0^2 = k_{-1}^2 + k_y^2 + k_z^2
\]

and \(k_0 = \omega/c\). We distinguish two extreme cases: i) \(k_y = 0\) results in the largest possible angle \(\theta = \pi/2 - \cos^{-1}(k_{-1}/(n_{core}k_0))\) and ii) \(k_z = 0\) results in the smallest possible angle \(\theta = 0\), i.e., the ray is totally internally reflected and a propagation loss of \(\alpha_{dB} = 0\) is obtained.

The requirement of an invariant relative power spectrum for all propagation distances \(x\) was implemented by enforcing

\[
|\varphi_{-1}|^2 / |\varphi_2|^2 = \text{const} = \gamma,
\]

where the power at the input \(x = 0\) is

\[
P(x = 0) = P_0 = |\varphi_{-1}|^2 + |\varphi_2|^2.
\]

The power of the simplified Bloch wave as a function of propagation distance \(x\) is

\[
P(x, \theta) = P_0 \left[ \left( \frac{\gamma}{\gamma + 1} \right) R_3(\theta) R_2(\theta) + \frac{1}{\gamma + 1} \right] \frac{x}{(2d \tan(\theta))}
\]

Because of the resulting power law, we can derive a propagation loss \(\alpha\)

\[
\alpha = \ln \left[ \left( \frac{\gamma}{\gamma + 1} \right) R_3(\theta) R_2(\theta) + \frac{1}{\gamma + 1} \right] / (2d \tan(\theta))
\]
Figure 4.31: Wave vector $k_{-1}$ of the spatial Fourier component of the Bloch wave in the first Brillouin zone A) and the ratio of the weights of the spatial Fourier components $\varphi_{-1}/\varphi_2$ B) obtained by a 2D COMSOL simulation of a W1 PhC waveguide with $n_{\text{eff}} = 2.87$. C) shows the power reflection coefficients for the interface $n_{\text{core}}, n_{\text{Air}}$ for both, p- and s-polarization. The propagation losses $\alpha_{dB}$ computed according to Eq. 4.72 ($\alpha_{dB} = -4.34\alpha$) and with the FDTD method are shown in D).

Fig. 4.31 shows the wave vector of the spatial Fourier component in the first Brillouin zone $k_{-1}$ (A) and the computed ratio of the spatial Fourier components $\varphi_{-1}/\varphi_2$ (B). The reflection coefficient as a function of frequency for both polarizations is shown in Fig. 4.31(C) for $k_y = 0$. The propagation losses $\alpha_{dB} = 4.34\alpha$ are computed for both polarizations and shown in Fig. 4.31 (D). Furthermore, the propagation loss obtained from a 3D FDTD simulation using the cutback method (cf. Sec. 5.3.2) is added for comparison. The accurately computed propagation losses for the TE-like PhC W1 mode has to be compared with the propagation loss $\alpha_{dB}$ for the s-polarization. It can be seen that the simple ray model over-estimates the propagation losses. However, as mentioned above, the propagation loss $\alpha$ for the case of $k_z = 0$ is zero. The real propagation loss is thus expected between the two extreme cases ($k_y = 0$ and $k_z = 0$). The accurately computed propagation loss by the FDTD method lies within that area. Even the trend of both propagation loss curves is similar. But, there is a difference in the cutoff frequency. This originates from the fact that the 2D COMSOL approximation with an effective refractive index of $n_{\text{eff}} = 2.87$ is not able to accurately model the frequency behavior for all frequencies.

We conclude that the propagation losses computed with this simplifying ray model deliver propagation loss values with the correct order of magnitude and the correct frequency trend as the one from the 3D FDTD simulation. This is an indication that the radiation losses are approximatively proportional to the relative weights $|\varphi|^2$ of the power spectrum of the propagating wave.

### 4.8 Conclusions

In this chapter, we discussed the loss mechanism in slab PhC waveguides. We saw that the conventional approaches based on perturbation theory cannot adequately handle systems with strong periodically modulated permittivities. Instead, we for-
mulated a new hypothesis about the loss mechanism in slab PhC waveguides. The hypothesis was substantiated by a number of numerical experiments. We were able to find many indications that support the claims made in I.) and II.) of Sec. 4.2. The perturbation model of a weak periodic wall distortion function developed by Marcuse [167] as well as the simple ray model developed in Sec. 4.7 support the claim 3.) of Sec. 4.2. Even so, a simple quantitative description of the radiation losses for slab PhC waveguides is still missing. We have reasons to believe that an analytical formula for such a description cannot be given. At the moment, advanced numerical methods have to be employed to accurately determine the radiation losses of substrate-type PhC waveguides.

Let us briefly review the citations on page 99 of Krauss [137] mentioned at the beginning of the chapter. We list them again

• «Out-of-plane leakage is the dominant loss mechanism for heterostructure waveguides. As all waveguide modes are situated above the light-line, there is always the possibility of coupling to radiation modes. In simple terms, the origin of these losses is a) the lack of waveguiding in the holes, with resulting diffraction loss and b) the fact that the holes are not etched sufficiently deeply, so the tail of the mode radiates into the substrate.»

• «All of the models conclude, that low-loss propagation above the light-line is indeed possible and that current waveguide designs are not yet optimized. The key parameters to improve are diffractive loss at the holes (reduced by smaller hole size), scattering into the substrate (reduced by deeper holes) and improvement of the waveguide geometry, away from the current asymmetric surface waveguides.»

According to our understanding, the dominant loss mechanism in substrate-type PhC waveguide is of a completely different nature. The loss mechanism consists of exciting a Bloch wave beyond the waveguide cutoff. A slab PhC waveguide is excited beyond cutoff, if one or more of the spatial Fourier components of the Bloch mode are situated above the background line. We consider the ‘lack of waveguiding in the holes’ to be irrelevant. For instance, ‘lack of waveguiding in the holes’ would be equally relevant for membrane-type PhC waveguides operated below the light-line. However, those waveguides have very low propagation losses. The experiment shown in Fig. 4.11(E) also shows that loss-less propagation of light is possible for slab waveguides with periodic holes penetrating through the core of the slab waveguide. On the other hand, we agree with the statement that insufficiently deeply etched holes result in an increased propagation loss. However, our explanation is quite different from the one cited above. We have shown in Sec. 4.3.3 that the holes (or their tails) cannot be treated as individual scatterers whose scattered powers add up hole by hole. Instead, the loss mechanism is related to the fact that the background line is only a strict separatrix for an etching depth \( d \rightarrow \infty \). For \( d < \infty \), the optical mode receives a weak oscillatory tail and is, strictly speaking, no longer a guided mode. The deeper we etch, the closer we are to a guided mode and the smaller are the propagation losses.

The proposed strategy to reduce the hole size to reduce the diffraction losses is not justified. The experiments shown in Fig. 4.11 demonstrate that there are cases, where increasing the size of the holes reduces the propagation loss. Relevant for
the propagation losses are only the relative magnitudes $|\varphi|^2$ of the spatial Fourier components of the Bloch mode above the background line.

Increasing the etch-depth reduces the propagation losses. But opposed to common belief, an infinitely deeply etched hole does only result in a loss free PhC waveguide mode, if all spatial Fourier components of the Bloch mode are situated below the background-line. Otherwise, a finite propagation loss persists even for infinitely deeply etched holes.

No predictions for the propagation losses of an asymmetric vertical layer stack can be deduced from the hypothesis. However, in a slab waveguide, the asymmetric layer structure introduces a cutoff frequency. A larger asymmetry tends to increase the cutoff frequency. We cannot give a conclusive answer at this point, but we will discuss this proposal for reducing the propagation losses later in Sec. 6.3.3.1.

As opposed to the other models referred by Krauss [137], our hypothesis suggests that low-loss propagation above the background line is very hard to achieve. The key parameters to reduce the propagation losses are:

- **Reduce the relative magnitudes of the spatial Fourier components of the Bloch mode that are located above the background-line.** An example of a PhC waveguide, which has a very small Fourier component above the background-line is the W3 PhC waveguide. In chapter 7, the proposed strategy is used to reduce the propagation losses of substrate-type PhC waveguides.

- **Shift the background-line to higher frequencies by engineering the PhC pattern of the background system.** This can be achieved, for example, by reducing the width of the PhC waveguide in the background or by increasing the refractive index contrast between the core and the cladding layers. In chapter 7 it is shown that the propagation losses of substrate-type PhC waveguides can be reduced considerably by modifying the radius of the holes in the substrate. Furthermore, an ultra low-loss PhC waveguide design can be obtained if narrow vertical slabs are used as the cladding layers. This waveguide design is presented in chapter 8.
Computation of the Propagation Losses of Line-Defect PhC Waveguides

A part of this chapter is published in Ref. [117].

Experimentally measured propagation losses range from less than 10 dB/cm [203, 173, 60] for single-mode membrane-type W1 PhC waveguides up to about 1800 dB/cm [295] for substrate-type W1 PhC waveguides. The propagation losses strongly depend on the design of the slab PhC waveguide as well as on fabrication imperfections (cf. Chapter 6). Reducing the propagation losses of substrate-type PhC waveguides is of key importance for the successful implementation of active PhC devices. The losses may be reduced by an optimization of the PhC device design and/or the fabrication process. An optimization by numerical means is preferred since it is faster and allows to investigate designs that are important for understanding the origin of the propagation losses, but are challenging to fabricate. For this purpose an numerical method has been developed that accurately models the propagation losses. Large 3D simulations are inevitable for the accurate modeling of the propagation losses in substrate-type line-defect PhC waveguides.

The chapter is organized in the following way: In Section 5.2, we motivate the numerical cutback-method to be used in combination with the FDTD method. In section 5.3 we present the numeric results from the proposed cutback-method. We perform a verification by applying the method 1) to numeric results of a membrane-type W1 PhC waveguide that is reported in literature and 2) to experimental measurements of a substrate-type W1 PhC waveguide. We discuss the frequency range of validity limited by estimating the errors made by the cutback-method and the error made by approximations (such as hole shape discretization and mode settling) used in the FDTD model.
5.1 Introduction

Propagation losses of PhC waveguides have been investigated numerically using various methods and an overview is compiled in Table 5.1. The dominant loss mechanism in substrate-type line-defect PhC waveguides is out-of-plane radiation due to the excitation of the line-defect PhC waveguide beyond the cutoff (cf. Chapter 4). Methods that operate in-plane (two dimensions) may be employed exclusively to waveguides, for which out-of-plane radiation is negligible such as membrane-type PhC waveguides operated below the air light-line. For this particular case, 2D methods have successfully been applied to investigate in-plane loss mechanisms, such as the Green function tensor method (GFT) \[95\] to investigate backscattering originating from disorder and the multiple multipole method (MMP) to compute the lateral radiation leakage \[247\]. But for the accurate modeling of the propagation losses in substrate-type line-defect PhC waveguides, 3D simulations are inevitable.

Numeric methods operating in two-dimensions using effective refractive indices \[70, 71, 19\] or relying on simplified assumptions – such as the guided-mode expansion method (GME) \[7, 76, 8\] – are not capable to cover the complexity of the propagation losses of substrate-type PhC waveguides. Particularly for those methods a comparison to experimental measurements is required to draw a conclusion about the accuracy of the employed method. However, Table 5.1 shows that quantitative comparisons of the obtained numeric results to experimentally obtained data for the propagation losses are rarely published. Actually, we are only aware of one comparison between numerically obtained propagation losses to experimentally measured values for the InP/InGaAsP material system by Sauvan et al. \[232\]. They measured propagation losses ranging from \(500 - 900\) dB/cm compared to \(250 - 500\) dB/cm obtained by the Fourier modal method (FMM).

In this chapter, we exclusively apply the finite difference time domain method (FDTD) aiming to accurately reproduce the experimentally obtained propagation losses of our PhC waveguides. There are mainly two different approaches to compute the propagation losses using FDTD \[270\]: one A) is based on the computation of the transmission \[47, 150, 60, 141\] through a long PhC waveguide and the other one B) on the computation of resonances in a super-cell \[141\]. The latter approach B) requires less memory, since the computational domain consists of only one period \(a\) in propagation direction. For the super-cell approach, the propagation losses are determined either by computing the quality factor \(Q\) and the group velocity \(v_g\) of the resonant modes \((\alpha = \omega_0/Qv_g)\) or by computing the ratio of out-of-plane power loss \(P_\perp\) to propagating power \(P_t\) \((\alpha = -\log(1 - P_\perp/P_t)/a)\). Above the light-line, as in the case of substrate type planar PhC waveguides, the method using the ratio of powers deviates considerably (in the order of \(400\) dB/cm) from the quality factor method \[140\]. The discrepancy is explained by the fact that the power ratio method only comprises out-of-plane radiation, whereas the quality factor method accounts for all loss mechanisms, such as in-plane backscattering. The quality factor method additionally requires a separate computation of the group velocity, which has to be re-performed for any variation of the hole shape. Furthermore, applying the FDTD

\[The\ GEM\ is\ based\ on\ a\ perturbation\ theory\ approach\ [201, 200]\ and\ relies\ on\ a\ weak\ periodic\ perturbation\]
Table 5.1: Numerical methods to compute the propagation losses of PhC and PhC waveguides. Note that only in three references a comparison of the simulated propagation loss to experimental data is made. To the best of our knowledge, the only comparison between numerical and optically measured propagation losses for our material system has been done by [232]. The numerically obtained propagation losses were about 50% lower then the measured propagation losses.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Method</th>
<th>Dimension</th>
<th>Investigated Effects</th>
<th>PhC WG</th>
<th>Material System</th>
<th>Measurements</th>
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<td>[95, 144]</td>
<td>GFT</td>
<td>2D</td>
<td>disorder, (backscattering)</td>
<td>X</td>
<td>Si membrane</td>
<td>sim: 30−1000 dB/cm meas: 30−1000 dB/cm</td>
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<td>2D/3D</td>
<td>etch depth</td>
<td>AlGaAs/GaAs</td>
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<td>sim: 250−500 dB/cm meas: 500−900 dB/cm</td>
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<td>InP/InGaAsP</td>
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<td>surface roughness</td>
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<td>2D/3D</td>
<td>hole-depth</td>
<td>GaAs/AlGaAs (substrate)</td>
<td>trans</td>
<td></td>
</tr>
<tr>
<td>[18]</td>
<td>ε''</td>
<td>2D</td>
<td>intrinsic</td>
<td>GaAs/AlGaAs</td>
<td>trans</td>
<td></td>
</tr>
<tr>
<td>[247]</td>
<td>MMP</td>
<td>2D</td>
<td>radiation leakage</td>
<td>X</td>
<td>Si membrane</td>
<td></td>
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<tr>
<td>[131]</td>
<td>FEM</td>
<td>3D</td>
<td>intrinsic</td>
<td>X</td>
<td>n = 1.45/2.3</td>
<td></td>
</tr>
<tr>
<td>[83]</td>
<td>FDFD</td>
<td>3D</td>
<td>intrinsic</td>
<td>X</td>
<td>AlOx/AlGaAs</td>
<td></td>
</tr>
<tr>
<td>[113]</td>
<td>FDTD</td>
<td>2D/3D</td>
<td>intrinsic, hole-depth</td>
<td>InP/InGaAsP</td>
<td></td>
<td></td>
</tr>
<tr>
<td>[47]</td>
<td>FDTD</td>
<td>3D</td>
<td>intrinsic</td>
<td>X</td>
<td>Si membrane</td>
<td></td>
</tr>
<tr>
<td>[150]</td>
<td>FDTD</td>
<td>3D</td>
<td>intrinsic</td>
<td>X</td>
<td>SOI (symmetric) sim: 1000 dB/cm meas: 1000 dB/cm ±200 dB/cm</td>
<td></td>
</tr>
<tr>
<td>[60]</td>
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<td>3D</td>
<td>intrinsic</td>
<td>X</td>
<td>SOI</td>
<td>trans</td>
</tr>
<tr>
<td>[141]</td>
<td>FDTD</td>
<td>3D</td>
<td>intrinsic</td>
<td>X</td>
<td>GaAs/AlGaAs, all types</td>
<td></td>
</tr>
<tr>
<td>[39]</td>
<td>FDTD</td>
<td>3D</td>
<td>intrinsic</td>
<td>X</td>
<td>Si membrane</td>
<td></td>
</tr>
<tr>
<td>[67]</td>
<td>FDTD</td>
<td>3D</td>
<td>hole-depth</td>
<td>X</td>
<td>InP/InGaAsP</td>
<td></td>
</tr>
<tr>
<td>[34]</td>
<td>FDTD</td>
<td>3D</td>
<td>finite-depth, conical holes</td>
<td>lithium niobate</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Legend. trans: transmission measurements, loss: propagation loss measurements
method in super-cells requires a careful investigation on where to place the source and the detectors in order to excite and detect all relevant modes [259]. Since we want to provide a tool that can eventually account for non-periodic lattice disorder (among other imperfections), we follow the first approach. To study the effect of imperfect hole shapes on the propagation losses, a three dimensional model is required. Both constraints, the three dimensionality and the long waveguides, lead to long simulations, and therefore the memory consumption and the simulation runtime are the limiting factors of the accuracy of our FDTD model (cf. Sec. 5.3.4.4). An advantageous feature of FDTD and other time domain methods is that only one simulation run is required to compute a large frequency spectrum if a broad-band pulse is propagated through the structure. We use the freely available MEEP program developed at MIT [206], which can be run on large distributed memory systems. A main limitation of brute-force methods, such as FDTD and FEM is that weak perturbations, such as surface roughness or small variations in radius and lattice disorder require a very fine resolution of the mesh to capture the small geometrical variations. In this case, semi-analytical methods in conjunction with coupled-wave theory are better suited [106].

5.2 The Cutback-Method

The numerical cutback-method is motivated from optical measurements. Experimentally, mainly two methods are applied to measure the waveguide propagation losses. The Fabry-Perot method relies on fringes originating from multiple reflections in a waveguide resonator and on known power reflection coefficients at the interfaces. Pronounced Fabry-Perot fringes are obtained for resonating structures

![Figure 5.1: The SEM image shows five PhC W1 waveguides of different lengths with the access trench waveguides. The cutout shows the cutback-method as it is used for the propagation loss characterization of the PhC W1 waveguides.](image)
having both, low propagation losses and substantial reflections at the waveguide interfaces. Typically, the interfaces consist of the cleaved chip facets having a power reflection coefficient of typically $\approx 30\%$. However, if the waveguide losses are large enough to damp the multiple reflection paths, the Fabry-Perot method is inadequate due to the weak fringe contrast. In this case the cutback-method can be applied. The cutback-method requires the measurement of the transmitted power of multiple waveguides of different lengths $L_i$ instead of only one waveguide. For our high-loss substrate-type PhC waveguides the cutback-method is better suited. Multiple reflections potentially arising at all transitions (access waveguide / PhC waveguide, chip facet) are sufficiently suppressed to be neglected. An quantitative analysis of the reflection coefficients and the propagation losses of dielectric waveguides is made in Sec. 5.3.4.1 to answer the question of ‘When the cutback-method can be applied?’

The cutback-method was one of the first experimental methods applied to measure the attenuation of light in a fiber. The idea is to use at least two fibers of the same type but of different length. If the shortest fiber is long enough to guarantee that the guided mode is well established and in case of negligible reflections within the waveguide, then the power attenuation can be obtained by

$$\text{Loss [dB/cm]} = \alpha_{dB} = 10 \log_{10} \left( \frac{P_2}{P_1} \right) / (L_2 - L_1), \quad (5.1)$$

where $P_1$ and $P_2$ are the transmitted powers and $L_1$ and $L_2$ the lengths of the short and the long fiber, respectively. Nowadays, the cutback technique is widely applied in integrated optics to characterize lossy optical devices [196, 173]. One reason is that the cutback-method allows to subtract all possible influences of the access structure as well as the coupling coefficients, because whatever factor appears in one measurement, it also appears in the other measurement. This property of the cutback technique is essential for our numeric model, since it also eliminates the unknown behavior of the trench waveguide / PhC waveguide interfaces. Theoretically, only two PhC waveguides of different length are required. Nevertheless, in our optical experiments more than two PhC waveguides of different length are used to increase the accuracy and to reduce measurement noise. Figure 5.1 shows the integrated W1 PhC waveguides that are used for the cutback measurements. In the following, we apply this technique to numerically computed power transmissions. Two different types of cutback approaches are presented in Secs. 5.2.4 and 5.2.5.

### 5.2.1 The Exponential Decay

The cutback-method relies on an exponential power decay as a function of propagation distance of the propagating wave. Many loss mechanisms in dielectric waveguides, such as absorption losses and scattering losses originating from small geometrical imperfections, are well described by an exponential power decay as a function of distance (cf. Sec. 4.1). However, the dominant loss mechanism in substrate-type line-defect PhC waveguides is due to the excitation of the waveguide beyond the cutoff. If a line-defect PhC waveguide is excited with a frequency,
for which no guided Bloch mode exists, then infinitely many radiative Bloch modes are excited at the input. A portion of the excited radiative Bloch modes results in a strong radiation pattern that rapidly diffracts. Thereafter a quasi stable wave is established in the line-defect PhC waveguide that is formed by the remaining radiative Bloch modes. The power of this quasi stable leaky wave approximately decays exponentially with propagation distance $x$. Three important consequences can be deduced:

- A realistic excitation is required to excite the same radiative Bloch modes as in the optical experiment.

- A strong mode settling behavior is expected at the input of the line-defect PhC waveguide due to the mode conversion from the trench waveguide to the PhC waveguide.

- The cutback-method delivers only accurate results for the propagation loss $\alpha$ if the power of the leaky wave decays exponentially with propagation distance. It is thus important to determine the frequency regions, for which the power is decaying approximately exponentially with propagation distance $x$.

### 5.2.2 Geometry of the Model

Our PhC waveguides are created by deeply etching a triangular lattice of circular holes into a layer stack consisting of an InP substrate of $\approx 300 \, \mu m$, acting as a bottom cladding, $(n=3.1496)$, a 522nm [69] thick quaternary InGaAsP core layer $(n = 3.3296)$ and an InP top cladding of 300nm [264]. For the simulation, we cover the stack by an air layer of $3 \cdot a = 1.305 \, \mu m$ thickness and use a finite substrate of thickness $5 \cdot a = 2.175 \, \mu m$. More than 99.998% of energy of the vertical mode profile (cf. Fig. 5.9) is contained in this vertical layer structure. In the simulation we use a radius of $r = 0.34 \cdot a = 148 \, nm$ and a lattice constant $a = 435 \, nm$ for a target wavelength of $\lambda = 1550 \, nm$. Figure 5.2 shows a horizontal cross section through the 3D computational domain of the reference trench waveguide (top) and a PhC waveguide (bottom) formed by one missing row of holes in the $\Gamma$-K direction. The reference trench waveguide is required to normalize the transmission spectra of the PhC waveguides (cf. Section 5.2.3). Figure 5.2 also depicts the sizes and positions of several power flux detectors (green and red) and the location of the excitation (blue). The power flux detectors compute the integral of the net Poynting vector (in the normal direction) of the fields in frequency domain over the sensor area. That is the net power flux of left and right propagating waves ($\vec{S}_i = \vec{P}_i - \vec{P}_i$, the arrows indicate the direction of propagation). The trench waveguide is excited by a pulse having a temporal Gaussian envelope, a normalized center frequency of $\omega_a/2\pi c = 0.28$ ($\lambda = 1554 \, nm$) and a normalized spectral width of $\Delta \omega_a/2\pi c = 0.2$ ($\Delta t = 3.2 \, fs$). Similar to optical experiments, where we excite the access trench waveguide with a spatial Gaussian mode profile, we also use a spatially Gaussian shaped source over the excitation area in the simulation. At all boundaries of

2The sensor area is chosen twice the dimensions of the trench waveguide core. Larger sensor areas yield the same numerical transmission spectra.
Figure 5.2: Horizontal cross section of both computational domains: 3D reference trench branch (top) as well as the 3D PhC waveguide (bottom). The gray area shows the regions of the pseudo-PML layer and it’s thickness, the air is illustrated as the black region and white is the dielectric. The waveguides are excited with a Gaussian pulse in time and with a Gaussian field distribution along the blue line. The green and red lines perpendicular to the waveguides indicate power flux sensors.
the computational domain, a perfectly matched layer (PML) [21] of one lattice constant thickness is superimposed. At the input and exit ports (trench waveguides), the PML thickness is increased to three times the lattice constant. By using access trench waveguides with this so-called pseudo-PML termination on both sides of the PhC waveguide we circumvent the delicate problem of designing suitable PhC boundaries [207]. Instead of PhC boundaries, there are two newly introduced trench waveguide/PhC waveguide interfaces with an additional unknown reflection coefficient originating from these interfaces. Note that these reflections are also present in our optical experiments.

The band diagram of the described PhC is computed with the 3D plane wave expansion method [110]. Fig. 5.3 shows those modes which have their energy localized in the PhC defect volume (cf. Section 3.2.2). The figure reveals two stop bands for the even mode (from $\omega_a/2\pi c = 0.2366$ to $\omega_a/2\pi c = 0.2401$ and from $\omega_a/2\pi c = 0.3238$ to $\omega_a/2\pi c = 0.3313$). Since the access trench waveguide is excited with an even mode, a low transmission is expected for frequencies within those stop bands (cf. Fig. 5.4).

### 5.2.3 Transmission and Reflection Coefficient

In the simulation, the field components in the time domain are recorded during the pulse propagation at the two red lines (sensors $S_2$ and $S_3$) drawn in Fig. 5.2. After the simulation, the recorded time-dependent pulse envelope for each field component is transformed into the frequency domain, in order to compute the frequency dependent Poynting vector. In the following, the power transmission coefficient is given by

$$T(\omega) = \frac{\vec{P}_{\text{trans}}(\omega)}{\vec{P}_{\text{in}}(\omega)} = \frac{S_3(\omega)}{S_1(\omega)}$$

(5.2)

Note that $S_1(\omega) = \vec{P}_1$ (from the reference waveguide) and $S_3(\omega) = \vec{P}_3$ because the absorber suppresses the backward propagating wave ($\vec{P}_1 = \vec{P}_3 = 0$). As opposed to sensors $S_1(\omega)$ and $S_3(\omega)$, sensor $S_2$ records both, the power of the incident ($\vec{P}_2$) and the reflected wave ($\vec{P}_2$). The power reflection coefficient is hence obtained by

$$R(\omega) = \frac{\vec{P}_{\text{refl}}(\omega)}{\vec{P}_{\text{in}}(\omega)} = \frac{S_1(\omega) - S_2(\omega)}{S_1(\omega)}$$

(5.3)

Practically, a perfectly matched layer consists of a continuation of the real part of the dielectric constant and an additional imaginary part that is added artificially in the absorbing layer. From a mathematical point of view, this is equivalent to a complex coordinate stretching [107]. Theoretically, a reflection free boundary can only be obtained if the continuation of the dielectric constant can be described by an analytic function. In a PhC, the material parameters cannot be described by an analytic function in the direction perpendicular to the boundary and thus a PML boundary does not represent a reflection free termination of a PhC. Alternatives consist of designing an impedance matched absorber [176] or by deriving an analytical continuation of a particular mode [186]. Oskooi et al. proposed in a recent paper [207] to gradually turn on a pseudo-PML layer. This resulted in substantially lower reflections at the PhCs boundaries. In summary, one can conclude that designing reflection free boundaries for PhC is not trivial and is still an active field of research.
The Cutback-Method

Figure 5.3: The band diagram for the substrate-type W1 PhC waveguide with \( r = 0.34a \) is obtained from 3D MPB simulations (plane wave expansion method), by selecting only the modes which have their energy confined in the waveguide core. The PhC waveguide modes with even and odd symmetry with respect to the x-z plane and TE-like polarization are shown in red and in blue color, respectively.

The trench waveguide (Fig. 5.2) is required to determine the incident power \( S_1 = \overrightarrow{P_1} = \overrightarrow{P_2} \). The power reflection and transmission coefficients are shown in Fig. 5.4 for five different lengths of the PhC waveguide. Whereas the spectral envelope of the reflection coefficient does not change for lengths longer than 20 periods, the transmitted power is monotonically decreasing with increasing length of the PhC waveguide.

5.2.4 Method A: The Cutback-Method of Transmissions

This approach is motivated by our experimental EndFire measurement setup [99, 196], where we have only access to the transmitted power. Hence, we restrict ourselves to employing only the computed transmitted power. The transmitted power including multiple reflections is given by

\[
P_{\text{out}}(L) = P_{\text{in}}T_{TP}T_{PT}e^{-\alpha L} \left( 1 + R_{PT}^2 e^{-2\alpha L} + \ldots \right) = \frac{P_{\text{in}}T_{TP}T_{PT}e^{-\alpha L}}{1 - R_{PT}e^{-\alpha L}}, \tag{5.4}
\]

where \( R_{PT} \) is the power reflection coefficient at the PhC waveguide / trench waveguide interface, \( T_{TP} \) is the power transmission coefficient from the trench waveguide into the line-defect PhC waveguide and \( T_{PT} \) is the power transmission coefficient from the line-defect PhC waveguide into the trench waveguide. The propagation loss \( \alpha_{dB} \) is computed by applying Eq. 5.1 to the transmission spectra (shown in Fig. 5.4, right) for a particular length \( L \). However, Eq. 5.1 can only be used for negligible reflections at the interface \( (R_{PT} \approx 0, T_{TP}T_{PT} \approx 1) \). More details are given in Sec. 5.3.4.1.
Fig. 5.4: The length-independent, normalized power reflection (left) and length-dependent, normalized transmission coefficient (right) spectra are shown for the structure given in Fig. 5.2 at the red power flux sensors. The inset shows an example of the $\Delta P = T(L) - T(10a)$ vs. $\Delta L$ data (red circles) in the dB-scale (cf. Eq. 5.8) for a particular frequency $\omega a / 2\pi c = 0.2667$ (indicated by the dotted black line). The black line in the inset is the linear fit to the computed data.

This method will be referred to as method A.

5.2.5 Method B: The Flux Distribution Method

As opposed to experimental measurements, where we only have access to the transmitted power, many power flux sensors can be distributed in the computational domain of the simulation without disturbing the propagation of the light. Instead of simulating many different lengths of the same PhC waveguide, one can think of using only one long PhC waveguide and record the data for multiple propagation lengths simultaneously. Therefore, a series of periodic power flux sensors is placed in the PhC crystal waveguide (illustrated as green lines in Fig. 5.2). The power flux sensors are separated by one lattice constant, i.e., they are placed at the same location relative to the PhC lattice. The sensors within the waveguide will record the net power, including all multiple reflections at the interfaces. The power flux $P(x)$ at location $x$ is given by two infinite sums of the forward and backward propagating waves

$$P(x) = \overline{P}(x) + \overline{P}(x)$$

$$P(x) = P_{in}T_{TP}e^{-\alpha x} + P_{in}T_{TP}R_{PT}e^{-\alpha(2L-x)} + \cdots$$

$$= \frac{P_{in}T_{TP}}{1 - R_{PT}^2e^{-2\alpha L}} \left[ e^{-\alpha x} + R_{PT}e^{-\alpha(2L-x)} \right].$$

For weak backscattering\(^4\) and if $R_{PT}$ is small, $P(x)$ can be approximated by a pure exponential function. This particular case will be referred to as method B.

\(^4\)There are two mechanisms resulting in a coupling to the backward propagating mode: inhibited propagation of a mode (e.g., for frequencies in stop bands or photonic band gaps) and scattering from disorder-induced imperfections. As long as no disorder is introduced in the numerical model, the backscattering is zero.
We include this method in the comparison, since it has the obvious advantage that only a single waveguide has to be simulated.

### 5.2.6 Method of Least Squares and the Coefficient of Determination

The exponential relation in case of low back reflections is

\[ P(x) = e^{-\alpha x} P_{in} \]  \hspace{1cm} (5.7)

where \( \alpha \) is the power loss figure. This equation can be related to Eq.5.1 by

\[ \alpha_{dB} = 10 \log_{10} \left( \frac{P(x)}{P_{in}} \right) \frac{1}{x} = \frac{10}{\ln(10)} \alpha. \]  \hspace{1cm} (5.8)

The linear fitting of the data in the dB-scale is solved by linear regression theory. The goodness of fit is quantified by the coefficient of determination \( R^2 \), a measure commonly used in statistics [254]. It is essentially determined by the squared residuals between each measured data point \( y_i = 10 \log_{10} \left( \frac{P(L_i)}{P_{in}} \right) \) and the fitted line \( f_i = \alpha_{dB} x + \text{const} \)

\[ R^2 = 1 - \frac{\sum_i (y_i - \bar{y})^2}{\sum_i (y_i - f_i)^2}, \]  \hspace{1cm} (5.9)

where \( \bar{y} \) is the mean value of the measured data points. Note that the coefficient of determination validates the exponential behavior of the data, but it contains no direct information about the potential FDTD simulation errors.

### 5.3 Results and Discussion

The first part of this section consists of a comparison of the two different cutback methods. In Secs. 5.3.2 and Section 5.3.3 the obtained results are compared first to a similar simulation applied to a membrane PhC waveguide and finally to experimental cutback measurements. In Section 5.3.4, we try to answer the question on how accurate our model is and which numerical error is introduced by the approximations such as geometry discretization.

#### 5.3.1 Comparison of the Cutback-Methods

In Fig. 5.5 the propagation loss spectra calculated by the two methods are shown for the frequency range of the even PhC waveguide mode (between \( \omega_a/2\pi c = 0.25 \) and 0.29): losses computed with the transmission data (method A, green) and losses computed using distributed power flux sensors (method B, red).

Method B results in a loss figure that is up to 248 dB/cm lower than method A for the range of \( \Delta \omega_a/2\pi c = 0.245 - 0.31 \). This difference can be understood if the raw data for each sensor in method B is analyzed. Two trends can be observed in
the sensor data: 1) an irregular behavior is obtained for the sensors that are close to
the input interface and an exponential behavior is obtained for the sensors that are
‘far’ away from the input interface. This has to do with mode settling in the PhC
waveguide [108, 209] as anticipated in Sec. 5.2.1 and can be observed in Fig. 5.12.
Therefore, the data from the first few sensors (e.g., 9 out of 49 sensors) have to be
removed from the data set that is used for the exponential fit. The black propa-
gation loss curve in Fig. 5.5 is obtained for the reduced data set. The same mode
settling behavior is observed for the line-defect PhC waveguides that are used for
method A. But since there the shortest length of the simulated line-defect PhC
waveguide is \( L = 10 \alpha \) long, it does not influence the propagation losses \( \alpha_{dB} \).

Figure 5.5: Propagation loss spectrum \( \alpha_{dB}(\omega) \) for the guided PhC waveguide mode
computed using the two described methods: losses computed with only the nor-
malized transmission (green, method A), losses computed using the field informa-
tion along a single PhC waveguide (red, method B). For a sensor set, where the first
nine sensors are omitted, method B results in the black curve.

In Fig. 5.6 the propagation loss spectrum \( \alpha_{dB}(\omega) \) is shown for both methods
separately. The corresponding coefficient of determination of the fit is depicted
below each propagation loss spectrum. The background in Fig. 5.6 is colored ac-
cording to the coefficient of determination: the white region \( (R^2 > 2/3) \) represents
a good exponential behavior, whereas green \( (R^2 < 2/3) \) represents poor exponen-
tial behavior. Method B has a lower coefficient of determination (smaller than 0.98
for all frequencies) than method A. For method A the coefficient of determination
is larger than 0.98 for most of the single mode regime.

An advantage of method B is that only a single simulation run is required, com-
pared to at least two simulation runs for method A. The same propagation losses
are obtained with method A and method B with the reduced data set. However, we
expect method B to be more sensitive on multiple reflections. The power \( P(x) \) at
position \( x \) in method B (Eq. 5.6) depends linearly on the reflection coefficient \( R_{PT} \).
Equation 5.4 reveals that the smallest order term in \( R_{PT} \) for the measured power
flux \( P_3 \) of method A is quadratic. Therefore, method A is more robust towards non-
vanishing reflection coefficients. A more detailed discussion on the induced error
Results and Discussion

1. Comparison of the Computed Propagation Loss to Other Simulation Results: The Membrane-Type W1 PhC Waveguide

To verify the validity of our model, we compare our cutback-method to well established results. We have chosen the free-standing Si membrane W1 PhC waveguide with a hexagonal lattice since it is one of the most widely used PhC waveguides. The comparison is based on the results published by Cryan et al. [47]. They investigated hexagonal lattice PhC W1 waveguide with $a = 430.55$ nm and $r = 0.3016 a$ implemented on free standing Si-membrane ($n = 3.4$) of thickness $t_{core} = 0.6 a = 258.3$ nm. We simulated the same PhC waveguide design with identical material parameters as reported in [47]. Using method A, the propagation loss spectrum $\alpha_{dB}(\omega)$ is computed from the transmission spectra of five different length of PhC waveguides (10a, 20a, 30a, 40a, 50a). The result is shown in Fig. 5.7 (thin black curve). The blue curve is the same as the black curve, but is additionally

\footnote{Philippe Lalanne advised me to benchmark my results to the ones obtained by Cryan et al. [47], since those results are considered by the PhC community to be the most accurate ones and as such are commonly used for benchmark tests.}

Due to multiple reflections can be found in Sec. 5.3.4.1.

Figure 5.6: Comparison of the propagation losses computed by the two described methods: losses computed with only the normalized transmission (left, method A) and losses computed using the field information along a single PhC waveguide (right, method B). In the lower row, the coefficient of determination is shown of the performed fit. The result within the white region has a goodness of fit $> 2/3$. The green region indicates a poor exponential (linear in log-scale) behavior of the propagation losses.
Computation of the Propagation Losses of PhC Waveguides

Figure 5.7: Computed propagation loss of a Si-membrane W1 PhC waveguide in triangular lattice by using the cutback-method A. The red curve is from Cryan et al. [47] and used as a reference.

smoothed (since the published data of Cryan et al. [47] has also been smoothed by using low pass filters) and the red one is taken from Fig. 2 of [47]. Our values above the light-line are 200dB/cm higher than the published ones but show a similar frequency behavior. The red propagation loss spectrum is wavelength-shifted by roughly 10-20nm compared to our simulation. A wavelength-shift in this order can result from a different approximation of the hole shape by the mesh. Above the light-line (left of light-line in Fig. 5.7) the propagation losses are in a similar order as for substrate-type PhC waveguides. McNab et al. [173, 183] measured the propagation losses of a similar membrane-type W1 PhC waveguide but with a filling factor $r = 0.35\alpha$. They obtained a similar propagation loss curve with values from 400 dB/cm to 1300 dB/cm for the frequency region above the light-line.

Membrane-type line-defect PhC waveguides typically exhibit a frequency range of guided Bloch modes, all spatial Fourier components of the Bloch mode are located below the light-line ($k_{x,m} > \omega_n/c\alpha$) for a given excitation frequency $\omega$. This so-called ‘below light-line’ condition leads to loss-free PhC waveguide modes for perfect PhCs (region right to the dotted black line in Fig. 5.7). However, instead of a constant propagation loss of $\alpha_{dB} = 0$ for frequencies below the air light-line, strong oscillations can be observed. These are Fabry-Perot fringes resulting from multiple reflections. The amplitude of the fringes increase towards the even mode cutoff indicating an increasing power reflection coefficient. Cryan [46] published a follow up article to [47] devoted to explain the poor performance of the cutback-method in the low-loss regime. By means of systematically excluding other loss mechanisms such as radiation leakage and potential numerical errors (e.g., positioning of the sensors and space- and time-discretization), he concluded that Fabry-Perot fringes are responsible for the inaccuracies observed in the low-loss regime, which confirms our observation.
Results and Discussion

5.3.3 Comparison of the Computed Propagation Loss to Optically Measured Propagation Losses: The InP/InGaAsP/InP Substrate-Type W1 PhC Waveguide

Our main interest are substrate-type W1 PhC waveguides. A detailed quantitative comparison between the FDTD simulation and optical measurements is presented here. The fabricated W1 PhC waveguides have to be modeled as accurately as possible for a comparison, i.e., a realistic hole shape have to be used in the following simulations. The experimental characterization of the hole shape was performed by SEM inspection of the cross-section of our etched PhC holes at the cleaved PhC facet as shown in Fig. 5.8. From this inspection, an approximation of the hole shape is deduced that consists of a cylindrical shape for the first 500 nm hole depth followed by a deep cone having a depth of 3.3 \( \mu \text{m} \). The gray line in Fig. 5.9 B) and D) is the measured propagation loss obtained by the EndFire setup: We coupled light from a lensed fiber into a 5 \( \mu \text{m} \) wide trench access waveguide. From this access waveguide the light is taper-coupled to the PhC waveguide under test. Since all waveguides are fabricated on the same chip, the total length (access waveguides + PhC waveguide) is the same for all waveguides. The only difference between two structures is the length of the PhC waveguide section and the length of the trench waveguide on the output side to complete the waveguide structure to the total chip length. Since the losses of the trench waveguides are in the order of 20 dB/cm, they are negligible compared to the PhC waveguide losses (\( \approx 1000 \) dB/cm) [123]. In the simulation we are not restricted to a fixed chip length and, therefore, only the length of the PhC waveguide is varied. Otherwise, there is no difference between the numerical model and the experiments. The propagation loss of a W1 PhC waveguide computed with method A is shown in Fig. 5.9 B) (blue curve) for the TE-like polarization. The measured propagation losses and simulated propagation losses
Figure 5.9: A and B shows the photonic bands of the even TE-like modes of a W1 and a W3 PhC waveguide. B) and D) show the computed propagation losses $\alpha_{dB}$ (method A) of a W1 and W3 PhC waveguide with holes given by a cylindrical shape of 500nm depth followed by a cone with a depth of 3.3 $\mu$m (blue). The corresponding EndFire measurements of the propagation loss are shown in gray.
agree for most of the single mode regime for the TE-like even mode. The same comparison of the measured and simulated propagation losses was made for a W3 PhC waveguide and is shown in Fig. 5.9 D). As opposed to the W1 PhC waveguide, the W3 PhC waveguide is not single moded. Nevertheless, the propagation losses $\alpha_{dB}$ obtained by the numeric cutback-method agree fairly well with the propagation losses $\alpha_{dB}$ obtained by optical measurements.

5.3.4 Accuracy of the Simulation Results

The emphasis on quantitative loss values requires a discussion of the errors induced by the numerical model. Time domain methods demand the investigation of at least the convergence in simulation runtime and the convergence in mesh resolution. Both figures converge and are not presented here. Nevertheless, we show the transmission spectra for different mesh resolutions in Section 5.3.4.2, where we point out that for certain frequencies, the error in the transmission can be substantial. Additionally, it is required for the computation of the reflection and transmission coefficients that the propagating mode in the access trench waveguide has settled to the stationary trench waveguide mode. This is discussed in the next subsection. Thereafter, the issue of spurious reflections from the trench waveguide / trench-pPML boundary is briefly addressed. A summary of all the possible numerical error contributions is given in Tab. 5.2.

5.3.4.1 Errors from Multiple Reflections

In Sec.5.2, we stipulated large propagation losses and low reflection coefficients at the PhC waveguide / trench waveguide interfaces. This allowed us to compute the propagation losses with the cutback-method. These two conditions are usually fulfilled for substrate-type PhC waveguides. However, we have seen large oscillations in the loss figure $\alpha_{dB}$ of the membrane-type W1 PhC waveguide originating from Fabry-Perot fringes below the light-line (cf. Sec. 5.3.2). Therefore, we try to identify the limits of the presented cutback-methods.

First, we estimate the validity of method A. We required a hypothetical exponential law for the transmitted power $P_{3,exp}$ at the output sensor $S_3$ with length of the PhC waveguide $L_{PhC}$

$$P_{3,exp}(L_{PhC}) = P_{in}T_T P_{PT} e^{-\alpha L_{PhC}}.$$  \hspace{1cm} (5.10)

This equation only holds if multiple reflections are negligible. For non-negligible power reflection coefficients $R_{PT}$, Eq. 5.4

$$P_{3,MR}(L_{PhC}) = \frac{P_{in}T_T P_{PT} e^{-\alpha L_{PhC}}}{1 - R_{PT} e^{-\alpha L_{PhC}}}.$$ \hspace{1cm} (5.11)

has to be used to compute the transmitted power. The power error $P_{error}$ that is made by using Eq. 5.10 instead of Eq. 5.11 can be expressed by
The power error $P_{\text{error}}$ is computed as a function of propagation loss $\alpha_{dB}$ and the power reflection coefficient $R_{PT}$ while assuming $P_{in}T_{TP}T_{PT} = 1$ and $L_{PhC} = 50 \ a$. The black line represents an expected error of 5% of the measured power flux. Thus, for $(\alpha_{dB}, R_{PT})$-pairs in the white area, the expected error due to multiple reflections is smaller. There the cutback-method is applicable.

$$P_{\text{error}}(L_{PhC}) = P_{3,MR}(L_{PhC}) - P_{3,exp}(L_{PhC})$$

$$= P_{in}T_{TP}T_{PT}e^{-\alpha L} \left( \frac{1}{1 - R_{PT}e^{-\alpha L_{PhC}}} - 1 \right).$$

(5.12)

$P_{\text{error}}$ can be computed for various pairs of $(\alpha_{dB}, R_{PT})$ for a specific $L_{PhC} = 50 \ a$ and for $P_{in}T_{TP}T_{PT} = \text{const} = 1$. The black curve in the right plot of Fig. 5.10 represents the values of $\alpha_{dB}$ and $R_{PT}$ for which the power error is 5% ($P_{\text{error}}(L_{PhC}) = 0.05$). The choice of a power error of 5% is arbitrary, but was motivated by the largest observed transmission error of $\Delta T/T = 6\%$ due to the grid resolution. For all pairs of $(\alpha_{dB}, R_{PT})$ below this black line the cutback-method results in an error $P_{\text{error}} \leq 5\%$ originating from multiple reflections.

The same investigation can be made for method B. Instead of computing the a power error for a single sensor $S_3$ at the output, the power error $P_{\text{error}}(x)$ is computed for all the sensors along the line-defect PhC waveguide. Equation 5.5 describes the power $P_{MR}(x)$ including all multiple reflections as a function of propagation distance $x$ in the PhC waveguide.

$$P_{MR}(x) = \frac{P_{in}T_{TP}}{1 - R_{PT}^2e^{-2\alpha L}} \left[ e^{-\alpha x} + R_{PT}e^{-\alpha(2L-x)} \right]$$

(5.13)

Analogous to the procedure for method A, we define the power error $P_{\text{error}}(x)$ as the difference of $P_{MR}(x)$ and the power obeying a pure exponential $P_{exp}(x)$.
\[ P_{\text{error}}(x) = P_{MR}(x) - P_{\text{exp}}(x) \]
\[ = P_{in} T_{TP} \left[ \frac{1}{1 - R_{PT}^2 e^{-2\alpha L}} \left( e^{-\alpha x} + R_{PT} e^{-\alpha(2L-x)} \right) - e^{-\alpha x} \right] \] (5.14)

\( P_{\text{error}}(x) \) is computed for \( P_{in} T_{TP} = 1 \) and \( L = 50a \) and various pairs of \((\alpha_{dB}, R_{PT})\). The white area in the right plot of Fig. 5.10 shows the regions of a \( P_{\text{error}} \leq 0.05 \) for all sensors for a \( L = 50a \) long PhC waveguide. The power error increases along the propagation distance \( x \), because the influence of the damped first order reflection is largest close to the output interface. As long as the reflection coefficient \( R_{PT} < 0.05 \) both methods may be used even for very low-loss devices. Fig. 5.10 shows that method A is more robust to multiple reflections than method B (e.g., for a power reflection coefficient of \( R_{PT} = 0.1 \) the minimum allowed propagation loss \( \alpha_{dB} \) is roughly factor 2 smaller for method A than for method B).

5.3.4.2 Mesh Resolution

The error which is introduced by the approximation of the circular holes by a rectangular mesh (cf. Fig. 5.11, left) not only leads to slight variations in the absolute value of the transmission, but also to a slightly different filling factor \( r/a \) for every grid resolution. The variance in the ratio \( r/a \) manifests itself in a slight shift of the band edge frequency of the PhC. For a frequency near the band edge, the difference of the transmission value for two different mesh resolutions can be large. The transmission spectra for various mesh resolutions are shown in Fig. 5.11. We found a maximum difference of \( \Delta T/T \leq 6\% \) in the transmission value for mesh resolutions \( > a/18 \). However, since all simulations required for the cutback-method only differ in the length of the PhC waveguide section, they have all the same mesh resolution and hence also the same filling factor. The same error in the approximation of the hole shape in all of these spectra.

By choosing finer grids, an arbitrarily small simulation error can be obtained. Unfortunately, doubling the mesh resolution leads to a \( 2^3 \)-fold increase of the number of unknowns and needs twice as many time steps for simulating the same propagation time – hence resulting in a 16-fold increase in simulation time. We have chosen a resolution of \( 1/20a \), simply because it is the highest resolution we can perform in a reasonable time (e.g. a single simulation run takes about a day with 20 parallel CPUs).

5.3.4.3 Excitation and Mode Settling in the Access Waveguide

The structure is excited by a Gaussian pulse in time and by a spatial Gaussian function laterally across the waveguide. Although the spatial function of the excitation is close to the stationary mode profile, some propagation distance has to be added for the mode settling of the trench waveguide mode. In Fig. 5.12 three plots are shown to determine the distance needed for mode settling. The \( H_z \)-field compo-
Figure 5.11: Top: The mesh is shown for various grid resolutions. The difference (error) of the filling factor (ratio of the hole area to the unit cell area) of the discretization to the ideal filling factor is given in percent below each plot. Bottom: The transmission spectra for different grid resolutions (from eight grid points up to 28 grid points per lattice constant a). The difference in the band edge frequency varies substantially especially for the lowest resolution. Within the range of the guided PhC waveguide mode, the amplitude of the transmission is within a range of 6% for mesh resolutions $> a/18$. 

Transmission Coefficient ($L_{PhC} = 30a$)
Figure 5.12: The upper most image shows three exemplary time snapshots of the pulse represented by the z-component of the magnetic field in the center of the waveguide along the propagation direction $x$. The center illustration shows the sum of all exported pulses to show the settling process in the trench waveguide. The lower plot shows the evolution of the pulse by plotting the difference of the $H_z$-field between subsequent time steps. The mode needs approximately 10 lattice periods of propagation to settle to the stationary in the input trench waveguide and about 5 lattice periods of propagation in the PhC waveguide.

Component was exported in time steps\(^6\) of $2 \frac{a}{c}$ for the lateral center of the waveguide ($y = 0$). All the exported $H_z$-field data (two of those time-snapshots are shown in the first plot of Fig. 5.12) are combined by a summation, such that it can be shown in a single figure (second plot in Fig. 5.12). It can be seen, that the maximum of the $H_z$-field component in the access trench waveguide moves first towards the top surface and finally converges close to the center of the core. To better quantify this wiggle at the beginning of the waveguide, the change of the mode profile $\Delta H_z$ is shown in the third plot of Fig. 5.12. To obtain this plot, the $H_z$-field component along a line in z-direction going through the maximum value - which moves from left to right as time progresses – is extracted for each export. Thereafter, the difference of these one dimensional vertical mode profiles of two subsequent time steps are plotted. Only a minor improvement can be observed after propagation distances longer than 10 lattice constants. Therefore, the input sensor $S_1$ is placed 10 periods after the excitation (cf. Fig. 5.2). A similar mode settling problem can be observed at the input of the PhC waveguide. After 5 lattice constants, the mode profile is stable. This graphically illustrates the need to omit the first few sensors for method B. No mode settling behavior is observed in the output trench waveguide. Therefore, the output trench waveguide is adjusted to the minimum length of 3 lattice constants and the output sensor is placed in the middle of the output trench waveguide.

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\(^6\)MEEP computes in units normalized to the lattice. The time scale is lattice constant $a$ divided by the speed of light $c$. 
5.3.4.4 Overall Error Estimation of the Numerical Model

The simulation is stopped when the magnetic field \( H_z \) component at the output sensor reaches a value, which is \( 5 \cdot 10^{-5} \) times smaller than the largest recorded one. This guarantees that the pulse did propagate through the PhC waveguide completely. Since we expect a large group velocity dispersion for certain frequencies (e.g., slow light waves) in the PhC waveguide, we used this small value for the stopping criterion. We expect an error in the propagation loss \( \Delta \alpha_{dB} < 0.34 \text{ dB/cm} \), arising from this stopping criterion (cf. Tab. 5.2).

In Fig. 5.13 the magnetic field reflection coefficient is plotted as a function of the trench-pPML thickness. To obtain an error of a similar magnitude as the one from the stopping criterion, a necessary thickness of three lattice constants for the trench-pPML boundary can be deduced from Fig. 5.13.

The error introduced by the mesh resolution cannot be determined exactly, since for that purpose an infinitely fine resolved mesh would be required. Therefore, we estimate the error by seeking the highest deviation of the transmission \( T \) for mesh resolutions from \( \frac{1}{18a} \) to \( \frac{1}{28a} \) within the band gap range (cf. Fig. 5.11) that is roughly \( \frac{\Delta T}{T} = 6\% \). The error for the mode settling in the access waveguide is estimated by the maximum deviation from the vertical mode profile at distance \( 10a \) and found to be roughly \( \frac{\Delta T}{T} = 1\% \). Because every simulation is excited with the same input sequence and because of an identical mesh discretization within one cutback-simulation, the same error is made in every simulation. This systematic error will hence be canceled by the cutback-method and will not

Table 5.2: The numbers below represent an estimation of the worst case of the error of the propagation loss \( \alpha_{dB} \). At the band edge (BE) a substantial error in the transmission coefficient can result because of the hole shape discretization. A specific frequency in the vicinity of the band edge may lay in the stop band for one mesh discretization and in the single mode region for another mesh discretization. The non-negligible errors in the transmission, which are induced by the mesh discretization and the mode settling in the access waveguide are canceled by the cutback-method and can hence not be translated to an error in \( \alpha_{dB} \).

<table>
<thead>
<tr>
<th>Transmission Error</th>
<th>( \Delta \alpha_{dB} ) [dB/cm]</th>
<th>Frequency Error</th>
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</thead>
<tbody>
<tr>
<td>Mesh Resolution</td>
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<td></td>
</tr>
<tr>
<td>Finite Runtime</td>
<td>( \Delta H_z = \pm 5 \cdot 10^{-5} \cdot \max(H_z) )</td>
<td>( \pm 0.34 )</td>
</tr>
<tr>
<td>Reflection at Boundary</td>
<td>( \Delta H_z = \pm 7 \cdot 10^{-7} \cdot \max(H_z) )</td>
<td>( \pm 0.48 )</td>
</tr>
<tr>
<td>Mode Setting</td>
<td>( &lt; \Delta H_z = 10^{-2} \cdot \max(H_z) )</td>
<td></td>
</tr>
<tr>
<td>BE: ( \Delta \omega a / 2\pi c = \pm 0.004 )</td>
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<td></td>
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<tr>
<td>BG: ( \Delta \omega a / 2\pi c = \pm 0.006 )</td>
<td></td>
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</tbody>
</table>

BG: single mode regime within the PhC band-gap \( (\omega a / 2\pi c \approx 0.240 - 0.336) \), BE: band-edge
Conclusions

Both presented methods reliably produce propagation losses $\alpha_{dB}$ that agree well with optically measured propagation losses $\alpha_{dB}$. The measured propagation losses $\alpha_{dB}$ are at the most 50% larger than the simulated values. For a rather large frequency range from $\Delta \omega_a/(2\pi c) = 0.2604 - 0.2927$ the measured propagation losses deviate less than 15% from the simulated values. In comparison, the previously published data for our material system by Sauvan et al. [232] disclose measured propagation loss values for the frequency range $\Delta \omega_a/(2\pi c) = 0.294 - 0.31$, which are roughly 80% to 105% larger than the simulated propagation losses. Because of the new level of achieved accuracy of our simulations, we can conclude, that the relevant loss mechanisms for our substrate-type PhC are well covered by our numerical method if a realistic hole shape is used. The hole shape is thus a relevant factor for the total propagation loss figure, whereas we can already exclude effects such as surface roughness, disorder effects and material absorption from the list of possible relevant loss mechanisms in our substrate-type PhC waveguides, since they have not yet been taken account for by the numerical model.

In the following chapters we will apply the presented method to further investigate the detailed influence of the imperfections of the hole shape on the propagation loss. Furthermore, the numerical method allows us to minimize the propagation losses by optimizing design parameters such as the thicknesses of the layers of the vertical slab waveguide. Finally we can use the method for the quest of new low-loss PhC waveguides, which are suitable for electrical contacting.

Figure 5.13: The magnetic $H_z$-field reflection coefficient for the trench/pPML interface decreases for thicker PML boundaries.

even appear for different hole-shape simulations. The error estimates are summarized in Tab. 5.2.
Computation of the Propagation Losses of PhC Waveguides
6

Loss-Relevant Structural Imperfections in Substrate-Type Photonic Crystal Waveguides

The chapter is based on Ref. [116].

Chapter 4 concludes that infinitely many radiative Bloch modes – a leaky wave – are excited in our substrate-type W1 PhC waveguides. Those leaky waves are inherently lossy and as such responsible for the intrinsic loss contribution\(^1\). In chapter 5, it was shown that the optically measured propagation loss can accurately be computed by using the cutback-method and realistic hole shapes. It follows that structural imperfections, such as the non-cylindrical hole shape, are responsible for the difference between the intrinsic losses and the substantially larger measured propagation losses. Numerical simulations can give insight into the quantitative contribution to the propagation losses originating from fabrication imperfections. We will see by the end of this chapter that the intrinsic losses originating from the waveguide design and the scattering losses originating from structural imperfections are coupled and cannot be treated independently of each other.

Because of the interplay of the intrinsic losses of a PhC waveguide design and the losses induced by structural imperfections, it is not possible to completely isolate a single loss channel in substrate-type PhC waveguides as opposed to membrane-type PhC waveguides. However, instead of investigating an isolated loss channel, we can address the various structural imperfections separately. These investigations allow us to answer a practically more relevant question for the reduction of the propagation losses in substrate-type PhC waveguides: Which structural imperfection is mainly responsible for the large discrepancy between the intrinsic losses and the measured propagation losses? This information is highly relevant for the device engineers, since it allows them to take specific measures to

\(^1\)We strictly use the term intrinsic losses for the losses that remain in a perfectly fabricated device – i.e., a PhC waveguide with indefinitely deep cylindrical holes.
prevent propagation losses. For this chapter, we performed a comprehensive set of numerical experiments with the 3D FDTD method to investigate the influences of imperfections, such as the finite etch-depth, a conical hole shape, the finite number of lateral layers of holes, the asymmetric vertical layer structure, lattice-disorder and variations of the hole radius. The main achievement of this chapter is hence the synthesis of a complete picture for a particular structure – a substrate-type W1 PhC waveguide – and to compare the propagation losses originating from a particular structural imperfection quantitatively. Only for this reason, we were able to identify the design parameter that is responsible for most of the propagation losses due to fabrication imperfections. It permits us to direct the efforts in further improving the fabrication technology.

Table 5.1 shows that many numerical studies have been performed in the past addressing a part of the question about the origin of the large propagation losses in substrate-type PhC waveguides. However, all of them lack the general overview, which is essential to identify the main source for the large propagation losses. Since those studies are performed with various numerical methods for many different PhC waveguide designs, a general overview cannot be reliably assembled from the literature. The most complete set of investigations have been performed by Ferrini and Benisty addressing radiation losses [18, 70, 19, 69], losses due to imperfect hole shapes [72, 19] such as a finite hole depth, conical and cylindro-conical hole shapes, and disorder induced losses [71] for the InP/InGaAsP/InP material system. Even though their material system is similar to ours, their results are of limited value for our goal to reduce the propagation losses of PhC waveguides: First, they did not investigate line-defect PhC waveguides but only defect-free PhCs. Secondly, they do not provide a comparison of the numerically obtained propagation losses to optical propagation loss measurements, which is essential to determine the accuracy of their numerical method – particularly because their method is not derived from first principles.

### 6.1 Phenomenological Loss Channels of Line-Defect Slab Photonic Crystal Waveguides

We start by summarizing the phenomenological loss channels for slab line-defect PhC waveguides that are reported in literature. The numerical experiments that follow in Sec. 6.3 were designed, such that the quantitative contribution of the reported loss channels to the total propagation loss can be determined. The goal is to identify the dominant loss channel in fabricated substrate-type line-defect PhC waveguides with fabrication imperfections.

#### 6.1.1 Material Absorption

Absorption of light in a material can occur, if the energy of the propagating photons coincides with electronic energy transitions of the material. Normally, passive dielectric waveguides are operated with photons of energies below the band gap
of the involved semiconductor materials and thus, material absorption in those waveguides can be neglected.

6.1.2 Out-of-Plane Losses

All radiation that scatters vertically (out of the plane) out of the PhC waveguide core is summarized with the term out-of-plane losses. The most prominent intrinsic contribution of out-of-plane losses is due to unconfined modes, i.e., Bloch modes of the PhC waveguide that have at least one of the spatial Fourier components above the light-line of the cladding [140, 141, 109]. But also random irregularities in the structure, such as surface roughness or process variations in the cross section of the etched holes can result in vertical (and lateral) extrinsic radiation.

6.1.3 Lateral Radiation Leakage

If a PhC waveguide were of infinite lateral extent, we could expect a decay to zero of the modal fields at infinity. For a finite lateral extent of the PhC-lattice, however, the fields decay only over a limited distance. The remaining fields, even if they might be very small, can freely oscillate outside of the PhC structure. In terms of lateral profile, planar PhC waveguides are always so-called W-type waveguides (cf. Fig. 6.1). Strictly speaking those waveguides support only radiation modes. However, if locally excited, a leaky wave as discussed in Sec. 4.1.2.4 is established in W-type waveguides [124]. A leaky wave is an ensemble of radiation modes that yield a strong light localization in the waveguide core. This wave does not maintain its transverse mode profile along the propagation direction and usually a decay constant along the propagation direction is associated with a leaky wave [94]. In practice, the magnitude of this decay can be controlled in PhC waveguides with the number of lateral layers of holes.

![Figure 6.1](image1.png)  
**Figure 6.1:** Left: a W-type waveguide is shown. Note that the waveguide does not support a guided mode but only radiation modes. Even so, a **nearly guided** mode resembling a guided mode will propagate in the core of the waveguide. Right: a cross-section of a PhC waveguide with finite lateral dimensions are shown. If the PhC waveguide is operated within the PBG, then the PhC sections yield an exponential decay of the lateral mode profile and the situation is similar to the W-waveguide (left).
6.1.4 Losses Due to Mode Coupling Caused by the Asymmetry

This loss channel may be described in terms of mode coupling theory. We consider the complete, orthonormal set of modes of a symmetric slab PhC waveguide as the modes of the initial, undisturbed system [218]. Our design is such that its complete set of modes comprises a continuous set of radiative modes and a discrete set of guided modes. Due to the mirror symmetry of the vertical layer stack, the modes can be classified into either TE-like and TM-like PhC modes (cf. Sec. 2.3.1) that exhibit different dispersion properties and most notably a different frequency range of the photonic band gap. According to mode coupling theory, the propagation of light in a waveguide with a slight geometrical deviation from the initial perfect symmetric planar slab PhC waveguide can be described by the mode set of the undisturbed system and by an additional set of non-zero coupling coefficients between those modes. If a perturbation is introduced that breaks the symmetry, TE-like and TM-like modes will be able to couple. A loss channel is opened if coupling from (band-gap) guided modes to radiative modes occurs. This loss mechanism has been reported by Tanaka et al. [277]. They could show numerically that a conical hole shape in an otherwise symmetric membrane-type PhC waveguide design leads to a propagation loss due to coupling from band gap guided TE-like modes to non-guided^{2} TM-like modes.

6.1.5 Scattering at Geometric Non-Uniformity

Similar to asymmetries (refer to Sec. 6.1.4), the scattering at localized non-uniformities enables the coupling between guided Bloch modes and radiative Bloch modes and to the backwards propagating modes. A typical situation for this process is scattering at rough surfaces or lattice disorder of the PhC.

6.1.6 Interface Losses

Poor mode matching at the interfaces of butt-coupled waveguides gives rise to reflections. The reflected light is not propagated through the PhC waveguide and will manifest itself in a length-independent loss contribution. In our case, those reflections are very small for most of the single mode frequency regime [117]. We measured a power reflection coefficient using the Fabry-Perot technique in the order of 0.02 for the trench waveguide/PhC waveguide interface. However, if the PhC waveguides are operated in the slow light regime, the mode profiles of the PhC waveguide can be substantially different from the access waveguide resulting in large power reflection coefficients. These reflections can be largely reduced by a proper design of the interfaces [171, 96, 216] or by adiabatic tapering [108]. Losses at the interfaces are not relevant for the propagation losses, but since they can’t be avoided in practical experiments they are listed here for the sake of completeness.

^{2}There is no band gap for the TM polarization for a PhC based on a hexagonal lattice of air holes in InP or Si for $r < 0.4 a$ [104, p. 247].
6.2 Correlations between Structural Properties, Loss Channels and Loss Mechanisms

These phenomenological loss channels originate from the notion that a specific structural imperfection gives rise to leakage via a specific loss channel. However, theoretically, there are only two fundamental scattering loss mechanisms – surface/volume scattering and leaky waves – that result in a waveguide propagation loss. To each phenomenological loss channel the involved loss mechanisms are listed in Table 6.1.

Throughout the chapter we distinguish between these phenomenological loss channels (described in Sec. 6.1) such as out-of-plane radiation on one hand and structure-related characteristics like the shape of PhC holes or lattice disorder on the other hand. The loss channels are connected to the question: “Where and how does the lost light go?”, whereas the structure properties are related to the question: “What can we do to minimize the losses?”. In general, a specific structural imperfection causes leakage of light via many loss channels simultaneously. Table 6.2 lists the considered items of each group and indicates the links between them. For example, if a structure property modifies the waveguide design, then the Bloch modes are modified as well and consequently the propagation losses are different. The purpose of Table 6.2 is to show that the loss mechanisms are linked and cannot be separated, e.g., if the conicity of the holes is increased, then the light may vanish laterally (lateral radiation leakage, scattering at geometric non-uniformities, mode coupling due to asymmetry) or vertically (due to deflection or coupling to radiative modes or scattering). This coupling between the effects makes it impossible to isolate a single loss channel. In the following sections, a numerical experiment for every structure property listed in Table 6.2 is performed with the aim to determine its influence on the propagation loss.

Table 6.1: The phenomenologically reported loss channels are based on only two fundamental physical loss mechanisms.

<table>
<thead>
<tr>
<th>Loss Channel</th>
<th>Loss Mechanism</th>
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<tbody>
<tr>
<td></td>
<td>Surface/Volume Scattering</td>
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<tr>
<td>Material Absorption</td>
<td>X</td>
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<tr>
<td>Out-of-plane Losses</td>
<td>X</td>
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<tr>
<td>Lateral Radiation Leakage</td>
<td>X</td>
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<tr>
<td>Losses Due to Mode Coupling Caused by the Asymmetry</td>
<td>X</td>
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<tr>
<td>Scattering at Geometric Non-Uniformity</td>
<td>X</td>
</tr>
<tr>
<td>Interface Losses</td>
<td>X</td>
</tr>
</tbody>
</table>
Table 6.2: Various structural properties are linked to their potential loss channels.

<table>
<thead>
<tr>
<th>Structural Imperfection</th>
<th>Loss Channel</th>
<th>material</th>
<th>absorbing material</th>
<th>asymmetric layer structure</th>
<th>finite number of lateral layers of holes</th>
<th>leaky waves</th>
<th>finite etch depth</th>
<th>conical hole shape</th>
<th>cylindro-conical hole shape</th>
<th>lattice disorder</th>
<th>variance of hole radii</th>
<th>surface roughness</th>
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<tbody>
<tr>
<td></td>
<td>material</td>
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<td>out-of-plane</td>
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Numerical Experiment presented in Section 6.3.3.1 6.3.3.2 (6.4.2) 6.3.3.3 6.3.3.4 6.3.3.5 6.3.4.1 6.3.4.2 -

### 6.3 Influence of the Structural Imperfections on the Propagation Losses

In this section, we present the numerical experiments for investigating the influence of the structural imperfections on the propagation losses. The propagation losses were computed using the cutback-method A together with the 3D FDTD method (cf. chapter 5 and [117]). First, we introduce the PhC waveguide of interest with all the necessary details. Thereafter, we divide the experiments into two classes of structural imperfections: the first class consists of imperfections that are periodically repeated, i.e., the periodicity of the PhC remains unchanged despite the additional imperfections. Even though the periodicity of the modified PhC remains unchanged, the unit cell is modified by the imperfections and consequently the set of guided Bloch modes and radiative Bloch modes of the new system is different. If the system is excited at the input, a different ensemble of propagating Bloch modes is excited, i.e., a different leaky wave with a different propagation loss.
In the second class, we summarize irregular (not-periodic) structural imperfections. The considered imperfections are small, randomly distributed, geometrical disturbances, such that the PhC waveguide design is not modified. Strictly speaking, the periodicity of the system with the imperfections is lost, because of the random nature of the imperfections. However, in case of small random imperfections, the set of Bloch modes remains changed and perturbation theory can be applied.

### 6.3.1 The W1 PhC Waveguide of Interest

The PhC waveguide of interest is based on a hexagonal lattice of cylindrical holes penetrating through a vertical layer stack consisting of an InP substrate ($n = 3.17$, $d \approx 300 \mu m$), an InGaAsP core layer of 522 nm [69] thickness ($n = 3.33$) and an InP top-cladding of 300 nm thickness. The W1 PhC waveguide is obtained by omitting a single row of holes along the Γ-K direction (cf. Fig. 6.3). The lattice constant is $a = 435$ nm and the radius is $r = 148$ nm. A cross section micro-graph of our PhC holes is shown in Fig. 6.2 and reveals a hole shape that can be approximated by a 500 nm deep cylindrical hole followed by a conical hole of 2.7 $\mu m$ to 3.5 $\mu m$ depth (the values depend on the radius and the lattice constant [264]). The standard deviation for the hole radius and the lattice constant can be computed by fitting circles to SEM micro-graphs of the top-cladding surface (cf. Appendix A.5). We found a standard deviation of the radii of $\sigma/r = 0.01 - 0.02$ for $r \sim 148$ nm and a standard deviation of the lattice constant of $\sigma/a = 0.01 - 0.012$ for $a \sim 435$ nm. The typical surface roughness was measured by P. Strasser [260] by scanning an AFM tip over

![Figure 6.2: This picture shows SEM images of our substrate-type PhC; a top-view (left) and a cross-section (right). The sidewall angle of the conical hole is roughly $\vartheta = 2.5^\circ$. It can be seen that the hole deviates from the lattice periodicity beyond a depth of about 2.8 $\mu m$.](image-url)
Figure 6.3: The super-cell used for the 3D MPB simulation as well as the band diagrams resulting from the simulation are shown. The vertical layer stack consists of an InP substrate, a 522nm thick InGaAsP core layer and a 300nm thick InP top-cladding layer. The TE-like modes are shown in red (even) and blue (odd) according to their mirror symmetry. Only the modes which have their energy confined to the waveguide core are shown. The TE-like even mode stop bands lead to pronounced dips in the transmission spectra.

Dependent on the gas flow concentrations during the dry-etching process he found roughness values of about 2.5 – 5 nm at the hole sidewalls [262].

The numerical band diagram of this waveguide is computed using 3D MPB (plane wave expansion method) [110]. The TE-like modes of the line-defect PhC waveguide are shown in Fig. 6.3. The transmission spectrum of a 50 period long W1 PhC waveguide is computed with 3D FDTD. The spectrum is dominated by the two TE-like even mode stop bands $\Delta \omega a / (2 \pi c) = 0.2366 - 0.2401$ and $\Delta \omega a / (2 \pi c) = 0.3238 - 0.3313$.

### 6.3.2 Intrinsic Propagation Loss

The remaining propagation losses of a perfectly fabricated device are referred to as **intrinsic losses**. **Extrinsic losses** are exclusively associated to fabrication-related propagation losses, i.e., the propagation losses that are caused by fabrication-related imperfections such as surface roughness, lattice-disorder and deviation from an ideal hole shape. Figure 6.4 shows the intrinsic propagation loss $\alpha_{W1}$ of the W1 PhC waveguide described above. The blue curve in Fig. 6.4 are the propagation losses obtained for a realistic hole shape. Those values agree nicely to experimentally measured propagation losses (cf. Fig. 5.9). The difference between the intrinsic propagation losses and the propagation losses obtained for a realistic hole shape correspond to the extrinsic propagation losses. This difference could potentially be reduced by improving the process technology.
6.3.3 Propagation Losses Originating From Periodic Imperfections

First we investigate structural imperfections that are strictly periodic in propagation direction, i.e., the imperfect hole shape is translated to any hole of the PhC lattice. The PhC remains strictly periodic. The structural imperfections/modifications alter the Bloch modes and their spatial Fourier spectrum. Since the propagation losses are related to the relative strengths of the spatial Fourier components of the excited Bloch modes above the background line with respect to the ones below the background-line. Furthermore, the background-line is also modified in some of the experiments. For example, it is expected that the background-line can be approximated by the fundamental mode of the 2D line-defect PhC waveguide in the substrate for a large etch depth. However, the background-line of the 2D line-defect PhC waveguide of the substrate is no longer a good approximation for shallow holes. Refer to Sec. 4.5.4 for more details.

6.3.3.1 Vertical Layer Structure

In our first numerical experiment, we consider a planar slab waveguide that has the same W1 PhC waveguide design in all three layers. The cladding layers are 1.74µm thick and are terminated by a PML layer. By varying the refractive index of the top cladding, a perfectly symmetric layer stack can be obtained for \( n_{\text{cladding}} = n_{\text{substrate}} \) (see the insets in Fig. 6.5). According to Qiu [218] and to Tanaka et al. [277] losses occur due to mode coupling between TE-like band gap guided modes and TM-like modes that are not band gap guided. Refer to Sec. 6.1.4 for the description of the loss channel. This loss channel can be excluded for the symmetric waveguide, and according to the findings of Qiu and Tanaka et al., it is expected that the symmetric waveguide exhibits the lowest propagation loss.
Figure 6.5: The refractive index of the top cladding material was varied from $n = 3.15$ (symmetric layer structure, dark red line) to $n = 1$ (strong asymmetry of the layer structure, dark blue line). The asymmetric layer structure exhibits a lower propagation loss for lower frequencies $\omega a / 2 \pi c < 0.285$, while the symmetric structure performs better for higher frequencies.

Figure 6.6 shows the cross-section of the vertical layer stacks and drawings of the band diagram and the background-lines. For example, the background-line of the PhC waveguide with the air top-cladding as shown in Fig. 6.6 A) is the air light-line. Light can only radiate into the top-cladding if spatial Fourier components of the Bloch modes of the PhC waveguide are located above the top-cladding background-line, i.e., the air light-line. On the other hand, for the symmetric vertical layer stack, the background line of the bottom-cladding and the top-cladding is the same. The symmetric waveguide will thus radiate equally into the top-cladding and the bottom-cladding layer. This explains the superior performance of the asymmetric waveguide for lower frequencies ($\omega a / (2 \pi c) < 0.285$). For those frequencies, the asymmetric PhC waveguide modes are located below the...
Figure 6.6: Band diagram and background-lines for the three different PhC waveguide designs: strong asymmetry $n = 1$ (A), weak asymmetry $n = 2.34$ (B) and symmetric $n = 3.15$ (C). For all vertical layer structures, radiation into the top and bottom cladding is expected – except for waveguide design (A) and for frequencies below the background line of the top cladding ($\omega a/2\pi c < 0.285$). Then, only radiation into the substrate layer occurs.
Structural Imperfections in Slab PhC Waveguides

background-line of the top-cladding but below the background-line of the bottom cladding and hence radiation only occurs into the substrate. The different vertical layer stacks result in a slightly different set of Bloch modes for each waveguide design and thus in different spatial Fourier spectra. This could explain the remaining differences that can be seen between the propagation loss spectra in Fig. 6.5.

We conclude that the asymmetric layer stack indeed has a significant influence on the propagation loss. The loss mechanism consisting of mode coupling from band gap guided to unguided modes is relevant for membrane-type PhC waveguides operated below the light-line [277, 218]. However, for substrate-type PhC waveguides, this mechanism is a second order effect. Instead, the different background-lines for the top-cladding and the slight change of the Bloch modes are dominating the propagation loss spectrum.

6.3.3.2 Finite Number of Lateral Layers of Holes

An ideal W1 PhC waveguide is of infinite lateral extent. However, a finite structure is required in all practical situations, whether it concerns a numerical method where a finite computational domain is required or a real device. Therefore, the question arises, where it is safe to truncate the PhC waveguide laterally in order to obtain an approximately infinite PhC waveguide structure.

This loss channel is addressed numerically by running a propagation loss computation for different numbers of lateral layers of PhC air holes. From Fig. 6.7 it is inferred that the required number of holes for a propagation loss close to the intrinsic loss depends strongly on the operating frequency of the PhC waveguide. Smajic et al. [247] already pointed out the astonishing fact that for a small frequency range in the center of the band gap, one single row of holes can guide the light. A single row of holes is no longer a 2D PhC with a hexagonal lattice and the band gap vanishes. In that case, the light is obviously not gap guided. This requires some further discussion. It is instructive to study the lateral mode profile of a PhC W1 waveguide as it is shown in Fig. 6.8. It can be seen that the slope of the dispersion – e. g., the group velocity of the PhC waveguide mode – is correlated to the lateral mode profile: the electric and magnetic fields of the slow light modes of the PhC waveguide penetrate deeper into the PhC cladding. The interaction of the light of those modes with the holes in the second or third row with respect to the waveguide core is intensified. On the other hand, the modes having a fast group velocity are characterized by a tight confinement of the lateral mode profile. Those modes seem almost exclusively to interact with the first row of holes.

The associated mechanism of the loss channel is explained in 6.1.3.: a laterally insufficiently extended PhC results in lateral radiation leakage and in propagating leaky waves in the PhC waveguide core [94]. If the PhC waveguide is excited with a frequency within the photonic band gap of the PhC, then the field amplitude decays exponentially in lateral direction (y-axis) in the PhC cladding. Therefore, an empirical exponential law is inferred that relates the propagation losses to the lateral dimension:

$$\alpha_{dB}(n) = \alpha_{W1} + \alpha_r e^{-\gamma_r n},$$  \hspace{1cm} (6.1)

where $\alpha_{W1}$ is the intrinsic loss of the W1 PhC waveguide. $n$ is an integer repre-
Influence of the Structural Imperfections on the Propagation Loss

Figure 6.7: A) The propagation losses for the W1 PhC waveguide as a function of the number of lateral hole layers is shown. The loss figure is almost independent of the number of layers for frequencies around \( \omega a/(2\pi c) \sim 0.28 \). In that range even a single row of holes guides the electromagnetic wave equally efficiently as an semi-infinite PhC. The more the frequencies approach the band-edges, the more lateral hole layers are required to guide the light. B) The decay constant \( \gamma_r \) of Eq. 6.1 for the same frequency range.
senting the number of lateral layers. $\alpha_r$ and $\gamma_r$ are empirical constants, which we used as fitting parameters. For the frequency ranges $\Delta \omega a/(2\pi c) = 0.2424 - 0.2684$ and $\Delta \omega a/(2\pi c) = 0.2877 - 0.31$ we were able to fit the model to the propagation loss data with a coefficient of determination $R^2 > 0.988$. This confirms the exponential dependence of the propagation loss with respect to the number of lateral layers of holes. Fig. 6.7, bottom shows $\gamma_r$ as a function of frequency. $\gamma_r$ is related to the lateral decay constant of the fields of a PhC W1 waveguide. Johnson et al. [109] emphasize that for the limiting case of a vanishing group velocity, infinitely many lateral layers are required theoretically. Thus, it is expected that $\gamma_r$ approaches a value close to zero for frequencies close to the stop band of the W1 PhC waveguide. It can further be seen that $\gamma_r$ increases rapidly for frequencies close to $\omega a/(2\pi c) \approx 0.27$ and $\Delta \omega a/(2\pi c) \approx 0.29$. This reflects the strong confinement of these modes to core of the W1 PhC waveguide.

Using the results above, we can finally answer the question of ‘How many lateral layers of holes are needed to approximate a PhC waveguide with two semi-infinite PhC claddings?’ From Fig. 6.7 we can infer that the propagation losses of PhC consisting of four layers of holes deviate less than 100 dB/cm from the intrinsic propagation losses for all frequencies. Furthermore, for most frequencies $\gamma_r \approx 1$ holds, i.e., if we want to half the propagation loss contribution due to lateral radiation leakage, then we only need to add $\Delta n \approx 0.7 \approx 1$ layer of holes.
6.3.3.3 Finite Etch-Depth of the Holes

The scattering of light at holes/trenches of finite depth has been studied for years for 1D PhC, such as Bragg gratings [41, 229]. We thus first compile an overview of the well-established perturbation theories. The usually studied slab waveguide layer stack consists of a substrate layer, a waveguide core layer with thickness $t_{\text{core}}$ and an air cover layer. David et al. [51] distinguishes between three different scattering regimes with respect to the depth $d$ of the periodic scatterer: the Rayleigh regime for $d \ll \lambda$, an intermediate regime for $(t_{\text{core}} - d) > \lambda/n$, and the deep hole regime for $d > t_{\text{core}}$, where $n$ is the refractive index of the slab, $\lambda$ is the wavelength of the light in free-space and $t_{\text{core}}$ is the thickness of the core layer. The scattering efficiency in the Rayleigh regime scales with the square of the dipole induced by the perturbation $\Delta \varepsilon$, i.e., to the square of the volume of the scatterer. Thus the scattering losses $\alpha$ is quadratic with hole-depth $d$

$$\alpha \sim (d \Delta \varepsilon)^2.$$ (6.2)

For the intermediate regime David et al. [51] derived a cubic relation to the thickness of the still unetched waveguide $(t_{\text{core}} - d)$ by following the perturbation approach developed by Streifer et al. [265]

$$\alpha \sim (t_{\text{core}} - d)^{-3}.$$ (6.3)

Both approaches above rely on perturbation theory and thus are valid for weak perturbations. Summarizing, the scattering losses increase quadratically with $d$ for $d \ll \lambda$ and cubically with $d$ for $(t_{\text{core}} - d) > \lambda/n$. Thereafter a reversal of the trend is observed, i.e., the scattering losses start to decrease again. The reason is that the assumption that all observed scattering at the hole transfers to scattering loss is not valid anymore. Furthermore, perturbation approaches cannot be applied for these cases, where $(t_{\text{core}} - d) < \lambda/n$. Instead, full 3D simulations have to be used. For the (very) deep holes regime, the fields are decaying exponentially in the substrate, and hence it is assumed that the scattering/radiation loss scale exponentially with the hole-depth $d$ [51]

$$\alpha \sim \alpha_0 + Ae^{-\gamma_d d},$$ (6.4)

where $\alpha_0$ represent the intrinsic losses of the slab PhC waveguide. The exponential behavior of the propagation losses with hole depth was confirmed by 3D simulations performed by Fasquel et al. [67] for a single wavelength $\lambda = 1550$ nm.

The propagation losses are computed for various hole depths and are shown in Fig. 6.9, left. Two trends can be observed: First, the propagation losses are larger for lower frequencies. We attribute this effect to the spatial Fourier components of the Bloch wave that lie above the background-line. Figure 6.10 reveals that the relative magnitude of the spatial Fourier components of the Bloch wave above the background-line are smaller for higher frequencies (until $\omega a/(2\pi c) < 0.3$) Secondly, the propagation losses decrease monotonically for increasing hole-depths as it is expected. We expect that the Bloch modes are hardly influenced for holes that penetrate through the core of the PhC waveguide into the substrate layer $d > (t_{\text{top}} + t_{\text{clad}})$. However, the background changes: for holes that are
Figure 6.9: A) propagation loss $\alpha_{dB}$ for a number of etch-depths. B) numerical fit to Eq. 6.4 of the propagation loss as a function of the etch-depth for numerous frequencies within $\Delta \omega a / 2\pi c = 0.24 - 0.31$. The red curve is the fit averaged over all frequencies. This curve approaches a constant behavior for an etch-depth of $1.5 \mu m$. The inset of the right figure shows the decay constant of Eq. 6.4 for the same frequency range.
Influence of the Structural Imperfections on the Propagation Loss

Figure 6.10: We excited a long 2D W1 PhC waveguide as shown in the inset numerically. Then, a Fourier transform was applied to the resulting magnetic field $H_z$ in the center of the W1 waveguide. The ratio $R$ of the strongest spatial Fourier component in the first Brillouin zone (component above the background-line) to the strongest spatial Fourier component in the second Brillouin zone (dominant Fourier component $\tilde{k}_x$) is shown above. A larger propagation loss is expected for a higher ratio $R$.

\[ d \lesssim (t_{\text{top}} + t_{\text{core}}), \] the background-line of the substrate is given by the substrate line $\omega = k_x \cdot c/\n_{\text{InP}}$. If we increase the hole depth, then the background-line will slowly make a transition to the background-line of a infinitely extruded 2D PhC W1 waveguide (cf. Sec. 4.5.4).

The statement made by David et al. [51] and Fasquel et al. [67] that the propagation losses decrease exponentially with increasing hole-depth $d$ (Eq. 6.4) is verified in the following. Therefore, the numerically obtained propagation losses are fitted to

\[ \alpha_{dB}(d) = \alpha_{W1} + \alpha_d e^{-\gamma_d d}, \] (6.5)

where $\gamma_d$ and $\alpha_d$ are fitting parameters and $\alpha_{W1}$ is the intrinsic propagation loss. The coefficient of determination is larger than $R^2 > 0.99$ for all fits in the shown frequency range. We thus can confirm the exponential dependence of the propagation losses on the etch-depth $d$ for all frequencies of the single mode regime of the PhC waveguide. $\gamma_d$ increases slowly from $2/a$ for the low frequencies up to about $3/a$ for the high frequencies.

In a dry-etching process, the maximum achievable etch-depth is limited by the etching selectivity between the mask and the waveguide materials. Thus we like to address the question of ‘How deep one has the etch to achieve a negligible low propagation loss due to a finite-etch depth?’ A clear transition from the exponential regime to the constant regime ($\lim_{d \to \infty} \alpha_{dB}(d) = \alpha_{W1}$) can be observed in the Fig. 6.9 for almost all $\alpha_{dB}(d)$-curves. This transition is roughly at $d \sim 1.5 \mu m$ for our W1 PhC waveguide in the InP/InGaAsP system. A similar value has been ob-
tained by Fasquel et al. [67] for a wavelength $\lambda = 1550$ nm.

### 6.3.3.4 Conical Hole Shape

It was recognized by Burr et al. [34] and Ferrini et al. [72, 70] that a conical hole-shape can have a tremendous impact on the propagation losses. We start the section by identifying differences between the W1 PhC waveguide with a perfect cylindrical hole shape and the PhC waveguide with a conical hole shape with cone height $d_{cone} = 2.175 \, \mu m$. First, the radius varies linearly along the out-of-plane direction for a conical hole. This has a moderate influence on the Bloch modes of the PhC waveguide (we found a ratio of the Fourier components of the first to the second Brillouin zone that was about 8% higher than for the intrinsic PhC waveguide).

Furthermore the substrate background is strongly modified. For instance, the radius can become very small in the substrate, such that the band gap of the PhC cladding disappears. Then, the lateral radiation leakage contribution is expected to be large even in case of many lateral layers of holes. Finally, the background-line of the substrate layer is difficult to determine: for very shallow conical holes, the background-line is given by the light line of the substrate material. For very deep holes, the background-line is approximated by the fundamental mode of the 2D W1 PhC waveguide with $n_{core} = n_{InP}$. We expect that this approximation breaks down quickly for non-negligible sidewall angles.

Figure 6.11 shows the cross-section ($y$-$z$-plane) of the magnetic field for equally spaced values $x_i = \{0 \cdot a, 1/6 \cdot a, \ldots, a\}$ along the propagation direction within a period of the PhC waveguide for $\omega a/2\pi c = 0.265$ for a reduced mesh resolution of $a/12$. The column on the left (right) side of Fig. 6.11 shows the permittivity and the field plots of the intrinsic PhC waveguide (PhC waveguide with conical holes of $d_{cone} = 2.175 \, \mu m$). The magnetic field plots of the PhC waveguide with the conical holes reveal a strong radiation into the substrate. Additionally, a significant lateral radiation can be observed for all magnetic field plots for the PhC waveguide with the conical hole shape compared to the fields of the intrinsic PhC W1 waveguide. We conclude that conical holes lead to large radiation into the substrate and in large lateral radiation.

We present a numerical experiment, where the depths of the cones are varied while the radius is kept constant at the top surface ($r = 148$ nm). Because of the finite dimensions of the computational domain, the holes are truncated after $4.35 \, \mu m$ in the simulation by the PML boundary layer. A drawback of the numerical experiment is that the hole radius at the center of the vertical mode profile changes in every simulation. Hence, the effective filling factor slightly changes for every hole depth.

The angle of the sidewall is given by

$$\vartheta_{sidewall} = \arctan \left( \frac{r}{d_{cone}} \right).$$

The results of the corresponding cutback-simulations are shown in Fig. 6.12. Two trends can be observed: For large sidewall angles, the propagation loss is very large for all frequencies. Then the propagation loss decreases with decreasing sidewall angle and for certain frequencies is even lower than the intrinsic propagation loss.
Figure 6.11: Cross-sections of the magnetic field $H_z$ equally spaced along the propagation direction. Left: the intrinsic PhC waveguide. Right: the PhC waveguide with a conical hole shape with $d_{cone} = 2.175 \mu m$. A strong radiation into the substrate and a lateral radiation leakage can be observed for the PhC waveguide with a conical hole shape. Note that plots have been generated for a reduced mesh resolution $\alpha/12$ of the FDTD simulation. The used mesh for the propagation loss computation is $\alpha/20$. 
Figure 6.12: The cone-depth is varied for cones with a constant radius at the top surface. Whereas propagation losses monotonically improve for deeper conical holes close to the band edges, they reach a minimum for a hole depth of roughly 10 µm for frequencies around ωa/2πc ∼ 0.28, which is even lower than the intrinsic losses of a W1 PhC waveguide.

αW1. For sidewall angles smaller than 0.05° the propagation loss starts to increase again until the intrinsic losses are reached. This behavior seems to be completely counter-intuitive at first glance. However, since the effective radius changes for every different cone, the transmission spectrum changes, as well. If the minimum of the propagation loss over the spectrum shown in Fig. 6.12 is traced in absolute value and in frequency, one can observe that the minimum propagation loss is monotonically decreasing with the hole-depth and that the frequency position of the minimum loss is moving from lower to higher frequencies (dotted curve in Fig. 6.12). Additionally, the propagation loss spectrum becomes broader, e.g., the frequency range having a propagation loss smaller than 1000 dB/cm becomes larger with increasing hole depth.

Tanaka et al. [277] presented a similar theoretical investigation of the influence of the conical hole shape on the propagation losses in a membrane-type W1 PhC waveguide. If this waveguide is operated below the light-line, the only remaining loss channel out of the list given in Tab. 6.2 is mode coupling due to the asymmetry of the conical holes. And indeed, they found that the asymmetry introduced by the conical shape enables coupling from the gap-guided TE-like to the TM-like mode that leaks laterally out of the crystal due to the missing band gap for TM modes. The plot of the continuous electric field for a PhC with conical holes (dcone = 8 µm) etched into a low index contrast lithium niobate slab waveguide shown by Burr et al. [34] even suggests a further loss channel that consists of ‘deflecting’ the light towards the substrate. We could neither observe a clear deflection of the light nor a clear mode coupling between the TE-like and the TM-like modes. Instead we observe an additional lateral radiation leakage of the TE-like
PhC waveguide mode for shallow holes. The dominant loss mechanism is thus composed of lateral radiation leakage and radiation into the substrate. The relative contribution to the total propagation losses of the two loss channels depends on the hole depth.

In summary, this experiment shows that the conical hole shape has a severe impact on the propagation losses, since additional lateral radiation leakage adds to even larger out-of-plane losses observed in PhC waveguides with conical hole shapes. For example the smallest investigated conical hole \( d_{cone} = 2.175 \mu m \) leads to a propagation loss that is about a factor of eight larger than the one from the simulation using cylindrical holes with the same depth.

### 6.3.3.5 Cylindro-Conical Hole Shape

The cylindro-conical hole shape as observed experimentally (see Fig. 6.2) can be decomposed into a cylindrical hole shape with a finite depth followed by a conical hole shape. Therefore it is not expected that a new loss channel is introduced for the cylindro-conical hole shape and from a theoretical perspective the numerical experiment is not too interesting. However, the cylindro-conical hole shape is of practical relevance since it can approximate the fabricated hole shape rather accurately. This hole shape is composed of a cylindrical hole of depth \( d_{top} = 500 \) nm at the top followed by a cone of depth \( d_{bot} = 3.3 \mu m \) (cf. Fig. 6.2). In the numerical experiment, the depth of the hole is kept constant at \( d = d_{top} + d_{bot} = 4.35 \mu m \).

![Cylindro-Conical Hole Shape](image)

Figure 6.13: The propagation losses are shown for cylindro-conical hole shapes having all the same depth of 4.35\( \mu m \) but a different share of the cylindrical part at the top. By increasing the depth of the cylindrical part the frequency position of the lowest propagation loss moves from lower frequencies to higher frequencies. For cylinders not penetrating completely through the guiding core layer (cylinder depth smaller than 822nm), the spectral behavior changes considerably and the propagation losses even increases with increasing cylinder depth.
which corresponds roughly to the maximum etch-depth achieved by our process for a radius of \( r = 435 \text{ nm} \) [264]. The cylindrical part of the hole is gradually increased from \( d_{\text{top}} = 0 \) until \( d_{\text{top}} = 0.5d \). The computed propagation losses can be seen in Fig. 6.13. For cylinders having a depth of less than \( d_{\text{top}} = 822 \text{ nm} \) (i.e., they do not completely penetrate through the core layer), the mode is considerably affected by the conical hole shape and the ‘effective radius’-effect. For these hole shapes, a substantial variation in the propagation loss spectrum can be observed as a function of \( d_{\text{top}} \): The position of the minimum propagation loss shifts from lower to higher frequencies and the propagation loss increases slightly with increasing \( d_{\text{top}} \). For cylinder depths above \( d_{\text{top}} > 822 \text{ nm} \), the propagation loss decreases steadily with increasing \( d_{\text{top}} \).

Because of the practical relevance, let us ask the question of ‘How large the upper, cylindrical part of the hole has to be for a negligible propagation loss contribution due to the imperfect hole shape for our W1 PhC waveguide?’ From Fig. 6.13 it can be deduced that an etch-depth of straight side-walls of roughly \( d_{\text{top}} > 1.1 \mu m \) is sufficient to obtain propagation losses that are comparable to the intrinsic W1 PhC waveguide, if the PhC waveguide is operated with frequencies larger than \( \omega a/2\pi c = 0.285 \).

### 6.3.4 Propagation Losses Originating From Randomly Distributed Imperfections

In a next step, we consider structural imperfections that are randomly distributed. The main differences of scattering at randomly introduced geometrical imperfections to periodic imperfections are

1. The Bloch modes of the PhC waveguide are not changed for small random imperfections and consequently the relative contribution of the spatial Fourier components above the background-line and the background-line are not changed.

2. The randomly distributed imperfections enable coupling between the excited Bloch modes along the propagation direction. As discussed in Sec. 4.1.2.3 we expect that the radiated power is proportional to the intensity \( I \) of the light that interacts with the small disturbances.

The procedure to obtain the numerical propagation losses is slightly different: Since we have to introduce randomly structural imperfections in our simulations, the resulting transmission spectra of the various length of PhC waveguides may exhibit small irregular, unpredictable frequency features. To reduce the influence of those features, three PhC waveguides were generated for each PhC waveguide length. Thereafter the average of the three obtained transmission values was computed and used for the subsequent fit to compute the propagation loss \( \alpha_{dB} \). Using only three randomly generated PhC waveguides of the same length is not accurate, however, using considerably more waveguides is not feasible because of the relatively costly numerical simulations.
6.3.4.1 Lattice Disorder

In the numerical experiment dedicated to lattice disorder, a random value has been added to the center position of the holes in both x and y direction ($\sigma_a^2 = \sigma_x^2 + \sigma_y^2$). The random value is generated according to a normal distribution with a mean coinciding with the center of the hole and a standard deviation of $\sigma = \sigma_a a$, where $\sigma_a$ is given in units of the lattice constant $a$. The propagation loss is computed by using transmission spectra that are averaged over three randomly generated PhC waveguides of the same length. The propagation losses are very high for frequencies in the slow wave regime ($\Delta\omega/\omega_c = 0.24 - 0.245$). For example, propagation losses larger than $-4500\,dB/cm$ are observed in the slow light regime for a standard deviation of $\sigma_a = 0.025$, whereas they are of similar magnitude as for the intrinsic W1 PhC waveguide in the center of the photonic band gap. The lateral mode profile of slow light modes typically extends further into the PhC claddings (cf. Fig. 6.8). The percentage of the mode intensity that interacts with the PhC holes is thus higher for slow light modes and a higher propagation loss is expected.

Lattice disorder of PhCs has been studied by various authors [71, 95, 202]. Hughes et al. [95] studied slow light modes in membrane-type PhC waveguides and predicted a square dependence of the propagation losses with the group velocity near the band edge due to disorder of the PhC lattice. That square law dependence of the propagation losses was established for the case of inexistent out-of-plane losses, i.e., it was assumed that light can only couple into the guided PhC waveguide mode propagating in either forward or backward direction. Recently, O’Faolain et al. [202] confirmed this phenomenon experimentally for membrane-type PhC waveguides. For slow light modes far away from the band edge, the scaling law is linear. For substrate-type PhC waveguides, the assumption made of inexistent out-of-plane losses does not hold and additional out-of-plane radiation into

![Figure 6.14: Propagation losses as a function of an artificially induced lattice disorder. The standard deviation $\sigma_a$ is normalized to the lattice constant $a$ (e.g. $\sigma_a = 0.025$ corresponds to $\sigma = \sigma_a \cdot a = 0.025 \cdot 435\,nm = 10.875\,nm$.](image-url)
the cladding layers is expected.

Even though large propagation losses are expected for slow light modes for moderate lattice disorders, the losses originating from lattice disorder are practically very small compared to out-of-plane losses. The reason is that displacement errors are very small after the etching-processes (in the order of $5.2\,nm \approx 0.01 - 0.012\,a$). Figure 6.14 shows that for such small lattice disorders, the fabrication related propagation losses are irrelevant.

### 6.3.4.2 Variations in the Hole Radii

A random number generated according to a normal distribution with a standard deviation of $\sigma_r = \sigma_r\,r$ and a mean equal to zero is added to the radius of every hole in the PhC waveguide. Three W1 PhC waveguides have been generated for each waveguide length. The propagation loss is computed by using the average transmission spectrum obtained from the transmission spectra of the three randomly generated samples. The propagation losses for standard deviations ranging from $\sigma_r = 0.025\,r$ to $\sigma_r = 0.1\,r$ are shown in Fig. 6.15. While frequencies in the range $\frac{\Delta\omega a}{2\pi c} = 0.275 - 0.305$ are hardly influenced, the frequency region close to the lower band-edge is strongly affected by the introduced radius disorder. We attribute this effect to the larger lateral extent of the PhC waveguide mode for slow light modes (cf. Fig. 6.8) and hence to a higher percentage of the intensity of the mode that interacts with the PhC holes. The standard deviation of the hole radius for our fabricated PhCs were measured from top-view micro-graphs and a variation of less than $\sigma_r < 0.02\,r$ is obtained (cf. [296] and appendix A.5). For this variance ($\sigma_r < 0.02$), no measurable effect on the propagation loss is expected from variations of the hole radii.

![Hole Radius Variations](image_url)

Figure 6.15: Propagation loss for artificially introduced variations of the hole radii. The propagation loss is most severely affected in the frequency range close to the lower band-edge.
6.3.4.3 Surface Roughness

The roughness at the surface is formed by the dry-etching process. A rough surface can scatter light of a guided mode into radiative modes. Strasser [262, 260] has characterized the surface roughness by scanning the surface of cleaved PhC holes with an atomic force microscope tip and found a roughness of 2-3 nm RMS for our process. To resolve such a roughness, a minimum grid resolution of the FDTD mesh of $\Delta x = \frac{435 \text{nm}}{3 \text{nm}} = 145 = \frac{a}{145}$ would be required which is beyond the feasibility of our method on the available computer resources. Therefore, other methods are required. For example, Johnson et al. [111] applied the volume-current method to investigate the effect of surface roughness on the propagation losses. They found that PhC waveguides are relatively robust against surface roughness, i.e., compared to disorder in the lattice constant or the hole radius of the same magnitude, the contribution of the surface roughness is negligible.

6.4 Discussion

The discussion is organized in two parts: First, the structure properties related to fabrication imperfections are discussed and – as a result – ‘demands on the process’ are deduced. The structural imperfection predominantly responsible for the large propagation losses is identified. Second, the remaining structural imperfections (the asymmetric vertical layer structure, the finite number of lateral layers of holes and the intrinsic losses of the PhC waveguide design) are analyzed aiming at a set of design rules. Furthermore, the most urgent question of ‘What can be done to reduced the large propagation losses?’ is addressed.

6.4.1 The Limiting Structural Imperfection

Because of the significance of the slow light mode for integrated optics and because of the fact that the influence of the structure properties are generally strongest in the slow light regime, two distinct frequency ranges are examined ($\Delta \omega / 2\pi c \simeq 0.27 - 0.30$ and $\Delta \omega / 2\pi c \simeq 0.24 - 0.245$). For both frequency ranges, the minimum requirements for a particular structure property are deduced by imposing the condition that the propagation losses shall not deviate more than 100 dB/cm from the value of the intrinsic propagation loss of the W1 PhC waveguide with a infinitely-deep cylindrical hole shape. The results for the structure properties related to fabrication are listed in Table 6.3 in the column titled ‘demands on the process’. Furthermore, we add the corresponding values obtained by measurements of our fabricated devices. As expected, the demands on the process are higher for slow light operation except for the etch-depth. By comparing the third and fourth columns of Table 6.3 to the measured values, it can be seen that our fabricated devices already fulfill the requirement for the etch-depth, the lattice disorder and the variance of the radius. The good agreement of the propagation loss measurements with the simulated propagation loss using the approximative cylindro-conical hole shape supports the claim that lattice-disorder, variances in the radii and surface roughness lead to negligible propagation loss contributions.
Table 6.3: Requirements for the fabrication and design rules for the W1 PhC waveguide etched into a InP/InGaAsP/InP layer stack with a 522 nm thick core and a 348 nm thick top-cladding layer for the operation in the passband and in the slow light mode. The limiting factor indicates, where the fabricated device does not meet the requirements up to a factor of ±100 dB/cm.

<table>
<thead>
<tr>
<th>structural imperfection</th>
<th>measured etch-depth</th>
<th>demands on the process</th>
<th>demands on the process</th>
<th>limiting factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>etch-depth</td>
<td>4.2 μm (r = 417 nm)</td>
<td>d &gt; 2.4 μm</td>
<td>d &gt; 2.4 μm</td>
<td>no</td>
</tr>
<tr>
<td>conicity</td>
<td>$\vartheta \sim 2.5^\circ$</td>
<td>$\vartheta \leq 0.78^\circ$</td>
<td>$\vartheta \leq 0.97^\circ$</td>
<td>yes</td>
</tr>
<tr>
<td>conical part of</td>
<td></td>
<td></td>
<td></td>
<td>yes</td>
</tr>
<tr>
<td>cylindro-conical shape</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>lattice disorder</td>
<td>$\sigma_a = 0.01 - 0.012$ (r = 5.2 nm)</td>
<td>$\sigma_a &lt; 0.025$</td>
<td>$\sigma_a &lt; 0.013$</td>
<td>no</td>
</tr>
<tr>
<td>variance of the radius</td>
<td>$\sigma_r = 0.01 - 0.02$ (r = 3 nm) [296]</td>
<td>$\sigma_r &lt; 0.1$</td>
<td>$\sigma_r &lt; 0.05$</td>
<td>no</td>
</tr>
<tr>
<td>surface roughness</td>
<td>$\sigma_R \approx 0.017$ (r = 2.5 nm) [262]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>number of lateral layers of</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>holes</td>
<td>-</td>
<td>$n \geq 4$</td>
<td>$n \geq 6$</td>
<td>no</td>
</tr>
</tbody>
</table>

The comparison further suggests that the imperfect hole shape is solely responsible for the difference between the measured propagation losses and the intrinsic propagation losses. Considering Table 6.3 again, it can be seen that the measured sidewall angle is larger than the required sidewall for a negligible influence originating from the conical or the cylindro-conical hole shape. Thus, from the fabrication point of view, the limiting factor are the angled sidewalls.

Actually, only the angled sidewalls in the uppermost part of the holes are responsible for the deviation of the propagation losses from the intrinsic losses. To support this claim, we compare the propagation losses of two devices having the same hole depth of 4.3 μm, but a different hole shape: one consist of a cylindrical hole of 500 nm followed by a cone of 3.85 μm height, and the other one is a cone with depth 4.35 μm. Note that the sidewall angle of the conical part of the first type of hole is larger than for the second. Even so, the propagation loss figure of the cylindro-conical hole shape is superior to the one of the conical hole shape.

There are two strategies that can be pursued to lower the propagation losses due to the imperfect hole shape: First, it can be tried to improve the fabrication process to increase the verticality of the holes in the uppermost part of the hole (≈ 1 μm). Kaspar [120] increased the hard mask from 400 nm to 1 μm to achieve...
even deeper holes with smaller sidewall angles. The measured propagation losses of those deep holes are as low as 400 dB/cm (cf. Fig. 7.3). Furthermore, we developed an annealing step in the MOVPE (as described in Sec. 7.4) that results in holes that are closer to a cylindrical hole shape. Second, alternative hole shapes may not only reduce the propagation losses due to the angled sidewalls, but may even improve the propagation loss figure of the PhC waveguide (cf. Sec. 7.3).

6.4.2 Intrinsic Propagation Losses of the PhC Waveguide Design

In a next step, we try to deduce rules for designing low (intrinsic-) loss PhC waveguides from the made numerical experiments. As discussed in chapter 4, intrinsic propagation losses in substrate-type PhC waveguides arise from the fact that the waveguide is excited beyond the cutoff. A leaky Bloch wave is excited if it contains spatial Fourier components above the background-lines of the cladding layers or if the PhC cladding layer is of finite extent laterally. From experiment 6.3.3.2 a minimum number of four (six) lateral layers of holes can be inferred for the passband (slow light) frequency range (also listed in Table. 6.3). On the other hand, no clear design rule can be derived from the experiments concerning the out-of-plane losses.

The numerical experiment of the etch-depth $d$ confirms the result obtained in Sec. 4.5.4, namely that a sufficiently deep hole-depth can approximate the background formed by infinitely deep holes. This approximation of the background line no longer applies for conical holes or cylindro-conical holes and high radiation losses into the substrate are observed for these hole shapes.

Chapter 7 is devoted to find better PhC waveguide designs, e.g., PhC waveguides that have smaller contributions of the spatial Fourier components above the background-line. However, we will discuss already here the influence of structural imperfections (a realistic cylindro-conical hole shape) on the propagation losses of two waveguides that have a lower intrinsic propagation loss. For instance, a propagating Bloch wave in a W3 PhC waveguide exhibits considerably smaller spatial Fourier components above the background-line. Experimentally measured propagation losses better than 20 dB/cm were reported [271, 248] for the multimoded W3 PhC waveguide. Therefore, we simulated the intrinsic propagation losses and the propagation losses of the W3 PhC waveguides with the realistic hole shape for our InP/InGaAsP/InP layer stack with the PhC parameters $r = 0.34a$ and $a = 435$ nm. The simulation is shown in Fig. 6.16 and reveals that the W3 PhC waveguide has propagation losses better than 150 dB/cm for all frequencies except for the frequency range of the even mode stop band at $\Delta \omega a / 2\pi c = 0.267 - 0.274$. The cylindro-conical hole shape mainly increases the propagation losses close to the stop bands.

A single mode waveguide design has been proposed by Kuang and O’Brien [141, 140], where one of the two PhC W1 waveguide boundaries is shifted by $a/2$ along the propagation direction. This design has only weak spatial Fourier components of the Bloch wave above the background-line. We will refer to it as the W1-$a/2$ waveguide. The simulated intrinsic propagation losses and the propagation losses of the PhC waveguides with the realistic hole shape for our InP/InGaAsP/InP layer stack with the PhC parameters $r = 0.34a$ and $a = 435$ nm are shown in Fig. 6.16.
Figure 6.16: The propagation losses are shown for a W1 PhC waveguide with laterally shifted PhC boundaries (bottom) and for a multimoded W3 PhC waveguide (top). For each design, the propagation losses have been computed using a perfectly cylindrical hole shape (blue) and a realistic cylindro-conical hole shape (red). The black curve represent the propagation loss for a standard W1 PhC with realistic hole shape, and is added for a direct comparison to the alternative waveguide designs.
First, we can confirm the relatively low propagation losses ($\approx 100 \text{ dB/cm}$) for an ideal, infinitely-deep cylindrical hole shape for the W1-\(a/2\) waveguide for a frequency of $\omega_{a/2}/2\pi c \approx 0.25$. Around this frequency the propagation loss is dramatically higher for the realistic cylindro-conical hole shape, whereas for frequencies close to $\omega_{a/2}/2\pi c \sim 0.325$ the hole shape hardly influences the propagation losses ($\alpha_{dB} \sim 270 \text{ dB/cm}$).

The main conclusion that can be drawn from these two additional experiments is that a realistic hole shape has a tremendous impact on performance of intrinsically low-loss PhC waveguide designs. Therefore, a systematic search for PhC waveguides exhibiting low propagation losses can not be divided into the two subproblems of i) finding a beneficial hole shape and ii) finding a beneficial PhC waveguide design. An optimization of the PhC waveguide design has to be performed with a costly numerically method in 3D that can simulate the propagation losses originating from the imperfect hole shape.

### 6.5 Conclusion

In summary, we have performed a set of numerical experiments to analyze the influence of fabrication imperfections and other structural properties. Since all experiments have been performed with the same numerical method on the same W1 PhC waveguide design, a quantitative comparison is possible. This allowed us to identify the angled sidewalls in the uppermost part of the holes to be the main source for propagation losses due to fabrication imperfections. Therefore, the main effort in improving the technology should be directed to reducing the conical sidewalls in the upper part (until a depth of about 1.1 $\mu$m) of the hole rather than to increasing the hole-depth or the smoothness of the sidewalls. Even if all demands on the fabrication could be met, a minimum achievable loss of about 300 dB/cm would remain for a W1 PhC waveguide. Alternative waveguide designs, such as the W3 PhC waveguide and the W1-\(a/2\) PhC waveguide exhibit substantially lower intrinsic propagation losses for our InP/InGaAsP layer stack. However, the alternative low-loss PhC waveguide designs can lose its favorable properties, if realistic hole shapes are considered.

Furthermore, many previously reported loss channels, such as mode coupling due to the asymmetry (cf. Sec. 6.1.4) and incoherent scattering at geometrical non-uniformities (cf. Sec. 6.1.5), can be dominant for membrane-type PhC waveguides operated below the light line. However they all play a subordinate role for substrate-type PhC waveguides. The large propagation losses observed in substrate-type PhC waveguides are largely due to out-of-plane radiation, i.e., the excitation of the substrate-type W1 PhC waveguide beyond the cutoff.
Reducing the Propagation Losses of Single-Mode Substrate-Type PhC Waveguides

Parts of this chapter are published in Ref. [118] and Ref. [119].

The high propagation losses of substrate-type PhC W1 waveguides in the order of 1000 dB/cm [260, 294] and the lack of efficient current injection schemes for membrane-type PhCs prevent the realization of efficient electrically pumped active PhC devices. A substantial part of the large propagation losses of substrate-type PhCs can be assigned to an imperfect hole shape (mainly the angled sidewalls of our fabricated holes [116]). This part of the losses may be reduced by further improving the process technology. However, a rather large propagation loss remains even for a perfectly fabricated device. This remaining propagation loss is a property of the PhC waveguide design.

In this chapter, we address the questions of ‘What can be done to reduce the large propagation losses of substrate-type PhC waveguides?’ and ‘Is it possible to improve the propagation loss figure of the substrate-type PhC waveguide technology to a competitive level ($\alpha_{dB} < 20$ dB/cm) with respect to membrane-type PhC waveguides?’ We start by summarizing the relevant achievements and insights gained in the previous chapters:

- We can accurately compute the propagation losses of substrate-type PhC waveguides without the need for fitting parameters (Chapter 5). The only simplification with respect to an experimental structure is the assumption that all holes are of identical shape.

- The reasons for the large propagation losses of substrate-type W1 PhC waveguides are a) the imperfect hole shape (extrinsic losses) and b) the PhC waveguide design, which does not provide a truly guided mode (intrinsic losses, see chapter 6).

- The relative position of the spatial Fourier components of the Bloch wave with respect to the background-line is relevant to determine regions of truly
Reducing the Propagation Losses of Substrate-Type PhC Waveguides

From these results, we can deduce the following strategies to improve the loss figure of single-mode PhC waveguides:

- Find a new PhC waveguide geometry that provides a Bloch wave with only small or ideally no spatial Fourier components above the background-line (Sec. 7.2).
- Find another background for which the separatrix lies above all Fourier components of the PhC waveguide modes (Sec. 7.3 and chapter 8).
- Improve the fabrication technology to yield holes with a lower sidewall angle (Sec. 7.4).

The focus of this chapter lies on measures to improve the propagation loss figure without a strong modification of the available fabrication process. Such measures are:

- modification of the pattern of the PhC waveguide (change of the mask for E-Beam lithography)
- modification of the layer stack (change of the MOVPE growth)

The main difficulty is that the loss mechanisms – losses due to fabrication imperfections and the excitation of unconfined modes – are not independent of each other. For instance, a PhC waveguide design may have a low propagation loss for ideal cylindrical holes, but is sensitive on an imperfect hole shape. The search for a better PhC waveguide design requires extensive numerical simulations in 3D, exclusively. Practically, a waveguide optimization including all relevant effects simultaneously is beyond the current capabilities of the available numerical resources. For the moment, there is no way around splitting the problem into smaller parts and optimizing them separately. However, such a procedure bears the risk that the combination of the optimization results not necessarily lead to the overall optimum design for our process technology.

First we address the question of an optimum layer stack for the hole shape given by our process. Then, the question about the existence of other PhC designs that exhibit lower propagation losses for an ideal, cylindrical hole shape is tackled. We explore possible PhC waveguide geometries in 2D with an algorithm that is motivated from evolutionary strategy. The target of the algorithm is to find new PhC waveguide designs such that the magnitude of the spatial Fourier components of the Bloch wave above the background-line is small. Thereafter, we pursue the strategy of modifying the substrate-background to reduce radiation into the substrate. We find promising results for a W1 PhC waveguide with an increased hole radius in the substrate.

Finally, two post-treatment steps were developed to reduce the propagation losses of substrate-type W1 PhC waveguides: A thermally driven mass transport process was established to reduce the sidewall-angles of the holes. Furthermore, for the implementation of the most promising design – a W1 PhC waveguide with an increased hole radius in the substrate layer – a very slow selective etch process was developed. By using the combination of both developed process steps, a W1 PhC waveguide is obtained that exhibits optically measured propagation losses of...
less than $\alpha_{dB} < 154 \text{ dB/cm}$. These propagation losses represent an improvement of more than a factor of three with respect to previously published state-of-the-art values [274, 260].

### 7.1 Optimization of the Layer Stack

In this subsection, we address the following question of ‘What are the minimum achievable propagation losses $\alpha_{dB}$ for a given, fixed hole shape but for varying thicknesses of the InP/InGaAsP/InP layers?’

The results in Sec. 6.3.3.5 suggest that the conical part of the hole is responsible for the propagation losses due to an imperfect hole shape. Thus, to improve the propagation losses, we either have to increase the verticality of the fabricated holes – which is a laborious task and may be accompanied by negative side effects such as a higher sidewall roughness – or by reducing the mode overlap with the conical hole shape. For instance, if the thicknesses of the top cladding and the core layer are reduced, then the center of the vertical mode profile is pushed towards the upper part of the hole and one would expect lower propagation losses. This argumen-
Reduction of Propagation Losses of Substrate-Type PhC Waveguides

Radiation originates from the notion, that the radiation losses are related to the mode overlap with localized imperfections (cf. Benisty [18] and Ferrini [72, 70, 71, 69]). This notion is conceptually wrong and leads to false predictions of the trends of the propagation losses as we will see in the following.

An optimization of the layer stack for the CAIBE [187] process has already been performed numerically by Ferrini et al. [69] using the empirical 2D ε″-model [18, 70, 72]. An optimum was found for a core thickness of \( t_{\text{core}} = 522 \text{ nm} \) and a top cladding thickness of \( t_{\text{clad}} = 300 \text{ nm} \). They assumed a cylindro-conical hole shape with a cone angle \( \alpha = 0.5^\circ \) in the substrate layer and a total hole depth of \( d = 4 \mu m \) [69]. Since we have the means to perform the optimization more rigorously with our accurate cutback technique based on FDTD, we reassess the optimization task for our technology and for our hole shape consisting of a 500 nm deep cylindrical hole followed by a conical hole of depth \( d_{\text{cone}} = 3.3 \mu m \). In Fig. 7.1 the propagation losses for four thicknesses of the core layer (400 nm (top left), 522 nm (top right) and 644 nm (bottom left) and 766 nm (bottom right)) and four top cladding thicknesses ranging from 0 \( \mu m \) to 1 \( \mu m \) are shown for realistic hole shapes. The propagation loss decreases for thicker core layers. The thickest core layer \( t_{\text{core}} = 766 \text{ nm} \) is close to the vertical single mode condition (cf. Fig. 7.2) such that the core layer cannot be increased much further. An optimum value for the top cladding thickness of \( t_{\text{clad}} = 348 \text{ nm} \) is found for all core layers. Furthermore, the frequency bandwidths\(^1\) of the propagation loss spectra are larger for thinner top claddings. The lowest propagation loss value \( \alpha_{dB, \text{best}} = 666.2 \text{ dB/cm} \) is found for a top cladding thickness of \( t_{\text{clad}} = 348 \text{ nm} \) and core layer thickness of \( t_{\text{core}} = 766 \text{ nm} \). Our currently used (non-optimum) layer stack (core layer thickness of \( t_{\text{core}} = 522 \text{ nm} \) and top cladding of \( t_{\text{clad}} = 348 \text{ nm} \)) that has been originally proposed by Ferrini et al. [69] exhibits a higher minimum propagation loss of

\[ \alpha_{dB, \text{best}} = 666.2 \text{ dB/cm} \]

\(^1\)Here, we use the term frequency bandwidth for the frequency range \( \Delta \omega \) of propagation loss values \( \alpha_{dB} \) that fulfill the condition \( \alpha_{\omega} < \alpha_{dB, \text{min}} \times 2 \).

![Figure 7.2: The vertical single mode condition for a four layer structure (InP, InGaAsP, InP, Air) computed by the 1D mode solver of M. Hammer [87].](image)

Figure 7.2: The vertical single mode condition for a four layer structure (InP, InGaAsP, InP, Air) computed by the 1D mode solver of M. Hammer [87].
Figure 7.3: Propagation losses $\alpha_{dB}$ as low as 400 dB/cm were measured by P. Kaspar for a layer stack with $t_{clad} = 300$ nm and $t_{core} = 640$ nm and $r \approx 0.263a$, experimentally [120]. The blue curves are the simulated propagation losses $\alpha_{dB}$ obtained by the cutback-method for a cylindrical hole shape with radius $r = 0.237a$ and $r = 0.25a$.

$\alpha_{dB} = 1073$ dB/cm.

In summary, we conclude that

- Reducing the layer thicknesses to move the mode profile towards the vertical, upper part of the hole does not yield lower propagation losses. In contrary, the smallest core layer thickness $t_{core} = 400$ nm results in the largest propagation losses. The perception that the propagation losses are determined by the mode overlap with imperfect local scatters as used by Ferrini et al. and Benisty et al. is not entirely correct as it is anticipated from Sec. 4.3.2.

- A new and optimum layer stack ($t_{core} = 766$ nm and $t_{clad} = 348$ nm) was found that has propagation losses as low as $\alpha_{dB} = 666.2$ dB/cm. This is a more than 400 dB/cm improvement of the propagation losses with respect to the alleged optimum computed by Ferrini et al. [69].

- The propagation loss measurements performed by P. Kaspar [120, 122] for a PhC waveguide using a layer stack of $t_{core} = 640$ nm and $t_{clad} = 300$ nm (motivated by this investigation) resulted in propagation losses as low as $\alpha_{dB} = 400$ dB/cm and supports our findings (cf. Fig. 7.3).

We conclude that a substantial reduction of the propagation losses of substrate-type W1 PhC waveguides can be achieved by optimizing the vertical layer stack.

### 7.2 Alternative PhC Waveguide Designs

In this section, we explore the potential of new in-plane PhC waveguide geometries. This investigation was motivated by the pioneering work of Kuang and...
O’Brien [141, 140]. They reported on a low-loss substrate-type PhC waveguide design for the AlGaAs/GaAs system with a theoretically predicted minimum value of $\alpha_{dB} = 46$ dB/cm. This proposed PhC waveguide is obtained by removing one row of holes from a hexagonal lattice and then shifting one side of the PhC cladding by half a period along the waveguide axis. The resulting PhC waveguide – we refer to it as the W1-$a/2$ waveguide – supports a Bloch wave with very small spatial Fourier components above the background-line. Kuang and O’Brien [141, 140] correctly realized, that this weak spatial Fourier component in the first Brillouin zone is responsible for the low intrinsic propagation losses observed in this waveguide. Their explanation for the discovered phenomenon is that «the fields in the PhC claddings are out of phase because of the spatial shift in the lattice». This cancellation, can be seen in the planar 2D Fourier transform of the magnetic field $H_z$ in the core layer that is shown in Fig. 7.4 (right). The spatial Fourier component in the first Brillouin zone seems to be completely missing for the W1-$a/2$ waveguide, whereas a small spatial Fourier component can be seen in the first Brillouin zone for the conventional W1 PhC waveguide (cf. Fig. 7.4, left). Further note that the 2D Fourier transform of the magnetic field results in rather sharp $k_x$-components and a large spread in the $k_y$-direction. The large spread in $k_y$ direction signifies a tight lateral confinement of the PhC waveguide mode. Kuang and O’Brien [141] pointed out that the proposed W1-$a/2$ may not be the optimum waveguide, and that even better waveguides may be found.

First, we compute the ratio $R = \varphi_{-1}/\varphi_2$ of the spatial Fourier component of the Bloch wave located in the first Brillouin zone $\varphi_{-1}$ and in the second Brillouin zone $\varphi_2$ for $k_y = 0$ for the standard waveguides as shown in Fig. 2.13. We include the waveguides, where one side of the PhC cladding is shifted by half a period, in our investigation. The results are shown in Fig. 7.5. The first thing to notice is that the standard W1 PhC waveguide has a relatively high ratio $R = \varphi_{-1}/\varphi_2$ for all

Figure 7.4: The 2D Fourier transform of the magnetic field $H_z$ of a W1 PhC waveguide (left) and the W1 – $a/2$ waveguide for an excitation frequency $\omega a/2\pi c = 0.25$. The white arrow points at the position, where the spatial Fourier component in the first Brillouin zone is expected.
Figure 7.5: The plots show the ratio $R = \varphi_1 / \varphi_2$ of the spatial Fourier component of the Bloch wave located in the first Brillouin zone $\varphi_1$ and in the second Brillouin zone. The gray shaded area corresponds mode stop bands, i.e., frequency regions, where the ratio $R$ is meaningless. A low ratio $R$ is found for the $W_1-a/2$, the $W_2$, the $W_2-a/2$ and the $W_3$ waveguide. Of these waveguides, only the $W_1-a/2$ waveguide is single-moded. The standard $W_1$ waveguide has a relatively large ratio $R$ as well as the $W_1$ waveguide oriented along the $\Gamma - M$ direction.
frequencies except for the range form $\omega a / 2\pi c = 0.29$ to $\omega a / 2\pi c = 0.3$. Also the waveguides oriented in $\Gamma - M$ direction exhibit rather large ratios $R$ except for a single frequency $\omega a / 2\pi c = 0.277$ ($W_1, \Gamma - M$) and $\omega a / 2\pi c = 0.299$ ($W_1 - a/2, \Gamma - M$). Therefore, the $\Gamma - M$ waveguides are discarded from the list of potential waveguide designs. All multimode waveguides, i.e., the $W_2$, the $W_2 - a/2$ and the $W_3$ waveguide exhibit very low ratios $R$ for all frequencies except for the mini-stop band frequency range. The lowest ratio $R = 0.000112$ was obtained for the $W_2 - a/2$ and for a frequency $\omega a / 2\pi c = 0.2420$. The $W_1 - a/2$ waveguide has similar low ratios $R$, but additionally provides single-mode operation.

To explore the potential of completely new PhC waveguide geometries, an exploration algorithm was implemented. The algorithm was inspired by evolutionary strategy. As opposed to an optimization routine, the aim of our algorithm is not to fine-tune a design, but to explore a large search space. Figure 7.6 explains the procedure of the employed algorithm. The PhC waveguide has 6 rows of holes on each side of the core of the waveguide. The positions of the outermost three rows of holes (filled with a black color in Fig. 7.6) are fixed intentionally in the exploration routine to guarantee a photonic band gap. But, this measure constrains the search

![Figure 7.6: Schematics of the exploration algorithm.](image)

**Geometry**: The position $x_i \in [0, 1] \cdot a$, $y_i \in [0, 1] \cdot \sqrt{3} \cdot a / 2 + y_{i0}$ of the three innermost holes $h_i$ with respect to the center of the PhC waveguide have been encoded into a genome.

**Algorithm**: The algorithm is initialized by randomly generating 50 individuals. The ten best solutions are used as the first parent population. Then two individuals are chosen randomly from the parent population. A cross-over is performed, followed by a mutation operation resulting in two new child individuals. This step is repeated until a child population of 20 individuals is reached. After the computation of the fitness for all children, the ten best individuals are selected. They replace the entire parent population.
Figure 7.7: The plots show the ratio $R = \frac{\varphi^{-1}}{\varphi^2}$ of the spatial Fourier component of the Bloch wave located in the first Brillouin zone $\varphi^{-1}$ and in the second Brillouin zone $\varphi^2$ for the best solutions obtained by four different runs of the exploration algorithm. The gray shaded area corresponds to mode stop bands, i.e., frequency regions, where the ratio $R$ is meaningless. The best solutions have common geometric properties: the first rows are shifted roughly by $a/2$ with respect to each others.

Table 7.1: Parameters for the structures shown in Fig. 7.7.

<table>
<thead>
<tr>
<th>Structure</th>
<th>$r [a]$</th>
<th>$x_1 [a]$</th>
<th>$x_2 [a]$</th>
<th>$x_3 [a]$</th>
<th>$x_4 [a]$</th>
<th>$x_5 [a]$</th>
<th>$x_6 [a]$</th>
</tr>
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<tr>
<td>A</td>
<td>0.2758</td>
<td>0.4965</td>
<td>0.8287</td>
<td>0.8386</td>
<td>0.2268</td>
<td>0.5645</td>
<td>0.1832</td>
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<tr>
<td>B</td>
<td>0.2929</td>
<td>0.0247</td>
<td>0.0118</td>
<td>0.5353</td>
<td>0.0095</td>
<td>0.5252</td>
<td>0.0219</td>
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<tr>
<td>C</td>
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<td>0.4161</td>
<td>0.3144</td>
<td>0.5191</td>
<td>0.9675</td>
<td>0.6209</td>
<td>0.3529</td>
</tr>
<tr>
<td>D</td>
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<td>0.9399</td>
<td>0.3732</td>
<td>0.4503</td>
<td>0.9060</td>
<td>0.2379</td>
<td>0.9962</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Structure</th>
<th>$y_1 \frac{\sqrt{3}}{2} a$</th>
<th>$y_2 \frac{\sqrt{3}}{2} a$</th>
<th>$y_3 \frac{\sqrt{3}}{2} a$</th>
<th>$y_4 \frac{\sqrt{3}}{2} a$</th>
<th>$y_5 \frac{\sqrt{3}}{2} a$</th>
<th>$y_6 \frac{\sqrt{3}}{2} a$</th>
<th>Fitness</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.6839</td>
<td>0.6498</td>
<td>0.5873</td>
<td>0.6423</td>
<td>0.6465</td>
</tr>
<tr>
<td>B</td>
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<td>0.4678</td>
<td>0.6223</td>
<td>0.6726</td>
<td>0.7452</td>
<td>0.5615</td>
<td>0.7048</td>
</tr>
<tr>
<td>C</td>
<td>...</td>
<td>0.6340</td>
<td>0.6833</td>
<td>0.6498</td>
<td>0.5873</td>
<td>0.5817</td>
<td>0.4362</td>
</tr>
<tr>
<td>D</td>
<td>...</td>
<td>0.0650</td>
<td>0.5182</td>
<td>0.6506</td>
<td>0.8068</td>
<td>0.7743</td>
<td>0.4704</td>
</tr>
</tbody>
</table>

A) Fitness value: 195
B) Fitness value: 246
C) Fitness value: 251
D) Fitness value: 669
Reducing the Propagation Losses of Substrate-Type PhC Waveguides

space to PhC waveguides that are based on a hexagonal lattice. The three rows of holes closest to the core of the PhC waveguide are encoded in a vector containing one radius \( r \) for all holes and the relative positions \( x_i, y_i \) of the six holes closest to the PhC waveguide core. Every hole \( h_i \) can have any position within its unit cell, i.e., \( x_i \in [x_{i,0} - a/2, x_{i,0} + a/2] \) and \( y_i \in [y_{i,0} - a\sqrt{3}/4, y_{i,0} + a\sqrt{3}/4] \). To evaluate the fitness, a PhC waveguide of length \( L = 60 \) periods is generated and excited at the input for three different frequencies \( \omega_a/2\pi c = \{0.245, 0.25, 0.255\} \). The 2D Fourier transform is applied to the resulting magnetic field \( H_z \) and the ratio of the spatial Fourier component \( \phi_1 \) in the 1st Brillouin zone to the one \( \phi_2 \) in the 2nd Brillouin zone for \( k_y = 0 \) is computed. The fitness is defined as

\[
\text{fitness} = 1/3 \sum_{i=1}^{3} \phi_{-1,i}/\phi_{2,i}.
\]

The best solutions obtained by four different runs of the algorithm are shown in Fig. 7.7. All solutions with a large fitness-value are characterized by a lateral displacement of about \( a/2 \) of the two rows of holes that are closest to the center of the PhC waveguide – independent on the different runs of the exploration algorithm. Therefore, we have reasons to believe that the W1-\( a/2 \) represents the fundamental design for the optimum PhC waveguide geometry for a hexagonal lattice oriented along the \( \Gamma - K \) direction. Another commonality between the solutions is that the radii of the designs is rather similar. The values for the radii of the holes range from \( r = 0.2758 \) to \( r = 0.2929 \) (cf. Tab. 7.1).

The low propagation losses of W1-\( a/2 \) PhC waveguides with a perfect cylindrical hole shape have already been confirmed in Fig. 6.16 and they are expected to be as low as \( \alpha_{dB} \gtrsim 77 \) dB/cm. We conclude that the best PhC waveguide designs in terms of a weak spatial Fourier components of the Bloch wave above the background-line are based on the W1-\( a/2 \) waveguide. A further optimization of the W1-\( a/2 \) waveguide design could result in even better line-defect PhC waveguides.

7.3 Suppressing Radiation Into the Substrate by Modifying the Substrate Layer

The importance to understand the propagation of modes in the background is discussed in Sec. 4.5. A background that does not support oscillatory fields for all spatial Fourier components of a Bloch wave enables loss-free propagation of PhC waveguide modes. For instance, we can theoretically replace the substrate layer by another three-dimensional PhC that has a photonic band gap for the same frequency region as for the planar PhC in the core layer. Then, no radiation from the PhC waveguide mode into the substrate would be allowed. This idea is not completely new since already Uranus et al. [286] and Bakir et al. [16] proposed to replace the substrate layer by a periodic, highly reflective layer stack. The idea was inspired by the VCSEL design, where such highly reflective vertical layer stacks are commonly used to force the light to leave the laser cavity at the top surface. The background concept is by far more general and rigorous: in principle it allows for all
Suppressing Radiation Into the Substrate

Figure 7.8: Simulated propagation loss spectra for a substrate-type PhC W1 waveguide with a hole radius $r = 0.34a$ but with a different hole radius in the substrate PhC waveguide.

kind of backgrounds, such as e.g., a vertical slab waveguide as presented in chapter 8. The background-line in our substrate-type PhC waveguide is approximated by the fundamental mode of the W1 PhC waveguide etched into the InP substrate (cf. Fig. 4.22). An imperfect background, such as a PhC with holes with a finite hole-depth, does not forbid the radiation into the background, but is able to suppress the leakage into the substrate considerably (see Sec. 4.5.4). In terms of fabrication, however, it is difficult to manipulate the substrate layer independently of the PhC waveguide core layer. Only a wafer bonding processes could offer a high enough freedom to design the substrate layer. Because of the currently not available accurate wafer bonding technique we were looking for alternatives.

Increasing the hole radius in the substrate would alter the optical properties of the substrate layer. The following numerical experiment was performed to test the idea: The propagation losses are computed for an ideal cylindrical-hole shape, where only the radius of the holes of the W1 PhC waveguide in the substrate is increased. The results are shown in Fig. 7.8. It can be seen that the propagation losses are hardly influenced for the high frequencies from $\omega a/(2\pi c) = 0.29$ to $\omega a/(2\pi c) = 0.32$. However, an improvement of the propagation losses $\alpha_{dB}$ up to values of about
Figure 7.9: The spatial Fourier components of the Bloch wave of a 2D W1 PhC waveguide with holes of radius $r = 0.34 \, a$ are computed by exciting with a frequency $\omega$ at the input. A) shows the photonic bands for an effective refractive index $n_{\text{eff}} = 3.24$ (cf. Sec. 2.3.2). The photonic bands for a 2D W1 PhC waveguide with refractive index $n_{\text{InP}} = 3.17$ and with different radii $r = 0.34 \, a$ (B), $r = 0.4 \, a$ (C) and $r = 0.46 \, a$ (D) are superimposed to the photonic bands with $n_{\text{eff}} = 3.24$. The photonic bands of the background W1 PhC waveguides exhibit a mode stop band.

$\alpha_{\text{dB}} = 150 \, \text{dB/cm}$ can be observed for frequencies $\omega/2\pi c \approx 0.26$ to $\omega/2\pi c \approx 0.29$ for substrate radii $r_{\text{sub}} = \{0.28, 0.38, 0.4, 0.42, 0.44, 0.46\} \cdot a$. Note that also an improvement of the propagation losses can be observed for a smaller radius in the substrate.

The excited waves in the slab PhC waveguide propagate strictly along the $x$-direction. These propagating waves in the core of the slab waveguide excite propagating waves in the cladding layers that predominantly propagate in $x$-direction as well. However they additionally have a small wave vector component in $z$-direction. Even so, it is conclusive to investigate the two-dimensional ‘in-plane’ situation ($x$-$y$-plane) only. We study the substrate layer and the core layer separately. The spatial Fourier components of the W1 PhC waveguide in the core and the spatial Fourier components of the W1 PhC waveguide in the substrate layer are shown in Fig. 7.9 for three different radii in the substrate layer $r_{\text{sub}} = \{0.34 \, a, 0.4 \, a, 0.46 \, a\}$. The photonic bands of the background W1 PhC waveguides are shifted towards higher frequencies for larger radii in the substrate layer. Furthermore, the photonic bands of the background W1 PhC waveguides exhibit a mode stop band that shifts into the passband of the slab W1 PhC waveguide modes. These mode stop bands suppress the propagation in the line-defect mode of the substrate W1 PhC waveguide. This is the reason for the observed low propagation losses in Fig. 7.8 for the
Suppressing Radiation Into the Substrate

Figure 7.10: Comparison of magnetic fields $H_z$ for two PhC waveguides (dielectric constant is shown on the left) and for two different frequencies $\omega a/(2\pi c) = 0.27$ (plots in the middle) and $\omega a/(2\pi c) = 0.3$ (plots on the right); the PhC waveguide shown in (A) has a radius of $r_{\text{sub}} = 0.34a$ in the substrate and the PhC waveguide in (B) has a radius $r_{\text{sub}} = 0.42a$ in the substrate. Radiation into the substrate is clearly suppressed by the PhC waveguide with an increase radius in the substrate.

Figure 7.11: Computed propagation loss spectra for the W1-$a/2$ waveguide for a perfect cylindrical hole shape ($r_{\text{core}} = r_{\text{sub}} = 0.34a$) and for three increased radii $r_{\text{sub}}$ in the substrate only. The W1-$a/2$ maintains its low propagation losses for this hole shape as opposed to a cylindro-conical hole shape (cf. Fig. 6.16).
Reducing the Propagation Losses of Substrate-Type PhC Waveguides

frequency range \( \omega a / 2 \pi c \approx 0.26 \) to \( \omega a / 2 \pi c \approx 0.29 \). Note that the obtained low-loss frequency ranges by means of the 2D band diagram simulations and the 3D propagation loss spectrum do not agree. This is due to two reasons: First, the effective refractive index that is used to compute the 2D photonic bands for the 3D slab PhC waveguide mode is altered if the radius in the substrate is changed and would have to be adjusted for every simulation. Furthermore, one would only expect an agreement of the frequency ranges for negligible wave vector components \( k_z \) of the substrate modes. This is not the case for a 3D slab PhC waveguide.

Figure 7.10 shows the magnetic field plots for a radius \( r_{\text{sub}} = 0.34 a \) (A) and radius \( r_{\text{sub}} = 0.44 a \) (B) in the substrate layer for two frequencies \( \omega a / 2 \pi c = 0.27 \) (center) and \( \omega a / 2 \pi c = 0.3 \) (right). The frequency \( \omega a / 2 \pi c = 0.27 \) lies within the mode stop band of the W1 PhC waveguide in the substrate layer with \( r_{\text{sub}} = 0.44 a \) and \( \omega a / 2 \pi c = 0.3 \) lies outside this mode stop band. Figure 7.10 shows that the out-of-plane radiation occurs predominantly via the line-defect of the PhC waveguide in the substrate. But, for the frequency \( \omega a / 2 \pi c = 0.27 \) and a radius \( r = 0.44 a \) in the substrate layer, the radiation into the substrate via the line-defect channel is clearly suppressed. This shows illustratively that an enlargement of the radius of the holes in the substrate layer can reduce the propagation losses.

One is tempted to argue that the effective refractive index is smaller for larger hole radii. A smaller effective refractive index would increase the contrast of the vertical slab waveguide and improve the vertical confinement of the mode. As a consequence, the propagation losses would be reduced. But, this explanation would not explain the strong frequency dependence — i.e., the modification of the radius in the substrate only affects the propagation losses for a limited frequency range of the obtained propagation loss spectra. Secondly, the reduction of the radius in the substrate layer would result in a larger propagation loss for the same frequency range. That is not true for the frequency range \( \omega a / 2 \pi c \approx 0.26 \) to \( \omega a / 2 \pi c \approx 0.29 \) for the radius \( r = 0.28 a \) in the substrate. Therefore, it is important to realize that this improvement of the propagation losses is not due to an effective refractive index phenomenon.

In a last numerical experiment, the influence of the enlargement of the radius of the holes in the substrate layer are investigated for the W1-\( a/2 \) waveguide. The replacement of the perfectly cylindrical hole shape by a realistic cylindro-conical hole shape led to a dramatic increase of the propagation losses of those waveguides and render them useless. Therefore, we also want to test the new hole shape with an enlarged radius in the substrate layer for the W1-\( a/2 \) PhC waveguide. Figure 7.11 shows the computed propagation losses for a W1-\( a/2 \) waveguide with a radius \( r = 0.34 a \) and three different radii \( r_{\text{sub}} \) in the substrate. The propagation losses are only slightly larger for the larger radii of the holes in the substrate. Therefore, we conclude that the low propagation loss properties of the W1-\( a/2 \) waveguides are maintained for larger holes in the substrate.

An attempt to compute the effective refractive index for the purpose to compute the propagation losses of a W1 photonic crystal waveguide by a simplified 2D model was performed by K. Rauscher [222]. It was found that already the transmission curves obtained by the 3D FDTD model and the simplified 2D model using the computed effective refractive index differ substantially and that the computed effective refractive index has to be corrected manually to achieve a reasonable agreement of the transmission curves.
We conclude that a larger radius in the substrate layer can enhance the propagation loss performance of a W1 PhC waveguide. In Sec. 7.4 we developed a post-etching process step that can selectively enlarge the hole radius in the substrate layer.

### 7.4 Improving the Process Technology to Yield a Better Hole Shape

In the following pages, we report on two newly developed fabrication processes to reduce the propagation losses of substrate-type PhC waveguides. The first process is a thermally driven mass transport process aiming at reducing the angled sidewalls of the etched holes. The angled sidewalls are the main source for fabrication related propagation losses (cf. Sec. 6.4.1). The second process consists of a selective InP etch aiming at implementing the promising idea of increasing the radius of the holes in the substrate. SEM micro-graphs of the resulting hole shapes can be seen in Fig. 7.12. Optically measured propagation losses will be shown below for both processes and we find propagation losses as low as 154 dB/cm.

![SEM micro-graphs showing the cross-sections of the fabricated holes after the ICP-etching A), with the additional annealing step B) and with both, the annealing step followed by the selective wet-etch step C) and D).](image)

**Figure 7.12**: SEM micro-graphs showing the cross-sections of the fabricated holes after the ICP-etching A), with the additional annealing step B) and with both, the annealing step followed by the selective wet-etch step C) and D).
7.4.1 Reducing the Sidewall-Angle of the Etched Holes

A substantial part of the losses can be assigned to fabrication imperfections and is mostly due to the angled sidewalls of our fabricated holes [116]. Recent progress in fabrication [240] promises a major improvement of the loss figure due to this effect. The process reported by Shahid et al. [240] consists of a post-etch annealing step at 630° C for 2 min in a PH3 atmosphere. This results in a mass transport of the material around the exposed surfaces of the etched holes. The reshaped holes lead to better spectral characteristics of their W3 waveguides: An extinction ratio of 30 – 35 dB was measured by Shahid et al. [240, 241] for the mini-stop band after the mass transport process compared to extinction ratios of about 20 dB/cm [50] without the mass transport process.

Our process consists of a cleaning step with H2SO4 at 10° C for 35 s, followed by an annealing step in the MOVPE (heating-up to 630° C for 13 min (≈ 3 min at 630° C) and cooling-down for 15 min under a PH3 atmosphere (pressure 160 mbar)).

Fig. 7.12 shows the hole shape after the ICP dry-etching process (A) and after the mass transport process (B). It can be seen in Fig. 7.12 B) that the hole depth is slightly reduced in exchange of a more cylindrical hole at the bottom of the hole. By analyzing the hole radius from top view SEM micro-graphs, an average of \( r = 0.324 \pm 0.005 a \) was found for all four implemented lattice constants \( a_i = \{364 \text{ nm}, 398 \text{ nm}, 435 \text{ nm}, 475 \text{ nm}\} \). A spectrum that covers the complete photonic band gap range is obtained by using lithographic tuning [196, 260] i.e., the lattice constants \( a_i \) are chosen in such a way that the frequencies covered by

![Figure 7.13: Optically measured propagation losses for W1 PhC waveguides after the ICP etching (red) (refer to Fig. 7.12 A) for an image of the hole shape) and after the thermally driven mass flow process (orange) (refer to Fig. 7.12 B). The blue propagation loss curves are obtained by a 3D FDTD simulation for a cylindrical hole shape and two different cylindro-conical hole shape as shown on the right.](image-url)
our two tunable lasers (Δλ = 1470 – 1630 nm) assemble to a continuous (broad) spectrum if they are scaled to reduced frequency units. The propagation losses are obtained by fitting an exponential function to the power transmission of six different lengths of PhC waveguides $L_i = \{30a, 60a, 120a, 240a, 480a, 960a\}$. Figure 7.13 shows the measured propagation losses for the hole shape after the ICP dry-etching process (red) and after the additional mass transport process (orange). Furthermore, we added the propagation losses computed by the 3D FDTD simulations for three different hole shapes to Fig. 7.13: a perfect cylindrical hole shape with $r = 0.32a$, and two more realistic cylindro-conical hole shapes as shown in Fig. 7.13. The first cylindro-concial hole shape ($d_{cone} = 7.1a$) corresponds to the measured depth of the hole $d_{hole} \approx 4\,\mu m$ and the second cylindro-conical hole shape ($d_{cone} = 10a$) corresponds to an approximated sidewall angle of the conical part of the hole that is closest to the optical mode. At a first glance, it seems that the improvement of the propagation losses for W1 PhC waveguide with the improved hole shape are only marginal. However for the frequency range from $\omega a/2\pi c = 0.24$ to $\omega a/2\pi c = 0.26$ the annealed holes result in an improvement of about 300 – 500 dB/cm. Actually, the propagation loss curve obtained with the annealed holes agree fairly well with the propagation losses of the PhC waveguide with perfectly cylindrical holes for a frequency range from $\omega a/2\pi c = 0.24$ to $\omega a/2\pi c = 0.29$ compared to a frequency range from $\omega a/2\pi c = 0.27$ to $\omega a/2\pi c = 0.29$ for the hole shape obtained after the ICP etching.

We conclude as follows: The developed mass transport process results in a hole shape that results in propagation losses that are similar to the ones of a W1 PhC waveguide with a perfect cylindrical hole shape for a frequency range as large as half the photonic band gap.

### 7.4.2 Increasing the Radius of the PhC Waveguide in the Substrate Layer

A further improvement of the propagation losses for the PhC waveguide is expected, if the radius of the holes in the substrate layer is increased as proposed in Sec. 7.3. To increase the radius in the substrate, a selective InP wet-etch process with a very low and controllable etch rate is required. Bandaru and Yablonovitch [17] found that adding organic acids such as tartaric, lactic, citric and malic acid to HCl

Table 7.2: Measured etch-rates of InP for different mixtures of HCl (concentration 32%), $H_2O$ and $C_6H_8O_7$ (concentration 10%). To determine the etch-rate, we measured the etch-depth with respect to an unetched pattern with the surface step profiler.

<table>
<thead>
<tr>
<th>HCl:H_2O:C_6H_8O_7</th>
<th>InP Etch Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:1:0</td>
<td>89 nm/min ± 7 nm/min</td>
</tr>
<tr>
<td>1:1.5:0</td>
<td>20.1 nm/min ± 1 nm/min</td>
</tr>
<tr>
<td>1:1:0.25</td>
<td>43.2 nm/min ± 1.5 nm/min</td>
</tr>
<tr>
<td>1:1:0.5</td>
<td>21.9 nm/min ± 0.4 nm/min</td>
</tr>
<tr>
<td>1:1.5:0.25</td>
<td>11.9 nm/min ± 0.2 nm/min</td>
</tr>
</tbody>
</table>
reduces the etch rate and results in smoother and defect-free surfaces compared to etch solutions based on inorganic acids alone. Based on these results we developed a slow selective wet etching solution for InP. Table 7.2 lists the obtained etch rates (etch-depth measured with the surface step profiler) for InP for five different mixtures of HCl, water and citric acid (C₆H₈O₇). The etch rate in the lateral directions is of similar magnitude but additionally depends on the crystal direction. A further reduction of the etch-rate can be achieved by cooling the etching solution. Fig. 7.12 shows SEM micrographs of the hole shape that is obtained by etching with a HCl:H₂O: C₆H₈O₇ at −2°C for 12.5 min. A rather complicated hole shape is obtained since the wet-etching is not isotropic. The cross-sections obtained for the W₁ PhC waveguide oriented along the [011] and the [110] axis of the InP wafer do not contain the complete information of the hole shape. To gather a more complete picture of the hole shape, we created an imprint of the fabricated structures by filling the holes with benzocyclobutene (BCB) and subsequently bonding the chips on a silicon wafer. The InP/InGaAsP layers (i.e., the complete III-V chips) can be removed by etching with HCl (to remove the InP substrate) and followed by an etching step with CH₃OOH:HCl:H₂O₂ (to remove the InGaAsP core layer and InP top cladding). The remaining BCB pattern consisting of the organic columns of the filled holes is shown in Fig. 7.14. Unfortunately, the high aspect ratio of the BCB pillars results in a bending of the BCB pillars, such that they all stick together. Nevertheless, from the top view (left plot) an irregular hexagon-shaped horizontal cross-section can be identified. A cylindrical hole shape is thus a reasonable approximation for the real hole shape obtained in the substrate layer.

The optically measured propagation losses obtained by fitting an exponential function to the transmission spectra of six different length of PhC waveguides \( L_i = \{30a, 60a, 120a, 240a, 480a, 960a\} \) are shown in Fig. 7.15. The propagation losses improve dramatically for the high frequency range \( \Delta \omega/2\pi c = 0.29 - 32 \). The best obtained propagation loss value \( \alpha_{dB} = 154 \text{ dB/cm} \) is found for \( \omega a/2\pi c = 0.319 \) – a more than a 50-fold improvement of the propagation losses compared to

Figure 7.14: BCB imprint of the W₁ PhC waveguide obtained after the annealing and the selective etching process. Because of the anisotropic wet-etch step, an irregular hexagonal hole shape is obtained.
Figure 7.15: Optically measured propagation losses for W1 PhC waveguides oriented along the (011)-direction (red) and oriented along the (110)-direction (orange) (refer to Fig. 7.12 C) and D) for an image of the cross-section of the holes). The blue propagation loss curves are obtained by a 3D FDTD simulation for a hole shape consisting of two consecutive cylinders with depth $d_{\text{top}} = 2a$ and $r_{\text{core}}$ for the two top-most layers and with depth $d_{\text{bottom}} = 8a$ and radius $r_2$ in the substrate layer.

the propagation losses of a PhC waveguide without the post-etching steps. Very similar propagation loss spectra are obtained for both crystal orientations, even tough the cross-sections of the PhC waveguide oriented along different crystal orientations of the InP wafer are very different. Thus the approximation of the irregular hexagonal hole shape by a cylindrical hole shape is legitimate. This is also confirmed by the computed propagation loss spectra for two different theoretical hole shapes consisting of only cylindrical hole shapes as sketched in Fig. 7.15: the computed propagation loss spectra are very close to the measured propagation losses. The effective radius of the holes in the substrate $r_{\text{eff}} \approx 0.365a$ was estimated by averaging the hole shape of the two cross-sections as shown in Fig. 7.12 C) and D). The used radii ($r_{\text{sub}} = 0.36a$ and $r_{\text{sub}} = 0.38a$) in the simulation represent roughly the lower and upper boundary of the effective radius of the holes in the substrate. The propagation losses are strongly reduced, even though the enlargement of the holes in the substrate is rather moderate (refer to Fig. 7.8). The measured propagation loss values are very close to the propagation losses obtained numerically for a W1 PhC waveguide with a perfect cylindrical hole shape. However, the expected low propagation losses for the frequency range from $\omega a/(2\pi c) \approx 0.26$ to $\omega a/(2\pi c) \approx 0.29$ that are obtained for $r_{\text{sub}} \geq 0.38a$ (cf. Fig. 7.8) can thus not be observed for the measured propagation losses of the PhC waveguides with the improved hole shape.

We conclude that the selective wet-etch process step results in a moderate enlargement of the holes in the substrate. The propagation losses of the W1 PhC...
Reducing the Propagation Losses of Substrate-Type PhC Waveguides

Waveguide with the enlarged holes results in strong improvements of the propagation losses for the frequency ranges close to the upper edge of the photonic band gap. The resulting propagation loss spectrum is very similar to the propagation loss spectrum of a W1 PhC waveguide with perfect cylindrical holes.

7.5 Discussion

Table 7.3 lists the propagation losses obtained by various authors for substrate-type W1 PhC waveguides etched into a InP/InGaAsP layer stack. The propagation losses depend strongly on the thickness of the used layers and also on the radius of the holes of the design. The very large propagation losses of about $\alpha_{dB} \approx 1800$ dB/cm measured by Wüest et al. [295] are due to the unfavorable layer stack of $t_{core} = 400$ nm and $t_{clad} = 200$ nm. A similar value of $\alpha_{dB} = 1803$ dB/cm has been obtained for $t_{core} = 400$ nm and $t_{clad} = 348$ nm and $r = 0.34\, a$ in Sec. 7.1 (cf. Fig. 7.1). Substantially lower propagation loss values of $\alpha_{dB} \approx 400$ dB/cm are obtained by P. Kaspar [120] for an optimized layer stack. The usage of an optimized layer stack is a necessity to achieve low propagation losses. The newly developed additional process steps, i.e., the thermally driven mass transport process and the selective wet-etch process, yield hole shapes that result in a substantial improve-

<table>
<thead>
<tr>
<th>Ref</th>
<th>Process</th>
<th>W1 PhC waveguide design parameters</th>
<th>$\alpha_{dB}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>[295]</td>
<td>ICP</td>
<td>$r = 0.415, a$, $a = 430$ nm, $t_{core} = 400$ nm, $t_{clad} = 200$ nm</td>
<td>1800 dB/cm</td>
</tr>
<tr>
<td>[260]</td>
<td>ICP</td>
<td>$r = 0.335, a$, $t_{core} = 522$ nm, $t_{clad} = 300$ nm</td>
<td>600 – 1600 dB/cm</td>
</tr>
<tr>
<td>[273]</td>
<td>CAIBE</td>
<td>$r = 0.333, a$, $a = 450$ nm, $t_{core} = 500$ nm, $t_{clad} = 0$ nm</td>
<td>600 – 1000 dB/cm</td>
</tr>
<tr>
<td>[274]</td>
<td>CAIBE</td>
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<td>600 – 1000 dB/cm</td>
</tr>
<tr>
<td>[120]</td>
<td>ICP with 1 $\mu$m SiNx hard-mask</td>
<td>$r = 0.263, a$, $a = 380$ nm, $t_{core} = 640$ nm, $t_{clad} = 300$ nm</td>
<td>400 – 1000 dB/cm</td>
</tr>
<tr>
<td>this work</td>
<td>ICP with annealing and selective wet etch</td>
<td>$r = 0.32, a$, $t_{core} = 522$ nm, $t_{clad} = 300$ nm</td>
<td>154 – 1000 dB/cm</td>
</tr>
</tbody>
</table>
Figure 7.16: Improvements of the propagation losses by the developed process steps: the propagation losses (black) measured for the W1 PhC waveguide with $r = 0.34a$ without any post-processing steps as shown in Fig. 5.9, the propagation losses for the W1 PhC waveguide with $r = 0.32a$ with an additional thermal anneal step (orange) and with an additional selective wet-etch process (red). The (blue) simulated propagation loss for a perfect cylindrical hole shape with $r = 0.32a$ is also shown.

ment of the experimental propagation losses for a W1 PhC waveguide: from formerly $600 - 1000 \text{ dB/cm}$ [273, 274, 260] to newly $\alpha_{dB} \approx 154 - 1000 \text{ dB/cm}$. Figure 7.16 shows the successive improvement of the propagation losses of a W1 PhC waveguide for the developed process steps. The computed propagation loss for a perfectly cylindrical hole shape with radius $r = 0.32a$ is also shown to demonstrate that the propagation losses obtained after the post-etch processes are very close to the theoretical optimum values. Therefore, we conclude that fabrication imperfections are not limiting the performance of our W1 PhC waveguides anymore.

However, the radius of the holes in the substrate can be enlarged even further by simply etching for a longer etch-time. For those waveguides, an even better propagation loss figure is expected. Therefore, the question arises of ‘What is the lowest propagation loss value that can be achieved for substrate-type PhC waveguides for the InP/InGaAsP system?’ There is no ultimate answer to this question. However, we can outline strategies to obtain even lower propagation losses.

We pointed out in the introduction that a combination of the results/designs of separate optimizations do not necessarily result in a superior PhC waveguide design if combined. Nevertheless, it is promising to test PhC waveguides based on a combination of the results. Therefore, we compute the propagation losses of a W1 and a W1-$a/2$ PhC waveguide for the optimum layer stack with $t_{\text{clad}} = 348 \text{ nm}$ and $t_{\text{core}} = 766 \text{ nm}$ and for a hole shape consisting of a realistic hole shape but with an
Reducing the Propagation Losses of Substrate-Type PhC Waveguides

Figure 7.17: Simulated propagation loss spectra using the 3D FDTD method for a W1 (left) and W1-$a/2$ (right) PhC waveguides with the optimum layer stack of $t_{clad} = 348 \text{ nm}$ and $t_{core} = 766 \text{ nm}$ and an increased radius of the holes in the substrate.

enlarged cylindrical hole shape ($r = 0.38 \alpha$) in the substrate. The results are shown in Fig. 7.17. The lowest propagation loss value $\alpha_{dB} = 110.7 \text{ dB/cm}$ for the W1 PhC waveguide was found for $\omega a/2\pi c = 0.303$. Furthermore, a low-loss frequency range with propagation losses as low as $150 \text{ dB/cm}$ can be observed for the frequency range from $\omega a/2\pi c = 0.245$ to $\omega a/2\pi c = 0.26$.

Another strategy is to further engineer the stop band of the line-defect PhC waveguide mode of the substrate layer. For instance, the stop band can be enlarged by larger radii or maybe by using another line-defect PhC waveguide design.

Single-mode line-defect PhC waveguides operated above the background-line will always exhibit propagation losses. Therefore, we have reasons to believe that the proposed devices in Fig. 7.17 are close to the lowest propagation losses achievable for our substrate-type PhC waveguide technology in the InP/InGaAsP system.

So far, we did not obtain propagation losses in the order of 20 dB/cm neither experimentally nor theoretically. Are propagation losses in the order of $\alpha_{dB} \approx 100 \text{ dB/cm}$ low enough for the realization of an electrically driven PhC laser? The ultimate answer to that question cannot be given either. However, the smallest lasing substrate-type line-defect PhC lasers with electrical current injection are about $w = 1.4 \mu \text{m}$ wide, i.e., W4 and W5 PhC waveguides [120, 272]. Already the W3 PhC waveguide does not exhibit a net gain anymore. The propagation losses of a W3 PhC waveguide are about $\alpha_{dB} \approx 20 - 50 \text{ dB/cm}$ (cf. Fig. 5.9 and Ref. [271]). This means that a propagation loss of 100 dB/cm is still too large for our current design with three InGaAs quantum wells and an InP/InGaAsP/InP layer stack [120]. It can be argued that the design can still be improved by e.g., increasing the number of quantum wells. However, the goal is to develop electrically driven active devices for integrated optics that have a smaller footprint (device size). Slow light operation is a necessity to obtain superior performance of PhC based devices. But substantially higher losses are expected for operating the devices in the slow light regime [144, 95]. We conclude that the electrically driven active PhC waveguides have to be operated below the background-line to exploit the benefits offered by the slow light modes. Even so, we cannot exclude other, better PhC waveguide
designs that would allow the realization of an electrically driven single-mode PhC laser with a net gain for the weak vertical index system. But, such a laser could probably not be operated in the slow light regime and hence would not have a superior performance in terms of device size, threshold current and achievable output power with respect to conventional ridge waveguide diode lasers.

7.6 Conclusion

We investigated four strategies to reduce the propagation losses. First, the propagation losses can be decreased from formerly 1073 dB/cm to 666 dB/cm by using a layer stack that is optimized for our hole shape as obtained after the ICP process. Then we investigated the potential of other waveguide designs: The W1-α/2 waveguide design is the best single-mode PhC waveguide geometry, since it has the lowest magnitude of the spatial Fourier component of the Bloch mode above the background-line. Furthermore, we found that by enlarging the radius of the holes in the substrate layer the background can be engineered such that radiation into the substrate is suppressed. In this way, the propagation losses can be reduced to about 150 dB/cm theoretically.

Finally, we developed two post-treatment processes to reduce the extrinsic propagation losses. The first process is a thermally driven mass transport process that reduces the hole depth slightly in exchange for a more cylindrical hole shape. The second process consists of a selective InP etch with etch-rates in the order of a few nm/min. The selective etching process allows to controllably increase the size of the holes in the substrate, such that even larger hole sizes in the substrate could be obtained. By using the two post-treatment processes, we experimentally could demonstrate propagation losses as low as 154 dB/cm for a substrate-type W1 PhC waveguide with moderately enlarged holes in the substrate.

By increasing the radius in the substrate layer further, the propagation losses of the W1 PhC waveguide can be reduced for the lower frequency range. It is expected that the new hole shape allows the implementation of other promising PhC waveguide geometries such as the W1-α/2 waveguide. We further expect that the combination of the discussed measures to reduce the propagation losses – i.e., using the optimum layer stack and the improved hole shape – can be used to reduce the propagation losses to values below 100 dB/cm.
Reducing the Propagation Losses of Substrate-Type PhC Waveguides
Cross-Hair Device for Low-Loss, Electrically Pumped In-Plane Active PhC Waveguides

The chapter is published in Ref. [115].

In the previous chapter, we investigated the feasibility to reduce the propagation losses by small modifications of the $W_1$ PhC waveguide design. Thereby, the focus was on a solution that could be quickly realized in the lab. Even though measured propagation losses as low as $154 \, \text{dB/cm}$ were achieved, those numbers are still an order of magnitude larger in the dB-scale than for membrane-type PhC waveguides. In this chapter we discuss a novel PhC waveguide design that is not yet compatible with our existing process, but is promising for electrically pumped active PhC devices. The proposed PhC waveguide can be electrically pumped with a vertical contacting scheme and simultaneously exhibits low propagation losses in the order of $< 20 \, \text{dB/cm}$.

The basic idea underlying the new design consists of using a background system that potentially allows to design a PhC waveguide, such that all spatial Fourier component of the Bloch wave are located below the background line. Kaspar et al. [121] already proposed to use narrow vertical slabs as the background system of a line-defect PhC waveguide. The proposed design is shown schematically in Fig. 8.1. The computed separatrices for the narrow slabs in [121] indicate that the width $w$ of a narrow slab has to be roughly $w < d_{W_1}/8 = (\sqrt{3}a - 2 \cdot r)/8 \approx 60 \, \text{nm}$ such that the PhC waveguide modes are located below the background-line. It is expected that the free-carriers in such narrow slabs are completely depleted and consequently they cannot provide an efficient conducting channel for carrier injection [22]. A careful investigation of the influence of the design parameters on the electronic and optical properties is required to answer the question of whether the idea of using narrow contacting channels can be used for vertical current injection of an active line-defect PhC waveguide.

The performance of the device will critically depend on the width $w$ of the con-
tact channel: The wider the channel \( w \), the more efficient is the current injection; but at the same time the optical losses will increase as we approach a substrate-type design. In this chapter we address the following questions: How small do we have to design the channel width \( w \) in order to obtain low optical propagation losses? And what is the maximum current density, \( J_{\text{max}}(w) \) that we can pump through this channel of width \( w \) without affecting the gain properties of the active material? The answer to the latter question depends on the amount of surface damage induced during dry-etching, and on heat dissipation and gain properties of the structure. Although we currently cannot experimentally determine those parameters and properties accurately from fabricated devices, we try to make realistic estimates of them from simple experiments in Sec. 8.4.

The chapter will lead to a proposal for a PhC waveguide design including specific numbers for the design parameters that provides both low propagation losses (< 20 dB/cm) and the capability of electrical pumping of the active material by a vertical contacting scheme. The proposed device is suitable for the implementation of in-plane active photonic crystal devices, such as semiconductor optical amplifiers and lasers.

8.1 Vertical vs. Horizontal Current Injection Schemes

The main interest regarding weak refractive index contrast slab PhC waveguides is the prospect to vertically electrically pump active PhC devices. The vertical layer structure allows a straightforward realization of a PIN diode that could be contacted similarly to conventional semiconductor lasers and amplifiers characterized by an efficient vertical current injection. However, research on weak refractive index systems – also known as substrate-type devices – has been abandoned by many research groups due to the high propagation losses of the PhC waveguides in the order of 600 – 1000 dB/cm [274, 117]. On the other hand, membrane-type PhC

Figure 8.1: The cross-hair device consists of an active line-defect membrane PhC waveguide with a quantum well. The membrane is pumped vertically through two small connecting posts. The InGaAs capping-layer is highly doped to allow for a low contact resistance to the metal contact. Furthermore the capping-layer is needed to cover the holes with SiNx for the formation of the contact.
waveguides exhibit low propagation losses below 10 dB/cm [267, 203, 173, 60] but for membrane-type PhC devices, the current has to be pumped laterally through the PhC [65, 211]. Unfortunately, the ohmic resistance experienced by the laterally injected carriers increases with the filling factor of the PhC [23]. Large filling factors are essential to provide large band gaps in the PhC based devices [104]. The proposed waveguide design (cf. Fig. 8.1) combines the advantages of both approaches: the low propagation losses of membrane-type PhC waveguides and the efficient vertical contacting scheme of substrate-type PhC devices. Note that the current injection scheme is largely independent on the PhC waveguide design. Particularly, large filling factors may be used in the new PhC waveguide design as opposed to horizontally pumped membrane-type PhC waveguides [65]. The novelty of the proposed design thus lies in the combination of the following properties: a) it is vertically pumped and b) it allows for in-plane operation as opposed to the devices shown in [65, 211] which are surface emitters.

8.2 Theoretical Foundations to Obtain Low Propagation Losses

The aim of this paragraph is to determine the relevant background-line of the system shown in Fig. 8.1. Once the background-line is found, we can compute the
dispersion of the PhC waveguide mode and decide, whether the PhC waveguide mode is expected to be guided loss-free. Therefore, the dispersion diagram in Fig. 8.2 is considered. It contains the eigen-modes of the background and of the PhC waveguide. The figure shows the modes propagating in a homogeneous medium with refractive index \( n_{\text{air}} = 1 \) (referred to as the light-line – black in Fig. 8.2) and \( n_{\text{InP}} = 3.17 \) (referred to as the substrate line – green in Fig. 8.2), the TE (orange) and TM (red) mode of the vertical slab waveguide (the contacting channels) and the modes of the PhC waveguide (blue) within the PhC band gap (gray area). Note that the Fourier representation [161, 141] of the Bloch mode is used in Fig. 8.2, which has non-zero contributions for all components \( k_{x,m} = \hat{k}_x + m \cdot \frac{2\pi}{a} \). If one spatial Fourier component of the PhC waveguide mode is located above the background-line, then the PhC waveguide mode has oscillatory fields in the claddings (vertical slab) resulting in a finite propagation loss. All shown dispersion curves – except the substrate line – mark a boundary, which enables a further loss channel. A further increase in the propagation losses can be expected when the PhC waveguide mode crosses the light-line of the air. Four different regions in the dispersion diagram (points A-D in Fig. 8.2) can be identified for the shown PhC waveguide mode. For each case, the mode profile is schematically drawn in Fig. 8.2 and the corresponding locations (A-D) in the dispersion diagram are indicated for the two Brillouin zones. Depending on the location of the PhC waveguide mode in the dispersion diagram, the regions around the waveguide core that contain oscillatory fields change. Simply put, this means that the losses depend on the location in the dispersion diagram.

The significance of the dispersion curves for the propagation losses is confirmed by the numerically computed propagation loss spectrum of the final device shown in Fig. 8.12. The lowest propagation loss values are obtained for the PhC waveguide mode located below the dispersion curve of the slab TM mode (We find the lowest propagation loss value for \( \frac{\omega a}{2\pi c} = 0.253 \). A significant increase of the propagation losses can be observed for both, PhC waveguide modes located above the slab TM mode and above the air light line. Above the air light-line, the loss spectrum is dominated by the radiating Fourier component in the first Brillouin zone.

Figure 8.3: Definitions of the polarization in 2D PhC structures (left) and in slab waveguides (right).
zone \([141]\). In other words, the rather low propagation losses observed above the air light-line (around \(\omega a / 2\pi c \approx 0.285\)) correspond to a small relative contribution of the spatial Fourier component of the Bloch wave in the first Brillouin zone with respect to the other Fourier components. It has to be noted that for the simulations of Fig. 8.12, the waveguide is excited by a \(H_z\)-field. In the PhC terminology this means that we excite TE-like modes. According to conventional slab waveguide theory, however, we have a TM mode excitation: The conventions are illustrated in Fig. 8.3. Due to the symmetry properties of our excitation, the loss-relevant separatrix is the dispersion curve of the TM slab mode.

We conclude that low propagation losses are obtained, if all spatial Fourier components of the Bloch wave are below the separatrix given by the fundamental TM mode of the vertical slab.

### 8.3 Optical Design Considerations

#### 8.3.1 Photonic Crystal Waveguide Design

Having identified the relevant separatrix, we are able to formulate the task for obtaining low propagation losses: the dispersion of the PhC waveguide mode has to be shifted below the dispersion curve of the fundamental TM mode of the vertical slab waveguide. This can be achieved by either reducing the contact channel width \(w\) to raise the dispersion curves of the vertical slab TM mode to higher frequencies or by tailoring (optimizing) the PhC waveguide, such that the dispersion of the PhC waveguide mode is moved below the background-line. For instance, a larger cross section of the core of the PhC waveguide allows the mode to spread more in the transverse direction and as a consequence lowers its frequency.

From an electronic point of view, the contact channel width \(w\) should be as large as possible. Therefore, we start by choosing one of the largest possible channel width \(w \approx 0.526a \approx 200\) nm, for which still low optical propagation losses can be achieved. The choice was made by overlaying the TM dispersion curves for a number of contact channel widths \(w\) with the band gaps of potential PhC waveguides and then requiring a region such that for all frequencies of the photonic band gap a wave vector \(k_x\) exists in the first Brillouin zone that is below the TM slab dispersion curve. This process is illustrated in Fig. 8.4, where the dispersion curves of the lowest order TM (solid lines) and TE modes (dashed line) of the vertical slab consisting of a InP core \((n_{InP} = 3.15)\) and air claddings \((n_{air} = 1)\) for three different slab widths \(w = \{100\) nm, 200 nm, 400 nm\} are shown. The light-lines (black dotted lines in Fig. 8.4) of the involved materials (air and InP) represent the limiting cases of the modes of the vertical slab with respect to the channel width \(w\): For a very thin slab \((w \rightarrow 0)\), the dispersion of the slab modes coincides with the light-line of air, whereas for a thick slab \((w \rightarrow \infty)\) the dispersion of the slab approaches the light-line of \(n_{InP}\). Fig. 8.4 also shows the photonic band gap (PBG) of a planar slab PhC with \(n_{core} = 3.32\), \(t_{core} = 0.6 \cdot a\) and \(r = 0.25 a\) (gray shading). It can be seen that the vertical slabs with width \(w = \{100\) nm, 200 nm\} meet the requirement, i.e., both slabs guarantee a frequency range, for which the PhC TE-like waveguide mode is below the dispersion curve of the TM mode of the con-
The Cross-Hair Device

The Cross-Hair Device

Figure 8.4: Left: The dispersion relations for the fundamental TM mode (solid lines) and the fundamental TE mode (dashed lines) of the vertical slab waveguide are shown for three different post widths. The photonic band gap was read-out from a 3D MPB simulation of the optimized PhC waveguide and for a membrane thickness of \( t_{\text{core}} = 0.6 \ a \) and a post width \( w = 0.526 \ a \).

Note that both slabs would not meet the requirement for the slab TE mode polarization, and hence the PhC waveguide cannot be operated efficiently with a \( E_z \)-excitation.

Unfortunately, for a standard PhC W1 waveguide with \( r = 0.34 \ a \) – as used in the previous chapters – the computed propagation loss spectrum does not exhibit a frequency range of very low propagation losses as it can be seen in Fig. 8.5. This is due to the photonic band of the PhC W1 waveguide mode that is flat (\( \partial \omega / \partial k \approx 0 \)) below the slab TM dispersion curve (cf. Fig. 8.5 left plot). As a consequence, the usable frequency range is very small. Furthermore, the propagation losses of those modes are expected to be large due to the low group velocity [144, 95].

To increase the usable bandwidth below the background-line, the frequencies of the dispersion curve of the PhC waveguide mode must be lowered. From the gap map plot (cf. Fig. 2.12) and the sensitivity analysis in Sec. 3.3 three design related measures can be deduced:

- reducing the radius of the PhC holes shifts the photonic band gap to lower frequencies.
- reducing the radius of the first row of holes shifts the PhC waveguide mode closer to the lower band edge of the photonic band gap of the PhC.
- increasing the width \( d_{W_1} \) of the line-defect PhC waveguide also shifts the PhC waveguide mode closer to the lower band edge of the photonic band gap of the PhC.

From Fig. 3.8 and Fig. 3.11 a waveguide design can be deduced that promises a dispersion relation of the PhC waveguide mode that is shifted towards lower frequen-
Figure 8.5: W1 PhC waveguide with radius $r = 0.34a$ with a contact channel width $w = 1/2(\sqrt{3}a - 2 \cdot r)$.
Left: band diagram obtained with MPB and a 3D super-cell. The size of the dot corresponds to the energy confinement within the core of the PhC waveguide. The straight black line represents the air light-line, the dotted red line represents the dispersion curve obtained from the vertical slab operated in TM mode.
Right: 3D FDTD simulations; the red curve is the transmission coefficient for a PhC waveguide of a length of 50 PhC periods. The thick black curve is the corresponding propagation loss $\alpha_{dB}$. The white (bright blue) background signifies reliable (unreliable) propagation losses according to [117].

The W1 PhC waveguide design is based on a hexagonal lattice of air holes with radius $r = 0.27a$ and a radius of the first row of holes with $r_1 = 0.24a$. For this design a frequency range of $\omega a/(2\pi c) = 0.0002$ with less than $< 20$ dB/cm has been computed using 3D FDTD simulations (not shown here).

To maximize the frequency bandwidth below the vertical slab TM waveguide mode an optimization is performed. Therefore, we use the findings that the dispersion relation of a PhC waveguide mode can be engineered to almost any desired characteristic by manipulating the radii or the positions of the holes in the first and the second row adjacent to the line-defect on both sides of the line-defect [73, 156]. Since it is challenging to reproducibly fabricate holes of different sizes on the same chip, a design consisting of only one size of holes with radius $r$ is preferred. Therefore only four different radii $r_1 = 0.23a$, $r_2 = 0.25a$, $r_3 = 0.27a$, $r_4 = 0.29a$ were considered for the optimization. For each of those radii, the parameter search space was restricted to a shift of the position of the holes in the first row $s_{y_1}$ and the second row $s_{y_2}$. Only shifts away from the center of the waveguide were considered mainly because of the fact that a wider waveguide tends to better confine the energy of the optical mode to the active core of the waveguide, i.e., the active region. Note that the designs are symmetric with respect to the $x - z$ plane.

The optimization is performed by using a 2D super-cell model implemented...
Figure 8.6: Each plot represents a parameter sweep in the $s y_1 - s y_2$-plane for a given radius $r_i$. The color in the map is related to the single mode frequency bandwidth below the TM background-line of the planar slab of width $w = 200 \text{nm}$. The largest bandwidth ($\Delta \omega a/(2\pi c) = 0.0135$) was found for a radius $r = 0.25 \cdot a$, $s y_1 = 0.02 \cdot a$ and $s y_2 = 0.07 \cdot a$.

The optimization results are shown in Fig. 8.6. The color in the $s y_1$-$s y_2$ plane in Fig. 8.6 denotes the available frequency bandwidth below the background-line of the contact channel with $w = 0.526 \cdot a$. The four plots correspond to the four radii $r_1$, $r_2$, $r_3$ and $r_4$. The waveguide with the largest usable frequency bandwidth of $\Delta \omega a/(2\pi c) = 0.0135$ ($\approx 82.8 \text{ nm}$ for $\lambda = 1550 \text{ nm}$) has the parameters $r = 0.25 a$, $s y_1 = 0.02 a$, $s y_2 = 0.07 a$. The band diagram of the 2D MPB simulation is shown in Fig. 8.7. The red shaded area is the frequency bandwidth below the TM mode of the contact channel.

A further improvement of the usable low-loss frequency bandwidth PhC waveguide can be achieved by increasing the thickness of the core layer $t_{\text{core}}$. However, if the vertical cross-section of the PhC waveguide becomes too large, higher order modes may be able to propagate. It is still not completely clear how a hard crite-
Optical Design Considerations

Figure 8.7: The band diagram (B) of the TE mode of the optimum PhC waveguide (A) having the largest frequency bandwidth of $\Delta \omega a/(2\pi c) = 0.0135$ (red area) with parameters $r = 0.25a$, $s_{y1} = 0.02a$ and $s_{y2} = 0.07a$ computed with MPB and a 2D super-cell.

Table 8.1: The frequency band width $\Delta \omega a/(2\pi c)$ obtained from 3D FDTD simulations, where the PhC waveguide with a contact channel width $w = 0.526a$ has a propagation loss lower than $-100$ dB/cm and $-20$ dB/cm, respectively is listed below.

<table>
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<th>$t_{core}$ [a]</th>
<th>$20$ dB/cm</th>
<th>$100$ dB/cm</th>
<th>$\Delta \omega a/(2\pi c)$</th>
<th>$\Delta \lambda$ [nm]</th>
<th>$\Delta \omega a/(2\pi c)$</th>
<th>$\Delta \lambda$ [nm]</th>
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<tr>
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<td>---</td>
<td>---</td>
<td>0.0110</td>
<td>56.7</td>
<td>7.54 dB</td>
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</tr>
<tr>
<td>0.6</td>
<td>0.0002</td>
<td>1.2</td>
<td>0.0138</td>
<td>77.4</td>
<td>6.63 dB</td>
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</tr>
<tr>
<td>0.7</td>
<td>0.0038</td>
<td>23.3</td>
<td>0.0163</td>
<td>99.6</td>
<td>9.82 dB</td>
<td></td>
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</tr>
<tr>
<td>0.8</td>
<td>0.0046</td>
<td>30.9</td>
<td>0.0157</td>
<td>99.8</td>
<td>9.14 dB</td>
<td></td>
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</tr>
<tr>
<td>1.0</td>
<td>0.0067</td>
<td>41.3</td>
<td>0.0152</td>
<td>99.2</td>
<td>8.50 dB</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*MSR: confinement ratio defined as the ratio of the percentages of the energy confined to the PhC waveguide core between the first order mode and the next higher order mode.

$\Delta \lambda$ is determined by evaluating $\omega_i a/(2\pi c)$ for the edges $\omega_i$ of the obtained frequency bands for $a = 392$ nm.
The Cross-Hair Device

The Cross-Hair Device can be defined to determine the single mode condition of a slab PhC waveguide by using 3D super-cell simulations [103]. Therefore, we introduce our own figure of merit based on the confinement factor of the simulated modes. Since we operate the PhC waveguide close to the cutoff of higher order modes, we expect that there is only one mode that has a significantly higher confinement factor than all other modes. Therefore, we use the ratio between the energy overlaps of the first and the second order mode as our figure of merit. We call it mode suppression ratio MSR. Here, a MSR of 10 dB means a ten times lower confinement factor of the next higher order mode with respect to the fundamental PhC waveguide mode. Table 8.1 lists the usable frequency bandwidth and the MSR for various core layer thicknesses $t_{\text{core}}$. For all further investigations we used the waveguide having a core layer thickness of $t_{\text{core}} = 0.8 a$, because it has the largest MSR and still provides a large usable bandwidth. By scaling the lattice constant $a$, the lowest propagation loss value ($\alpha_{dB} = 5.4$ dB/cm) can be tuned to match the operation wavelength $\lambda_0 = 1550$ nm. A lattice constant $a = 392$ nm is found.

### 8.3.2 Material and Free-Carrier Absorption

The metallic contact layers and the doped contacting channels in close proximity to the optical mode can result in very large propagation losses [123]. By increasing the channel height $h_{\text{top}}$, the absorption in the metallic contact layer can be reduced, however, this comes with two undesired side effects: First, the thermal and electronic resistances increase with the channel height $h_{\text{top}}$. Second, the holes created by our dry-etching process have a cylindro-conical hole shape rather than the desired cylindrical shape. The angled sidewalls are largely responsible for the losses induced by fabrication imperfections [116]. By increasing the height of the upper channel $h_{\text{top}}$, the absorption in the metallic contact layer can be reduced.

![Mode Profile
htop
tcore
wcore
wn-InP
Au
p-InGaAsp-InP
i-InGaAsP
InGaAsPn $= 3.33$
InPn $= 2.99+i 2.48e-4$ (n:2e18).
Au
Used Refractive Indeces:
$n_{\text{Au}} = 1.96+i 22.5$
$n_{\text{InGaAs}} = 2.85+i 1.6e-3$ (p:2e19)
$n_{\text{InP}} = 3.03+i 5.9e-5$ (p:1e18)
$n_{\text{InGaAsP}} = 3.33$
$n_{\text{InP}} = 2.99+i 2.48e-4$ (n:2e18)
Figure 8.8: Left: A simplified 2D model of the device to estimate the height of the contact channel $h_{\text{top}}$ that minimizes the losses originating from the metallic contact and the doped cladding layers. Right: The propagation losses of the TE mode for $\lambda = 1550\text{nm}$ and for four different core layer thicknesses $t_{\text{core}}$ as a function of channel height $h_{\text{top}}$, computed with Lumerical, a commercial mode solver.
Electronic Design Considerations

8.4 Electronic Design Considerations

8.4.1 Depletion Width and Surface Space Charge Density of Our Etching Process

The InP dry-etching step for hole formation induces damages on the etched surfaces that manifest themselves by a surface charge density and a depletion zone at the surface boundary [148]. This effect reduces the effective width of the contacting channel that is usable for current conduction and is one of the main limitations in down-scaling the contact channel width $w$. In a first step, we try to extract realistic numbers of the depletion width and the resistivity of the narrow channels from a simple experiment: Narrow channels have been fabricated by deeply etching trenches into a 1.5 $\mu$m thick InP layer (measured doping concentration $4.5 \cdot 10^{17}$ cm$^{-3}$, resistivity of the conducting layer $\rho = 3.24 \cdot 10^{-5}$ $\Omega$m) grown on a semi-insulating Fe-doped InP substrate. A 3D illustration is shown in Fig. 8.9(B). Figure 8.9(A) shows the measured resistance and the conductivity of the etched channels for various channel widths $w$. The smaller the channel width $w$, the higher is the measured resistance. The smallest channel with a width $w = 100$ nm does...
The Cross-Hair Device

\[ R_{\text{meas}} - R_{\text{pad}} = \rho \cdot \frac{L_{\text{trench}}}{w} \cdot \frac{1}{w - 2w_d} = 5.24 \cdot 10^{-5} \Omega \text{m} \]

\[ 2w_d = 11.17 \text{ nm} \]

**Figure 8.9**: A: v-i curves for 320 \( \mu \text{m} \) long trenches of various widths \( w \). The smallest measurable channel width was \( w = 200 \text{ nm} \). B: schematic of the etched trench waveguides.

not allow current conduction. This is due to the fact that the usable width of the channel for current conduction is reduced by a depletion layer formed at the rough surface resulting from the dry-etching process. The depletion width of our process was found \( w_d = 56 \text{ nm} \pm 3 \text{ nm} \) for a doping of \( 4.5 \cdot 10^{17} \text{ cm}^{-3} \). Thus, the effective contact channel width that can be used for carrier conduction is reduced to \( w_{eff} = w - 2w_d \), and accordingly the smallest contact channel with \( w = 100 \text{ nm} \) is completely depleted. The smallest channel width \( w \) of our experiment allowing for current injection is \( w = 200 \text{ nm} \).

The measured doping concentration of \( n = 4.5 \cdot 10^{17} \text{ cm}^{-3} \) is rather low for the purpose of pumping an active device with a low series resistance. If we assume a constant surface charge density (approximatively given by the deep etching process only), then a higher doping concentration results in a smaller depletion width \( w_d \) and simultaneously reduces the resistivity \( \rho \). Additionally, the surface charge densities resulting from a wet-etching process (needed for the under-etching) are typically lower than the ones from the dry-etching process. Thus, the here presented parameters for the carrier conduction properties represent a worst-case scenario.

We conclude that the depletion zone formed by the dry-etching process in this experiment dominates the current conduction properties for channel widths in the order of \( w \approx 2w_d \). Note that the largest measured current density for the trench with width \( w = 200 \text{ nm} \) is \( J = 67 \text{ kA/cm}^2 \) and thus we conclude that a contact channel width of \( w = 200 \text{ nm} \) (as used in the PhC waveguide design to obtain low propagation losses) is able to conduct typical current densities for lasing devices of \( J \approx 0.5 - 5 \text{ kA/cm}^2 \).

### 8.4.2 Gain of the Active Device

In a next step, we estimate how much current will be necessary to pump the active waveguide to transparency. This, of course, depends on the design of the active gain material. If the active material is composed of quantum wells (QW), the number of wells is a crucial parameter. Therefore we are interested in the number of
QWs that minimizes the transparency current density – and in the corresponding current density. We apply the procedure developed by P. Kaspar [120, p. 98] to determine the number of QW’s for the proposed cross-hair device for the case of a semiconductor optical amplifier (SOA).

We model the gain of a single QW with a logarithmic relation \( g = g_0 \cdot \ln(J/J_0) \), where \( g_0 \) is the gain coefficient, \( J \) is the current density, and \( J_0 \) is the material transparency current density. In the presence of a number \( N \) of QWs, we assume that the current is evenly distributed among the QWs and that the optical mode overlap with all QWs is the same. The gain of \( N \) QWs can then be written as

\[
g = N \cdot g_0 \cdot \ln(J/(N \cdot J_0)). \tag{8.1}
\]

In case of a semiconductor optical amplifier, transparency of the waveguide is reached if \( g = \alpha_{WG} \), where \( \alpha_{WG} \) are the waveguide losses. The waveguide transparency current density is, therefore, given by

\[
J_{tr} = N \cdot J_0 \cdot e^{\alpha_{WG}/(N \cdot g_0)}. \tag{8.2}
\]

We find \( N = \alpha_{WG}/g_0 \) as the number of QWs that minimizes the waveguide transparency current density. Experimental data of our QWs (7.5 nm InGaAs layers separated by 12 nm InGaAsP barrier layers) yield a gain coefficient of \( g_0 \approx 39 \text{ dB/cm} \) for a single QW [120, p. 111]. Assuming that \( \alpha_{tot} \approx \alpha_{WG} < 20 \text{ dB/cm} \) we find the number of QW minimizing the waveguide transparency density to be \( N = 1 \). By using Eq. 8.2 a transparency current density of \( J_{tr} \approx 2.7 \cdot J_0 \) is found. The precise value of \( J_0 \) is hard to determine experimentally if the waveguide loss is not exactly known. For our QW material we estimate it to be \( J_0 < 0.2 \text{ kA/cm}^2 \) [120, p. 114]. Since only one QW has to be pumped to transparency for a net gain, we can estimate the transparency current density to be \( J_{tr} < 0.54 \text{ kA/cm}^2 \). Similar current densities have been measured in the fabricated trench waveguide based laser devices and the required current conduction can be supplied by the narrow contact channels – provided that the gain of the active device is not degraded by excessive thermal heating.

### 8.4.3 Self-Heating and Heat Dissipation

An insufficient heat conduction may reduce the gain and prevent the devices from functioning. For instance, the transparency current density \( J_{tr} \) critically depends on the temperature in the active region [10][41, pp. 57-59]. We thus investigate the steady state heat conduction equation [291, 276]

\[
\nabla \cdot (-k \nabla T) = H, \tag{8.3}
\]

where \( T \) denotes the temperature, \( k \) the thermal conductivity and \( H \) the heat generation rate for the transparency condition of the cross-hair device. The heat is predominantly generated by Joule heating and by non-radiative recombination processes. For low current densities, i.e., at typical transparency current densities of \( J_{tr} \approx 0.5 - 1 \text{ kA/cm}^2 \), Auger recombination is known to be the dominant heat generation process for the InP/InGaAsP system with InGaAs QW’s [214][74, pp. 316-319].
Therefore, we assume that all heat is generated in the QW. To make things worse, we further assume that all electrical power given by the drive current $I_{op}$ and the total voltage across the diode terminals $V_{diode}$ ($P_{el} = I_{op} \cdot V_{diode}$) is transferred into heat in the QW. After having located the heat source, we discuss the dissipation of the generated heat in the cross-hair device. Because of the low thermal conductivities of the surrounding air layers and the perforated InGaAsP membrane PhC layer ($k_{InGaAsP} = 0.05$ W/cm), the generated heat in the active region is only dissipated through the InP contacting channels ($k_{InP} = 0.68$ W/cm) approximately. Furthermore, it is expected that the heat is less efficiently dissipated via the top contact channel, because of the thin InGaAs capping layer that has a low thermal conductivity $k_{InGaAs}$. Additionally, the Au contact layer only serves as an ideal heat sink, if the Au layer is very thick. To be on the safe side, we assume that the heat can only dissipate through the bottom contacting channel as shown in the simplified thermal conduction model in Fig. 8.10 (center).

The heat conduction can be modeled by analogy to an electrical circuit where the heat flow corresponds to the current and the temperatures correspond to the voltages, respectively. The circuit analogon of our simplified thermal model is also shown in Fig. 8.10 (right). The temperature rise $\Delta T$ is given by [41, p. 56]

$$\Delta T = T_{max} - T_{sink} = P_{el} \cdot Z,$$  \hspace{1cm} (8.4)

where $P_{el}$ is the electrical power of the diode and $Z$ is the thermal impedance. The total thermal impedance $Z$ is composed of three thermal impedances in series: $Z_{core}$ represents the heat conduction in the InGaAsP core layer, $Z_{bot}$ represents the thermal impedance of the bottom contacting channel and $Z_{sub}$ models the heat conduction in the substrate layer. The maximum temperature $T_{max}$ in the center of the QW is then given by

$$T_{max} = T_{sink} + I_{op} \cdot V_{diode} \cdot (Z_{core} + Z_{bot} + Z_{sub}),$$  \hspace{1cm} (8.5)
The maximum temperature $T_{\text{max}}$ in the center of the QW computed as a function of applied current density according to Eq. 8.9 and computed with two different 2D COMSOL models. The first COMSOL model (B) is equivalent to the thermal impedance model and results in the same maximum temperature $T_{\text{max}}$. The second COMSOL model (C) takes a more realistic geometry of the active region into account and yields a slightly lower maximum temperature than the other two models.

with

$$Z_{\text{core}} = \frac{t_{\text{core}}}{2k_{\text{InGaAsP}}Lw} \approx 337.9^\circ C/W$$ \hspace{1cm} (8.6)

$$Z_{\text{bot}} = \frac{h_{\text{bot}}}{k_{\text{InP}}Lw} \approx 142.8^\circ C/W$$ \hspace{1cm} (8.7)

$$Z_{\text{sub}} = \frac{\ln\left(\frac{16h_{\text{sub}}}{\pi w}\right)}{\pi k_{\text{InP}}L} \approx 51.6^\circ C/W$$ \hspace{1cm} (8.8)

where $L$ is the length of the waveguide and $k_{\text{InP}} = 0.68$ W/cm and $k_{\text{InGaAsP}} = 0.05$ W/cm are the thermal conductivities of InP and InGaAsP, respectively. $Z_{\text{core}}$ and $Z_{\text{bot}}$ can be approximated by the thermal impedance of a one-dimensional heat conductor [41, p. 56]. The heat conduction in the substrate layer can be modeled by an analytical formula for the thermal impedance (Eq. 8.8) that was derived by Amann [5] for a linear stripe of width $w$ and a thick substrate layer. This approximation is suitable to describe the heat conduction in our substrate layer. Finally, we obtain an expression for temperature $T_{\text{max}}$ in the QW as a function of the current density $J$ and the geometrical parameters $w$ and $h_{\text{bot}}$ of the bottom contacting channel

$$T_{\text{max}} = T_{\text{sink}} + J \cdot V_{\text{diode}} \cdot \left[ \frac{t_{\text{core}}}{2k_{\text{InGaAsP}}} + \frac{h_{\text{bot}}}{k_{\text{InP}}} + \frac{w}{\pi k_{\text{InP}}} \ln\left(\frac{16h_{\text{sub}}}{\pi w}\right) \right].$$ \hspace{1cm} (8.9)

The maximum temperature $T_{\text{max}}$ in the QW according to Eq. 8.9 is depicted in Fig. 8.11 for an constant applied voltage of $V_{\text{diode}} = 1$ V and various current densi-
ties $J$ ranging from 500 A/cm$^2$ to 20 kA/cm$^2$. To verify the validity of the developed heat dissipation model, the temperature $T_{\text{max}}$ was computed by 2D COMSOL simulations for (B) the same simplified model (also shown in Fig. 8.10) and for a more realistic model (C) that takes the larger width $w_{\text{act}} \approx 535$ nm of the active region into account. An excellent agreement of the temperature $T_{\text{max}}$ computed by 2D COMSOL and the analytical expression Eq. 8.9 is found. For a realistic transparency current density of $J_{\text{tr}} \approx 1$ kA/cm$^2$ the maximum temperature increase is at the most $\Delta T \approx 1.5$ °C. Similar temperature values for ridge diode lasers at threshold have been obtained by self-consistent models [276, 75]. This simplified model depicts the worst case, i.e., the found temperature increase $\Delta T$ is expected to be an upper bound of the temperature in the QW of a real device. In a real device, we expect that a substantial part of the electrical power is transferred to optical output power, which does not contribute to the heat generation. Furthermore, in a fabricated device, some of the generated heat will radiate into the air layers and dissipate through the top contact channel and the InGaAsP membrane layer.

We thus conclude that the narrow contact channels – although surrounded by air – provide sufficient heat conduction for an operating active device with waveguide losses $\alpha_{\text{dB}} < 20$ dB/cm.

### 8.5 Summary of the Parameters and Performance of the Cross-Hair Device

The structure presented in Fig. 8.1 shows a design that is promising for a practical device at least from a theoretical point of view. The detailed structure parameters determined in the preceding paragraphs are summarized in Table 8.2. This PhC waveguide design exhibits low (passive) propagation losses: The propagation loss spectrum (cf. Fig. 8.12, right panel) shows propagation losses of less than 20 dB/cm for a wavelength bandwidth of $\Delta \lambda = 23.3$ nm and less than 100 dB/cm for a wavelength bandwidth of $\Delta \lambda = 99.6$ nm for a center wavelength $\lambda_0 = 1550$ nm. Despite the low propagation losses, the contact channel width is still as large as $w = 206$ nm, which is sufficient to achieve a typical current density for active de-

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value [a]</th>
<th>Value [nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Post width</td>
<td>$w = 0.526$</td>
<td>$w = 206$ nm</td>
</tr>
<tr>
<td>Post height</td>
<td>$h_{\text{top}} = 500$ nm</td>
<td></td>
</tr>
<tr>
<td>Core layer thickness</td>
<td>$t_{\text{core}} = 0.8$</td>
<td>$t_{\text{core}} = 313$ nm</td>
</tr>
<tr>
<td>Capping layer thickness</td>
<td>$t_{\text{cap}} = 150$ nm</td>
<td></td>
</tr>
<tr>
<td>Hole radius</td>
<td>$r = 0.25$</td>
<td>$r = 98$ nm</td>
</tr>
<tr>
<td>Lattice constant</td>
<td>$a = 1$</td>
<td>$a = 392$ nm</td>
</tr>
<tr>
<td>Shift of first row of holes</td>
<td>$s_{y1} = 0.02$</td>
<td>$s_{y1} = 0.02$</td>
</tr>
<tr>
<td>Shift of second row of holes</td>
<td>$s_{y2} = 0.07$</td>
<td>$s_{y2} = 0.07$</td>
</tr>
</tbody>
</table>

Table 8.2: Parameters for the proposed design of Fig. 8.1. The values given in [nm] are scaled, such that the best obtained propagation loss value ($\omega a/2\pi c = 0.253$) coincides with a operation wavelength of $\lambda = 1550$ nm.
Figure 8.12: Left: band diagram obtained with MPB and a 3D super-cell. The size of the dot corresponds to the energy confinement within the core of the PhC waveguide. The straight black line represents the air light-line, the dotted red (orange) line represents the dispersion curve obtained from the vertical slab operated in TM (TE) mode.

Right: 3D FDTD simulations; the red curve is the transmission coefficient for a PhC waveguide of a length of 50 PhC periods. The thick black curve is the corresponding propagation loss $\alpha_{dB}$. The white background signifies reliable propagation losses and the bright blue background signifies unreliable propagation losses (according to [117]).
The Cross-Hair Device

8.6 Discussion

Table 8.3 gives an overview over a few electrically pumped PhC lasers reported in literature. Only two of the PhC lasers [211, 65] are based on membrane PhCs. Both membrane-type PhC lasers are pumped laterally through the PhC device and emit light through the top surface. A characteristic of those membrane PhC lasers are a small footprint, a low threshold current density and extremely low optical output powers ($P_{opt} < 2$ nW). Our approach bears some similarity to the cavity laser reported by Park et al. [211]: in both cases carriers have to be pumped through a narrow contact channel. The reliable fabrication of a rod-like channel as used by Park et al. [238, 211] poses much higher demands on the technology than the ones required for the etching of the proposed slab-like contact channels. To obtain the 1D pedestal, the etching has to be controlled in two crystal directions. On the other hand, the etching has to be controlled in only one crystal direction for the pro-

Figure 8.13: The first two SEM micro-graphs A) and B) were obtained after wet-etching in HCl:H$_2$O:C$_6$H$_8$O$_7$ (1:1.5:0.25) for 10 min at room temperature. The reproducibility is high due to the low etch rate. But unfortunately, a rough surface results from the etch process. The SEM micro-graph in C) was obtained by P. Kaspar after etching with HCl for 1 min. Because of the short etch time, the accurate control of the channel width $w$ is not simple. Thus a new selective wet etch solutions is required, which provides both, high reproducibility and smooth surfaces.
Table 8.3: Electrically pumped active PhC devices (laser) reported in literature. The surface-emitting membrane-type PhC lasers are characterized by very low threshold currents $I_{\text{threshold}}$ and low optical output powers $P_{\text{out}}$. On the other hand, substrate-type PhC lasers have threshold currents in the mA-range and output powers in the order of a few mW.

<table>
<thead>
<tr>
<th>Ref.</th>
<th>Description of the Design</th>
<th>Active Material</th>
<th>Footprint</th>
<th>Pumping</th>
<th>$I_{\text{threshold}}$</th>
<th>$P_{\text{out}}$</th>
<th>SM/MM</th>
</tr>
</thead>
<tbody>
<tr>
<td>[211]</td>
<td>suspended PhC cavity, surface emitter</td>
<td>6 InGaAsP QWs (strained)</td>
<td>10 $\mu$m x 10 $\mu$m</td>
<td>h/v</td>
<td>260 $\mu$A</td>
<td>2nW</td>
<td>SM</td>
</tr>
<tr>
<td>[65]</td>
<td>suspended PhC W1 waveguide cavity, surface emitter</td>
<td>InGa QDots</td>
<td>10 $\mu$m x 10 $\mu$m</td>
<td>h</td>
<td>181 nA ($50^\circ$K), 287 nA ($150^\circ$K)</td>
<td>0.7pW</td>
<td>SM</td>
</tr>
<tr>
<td>[283, 24, 303]</td>
<td>PhC cavity LED that couples into a W1-W5 PhC waveguide, edge-emitter, pulsed operation @ room temperature</td>
<td>Q-Dots</td>
<td>20 $\mu$m x 10 $\mu$m</td>
<td>v</td>
<td>not specified</td>
<td>not specified</td>
<td>SM</td>
</tr>
<tr>
<td>[120]</td>
<td>W4-W20 PhC waveguides, edge-emitter</td>
<td>3 InGaAs QWs, 1 $\mu$m top cladding</td>
<td>20 $\mu$m x 2 mm</td>
<td>v</td>
<td>209 – 470 mA</td>
<td>0.5 – 2mW</td>
<td>MM</td>
</tr>
<tr>
<td>[53, 272]</td>
<td>W5-W7 PhC waveguides / ridge waveguide with a constriction, edge-emitter, pulsed operation @ room temperature</td>
<td>6 InGaASP QWs (strained), 1.5 $\mu$m top cladding</td>
<td>chip length x 20 $\mu$m</td>
<td>v</td>
<td>not specified</td>
<td>not specified</td>
<td>MM</td>
</tr>
<tr>
<td>[308, 309]</td>
<td>2D PhC (defect free PhC)</td>
<td>4 InGaAsP QW, 450 nm top cladding</td>
<td>100 $\mu$m x 550 $\mu$m</td>
<td>v</td>
<td>560 mA</td>
<td>40mW</td>
<td>-</td>
</tr>
<tr>
<td>[89]</td>
<td>coupled PhC cavities, edge-emitters</td>
<td>4 InGaAsP QWs (strained), 1.6 $\mu$m top cladding</td>
<td>150 $\mu$m x 20 $\mu$m</td>
<td>v</td>
<td>15 mA</td>
<td>2.6mW (thermally limited)</td>
<td>MM</td>
</tr>
<tr>
<td>[165]</td>
<td>coupled PhC cavities, G-M waveguides, edge-emitter</td>
<td>QWs</td>
<td>150 $\mu$m x 20 $\mu$m</td>
<td>v</td>
<td>13 mA</td>
<td>2.7mW (W11)</td>
<td>MM</td>
</tr>
</tbody>
</table>

Legend: h: horizontal carrier injection (membrane-type PhC devices); v: vertical current injection (substrate-type PhC devices); Footprint: the size of the physical layout of the PhC devices including the PhC cladding layers; SM: single-mode; MM: multimode
posed cross-hair device, which is a significant simplification. But, the etching has to be controlled in two different layers as opposed to Ref. [238, 211], where only one layer is etched. Nevertheless, we have promising preliminary results, which suggest that a reproducible fabrication of the proposed cross-hair device will be possible (see Fig. 8.13 for some SEM micro-graphs of preliminary etch-tests). When using membranes and lateral current injection, the PhC designs are restricted to relatively small filling factors to obtain low ohmic resistances. As opposed to that, the ohmic resistance of our cross-hair device mainly depends on the width of the contact channel \( w \), and hence the design freedom for the PhC geometry is preserved.

The vertically injected in-plane PhC waveguide lasers [120, 53, 89, 165, 272] are typically multi-moded (\( \gtrsim W_4 \) PhC waveguide). Either cavities [165, 89] or constrictions [53] have been added to the multimode PhC waveguides to achieve monomode operation. Those devices achieve output powers in the order of a few mW, which is considerably larger than the achieved output powers for membrane based PhC lasers. The PhC waveguide lasers typically emit at wavelengths corresponding to flat bands originating from mini-stop bands. The flat bands lead to a gain enhancement [59]. Because of the small frequency ranges of flat bands and the sharp PhC cavity resonances, the reported active PhC designs can only be used for lasing and not for broad band amplification. As opposed to that, our design has the advantage of providing a single-mode frequency range. This allows to tailor the PhC waveguide mode to exhibit flat bands with a moderate slow down factor (to increase the frequency band width) and with a negligible group velocity dispersion [156, 142]. Furthermore, by shifting the flat bands away from the Brillouin zone edge, it is possible to benefit from the gain enhancement effect [59] without suffering from additional losses due to backscattering [202, 95, 144, 44, 156]. The enhanced gain of the optical amplifier can be used to reduce the length of the amplifier device (cf. Sec.2.2.2.3). To our knowledge, our design is the only line-defect PhC waveguide that can be be used for the implementation of a broad band (\( \Delta \lambda \approx 25 – 100 \) nm) amplifier (SOA).

8.7 Conclusion

We presented an active low-loss PhC waveguide design with a vertical contacting scheme that promises a net gain for an electrically pumped active in-plane PhC waveguide. The optical performance was determined by a 3D FDTD simulation. A loss figure of less than 20 dB/cm for a wavelength bandwidth of \( \Delta \lambda = 23.3 \) nm was computed. For the electrical performance and the assessment of the waveguides potential for optical gain, a number of approximations were necessary to realistically estimate parameters such as material and free-carrier absorption, heat conduction, gain material and optical propagation losses. Our design has the advantage of having a true single mode operation range with low propagation losses. To our knowledge, the proposed design is the first single-mode PhC waveguide design with a vertical carrier injection scheme that can be used for the implementation of an electrically pumped broad-band (\( \Delta \lambda \approx 25 – 100 \) nm) semiconductor optical amplifier.
Conclusions and Outlook

The original aim of this thesis was the successful implementation of electrically pumped PhC devices such as an SOA or a laser. A successful implementation of an electrically driven single-mode line-defect PhC waveguide has not been achieved so far, due to the large propagation losses in the order of $\alpha_{dB} = 600 - 1000 \text{ dB/cm}$ observed in substrate-type PhC waveguides. To the best of our knowledge, the smallest working electrically pumped line-defect PhC waveguide lasers in our material system have a waveguide core width of $w \approx 1.4 \mu\text{m}$ [120, 272, 53]. These PhC waveguides are multimoded. Thus, the focus of this work lies on the fundamental question if substrate-type single-mode line-defect PhC waveguides can be realized that exhibit propagation losses comparable to the propagation losses $\alpha_{dB} \approx 20 \text{ dB/cm}$ of working devices, e.g., the W4 [120] and the W5 PhC waveguides [272, 53].

Before we discuss the question, we pass the thesis in review and put the emphasis on i) the contributions of this work to the state-of-the-art and ii) hitherto open questions that have been answered within the thesis.

9.1 Achievements and Contributions of this Work

- **Mode-map plots for engineering the dispersion relation of line-defect PhC waveguides.** The mode-map plots introduced in Sec. 3.3 show the influence of a specific PhC design parameter on the dispersion curve of the line-defect PhC waveguide modes. A set of mode-map plots can be used to identify the relevant design parameters to modify the dispersion of the line-defect PhC waveguide according to specific needs. Mode-map plots are suitable to reduce the search space of a design optimization algorithm.

- **Development of an efficient eigen-mode solver including dispersive materials.** The optimization of PhCs and PhC waveguides is a key acquirement for successfully engineering PhC devices. Since this design task is computationally expensive, efficient methods are required. A method based on high order finite elements with curved cells has been developed that allows us to solve for the band structure taking dispersive materials into account. The new
Conclusions and Outlook

- **Progressing the theory of propagation losses in substrate-type PhC waveguides.** We formulated a set of hypotheses about the loss mechanism in slab PhC waveguides. The theory consists of five statements (cf. Sec. 4.2) explaining i) when radiation losses have to be expected, ii) how the light is lost and iii) how much light is lost. A Bloch mode is only guided, if the wave vectors $k_m$ of all spatial Fourier components $m$ are larger than the largest wave vector $k_{clad}$ of oscillatory modes of the cladding. We computed the separatrix that borders the domain of these modes with oscillatory fields in the cladding for substrate-type W1 PhC waveguides. We find that one spatial Fourier component of the Bloch mode of our substrate-type W1 PhC waveguide is always located within the domain of radiation modes. Therefore a set of radiative Bloch modes – forming a leaky Bloch wave – is excited for an excitation frequency within the photonic band gap of the PhC. According to the hypotheses, the large measured propagation losses of our substrate-type W1 PhC waveguides originate from the fact that we excite the waveguide with a frequency, for which no guided Bloch mode exists. The radiation losses are proportional to the square of the magnitude of the spatial Fourier component of the Bloch mode within the domain of radiation modes. The hypotheses were verified by a set of numerical experiments and no contradiction of the hypotheses were found so far.

- **Development of a numerical method to accurately compute propagation losses.** A numerical method was developed that employs the cutback-method on the basis of an FDTD code. Although inefficient, the method is able to accurately predict the propagation losses of substrate-type line-defect PhC waveguides. A remarkable agreement was found between the computed propagation losses and experimental data for almost the entire single-mode regime of the W1 PhC waveguide.

- **Systematic study of structural imperfections to reduce the propagation losses due to fabrication imperfections.** The method developed to accurately compute the propagation losses was applied on a variety of structural imperfections to systematically investigate the influence of fabrication imperfections and design considerations on the propagation losses. The performed numerical experiments allowed us to identify the angled sidewalls of the cylindro-conical hole shape to be the main fabrication-related source of the propagation losses. In most cases the dominant loss mechanism is due to the fact that the waveguide is operated beyond the cutoff.

- **Reducing the propagation losses by optimizing the PhC waveguide design.** We optimized the thicknesses of the layers of the vertical InP/InGaAsP/InP structure for a realistic cylindro-concial hole shape and found that the propagation losses can be reduced from about 1000 dB/cm to roughly 600 dB/cm by using a thicker core layer thickness of about $d_{core} \approx 750$ nm. Furthermore, we pursued the approach to reduce the magnitudes of the spatial Fourier components of the Bloch wave above the background-line. We found that shifting one side of the PhC cladding of the line-defect PhC waveguides by half a period along the waveguide axis generally results in

numerical method exhibits an exponential convergence.
a very low spatial Fourier component of the Bloch mode in the first Brillouin zone. These so called W1-$\alpha/2$ waveguides exhibit propagation losses below $\alpha_{dB} < 100 \, \text{dB/cm}$ for a perfect cylindrical hole shape, theoretically. Furthermore, we discovered that increasing the radius of the holes in the substrate layer with respect to the radius of the holes in the core layer results in a reduction of the propagation losses of the W1 PhC waveguides to values of $\alpha_{dB} < 150 \, \text{dB/cm}$.

- Development of two post-processing steps to reduce the propagation losses of substrate-type W1 PhC waveguides. To reduce the sidewall angle of the etched holes, a thermally driven mass transport process in the MOVPE was developed. The process yields a more cylindrical hole shape in the substrate layer. The optically measured propagation losses are reduced from about 1000 dB/cm to roughly 500 dB/cm (a factor of two) for some frequency ranges. Then, a selective wet-etching process based on HCl and citric acid was developed to controllably increase the radius of the holes in the substrate layer only. Even though the enlargement of the holes is moderate for the fabricated samples, the propagation losses reduce to the propagation losses of a W1 PhC waveguide with a perfect cylindrical hole shape. For those samples we experimentally measured propagation losses as low as $154 \, \text{dB/cm}$. So far, the lowest measured propagation loss value for substrate-type W1 PhC waveguide in the InP/InGaAsP reported in literature has been $\alpha_{dB} \approx 600 \, \text{dB/cm}$ [274, 260]. Our record-low propagation loss value of $\alpha_{dB} = 154 \, \text{dB/cm}$ thus represents the currently lowest measured propagation loss for a substrate-type W1 PhC waveguide in the InP/InGaAsP system.

- Design proposal for low-loss, electrically pumped in-plane active PhC waveguides. We have proposed an active low-loss PhC waveguide design with a vertical contacting scheme that promises a net gain for an electrically pumped active in-plane PhC waveguide. The proposed theoretical cross-hair design exhibits propagation losses of less than 20 dB/cm for a wavelength bandwidth of $\Delta \lambda = 23.3 \, \text{nm}$. The design essentially consists of a modified membrane-type W1 PhC waveguide with two narrow vertical contact channels. The channels are wide enough to support the estimated threshold current density of $J_{tr} < 0.54 \, \text{kA/cm}^2$ and simultaneously provide truly guided line-defect PhC waveguide modes: all spatial Fourier components of the Bloch mode are located below the background-line that is given by the fundamental TM mode of the vertical slab waveguide (contact channel). The new design has a true single mode operation range with low propagation losses. Therefore, the proposed design is suited for the implementation of an electrically pumped broadband ($\Delta \lambda \approx 25 – 100 \, \text{nm}$) semiconductor optical amplifier.
9.2 Conclusions

The improved theoretical understanding as well as the accurate computation of the propagation losses of line-defect PhC waveguides allowed us to answer the following important questions:

- **How much propagation loss remains even for the perfectly fabricated PhC waveguide?**
  The remaining (intrinsic) propagation losses depend on the PhC waveguide design. The minimum achievable propagation loss for a W1 PhC waveguide with a core layer thickness $d_{\text{core}} = 522$ nm and a top-cladding thickness $d_{\text{clad}} = 300$ nm depends on the hole radius and is roughly between $\alpha_{\text{dB}} = 150$ dB/cm ($r = 0.32a$) and $\alpha_{\text{dB}} = 300$ dB/cm ($r = 0.34a$) (cf. chapter 6 and chapter 7).

- **What is the lowest propagation loss that can be obtained with the substrate-type PhC waveguide technology?**
  By increasing the radius of the holes in the substrate layer only, propagation losses in the order of $\alpha_{\text{dB}} \approx 150$ dB/cm are obtained for almost the complete photonic band gap of the PhC, theoretically. Experimentally, we observed that already a modest enlargement of the holes in the substrate layer results in propagation losses that are very similar to the intrinsic losses of substrate-type PhC waveguides. Therefore, we expect that the W1-$a/2$ PhC waveguide maintains its low-loss properties for an increased radius in the substrate. Numerical simulations support this expectation. We expect that propagation losses as low as about $\alpha_{\text{dB}} \approx 80$ dB/cm can be achieved for practical devices, experimentally.

- **Which structural imperfection resulting from our fabrication process is responsible for the large propagation loss?**
  The angled sidewalls in the uppermost part of the holes are the main source for propagation losses due to fabrication imperfections (chapter 6). The lowest measured propagation losses for realistic cylindro-conical holes and a radius $r = 0.34a$ are roughly $\alpha_{\text{dB}} \approx 1000$ dB/cm. For the same W1 PhC waveguide but with perfect cylindrical holes, propagation losses of about $\alpha_{\text{dB}} = 300$ dB/cm are expected according to our simulations. In other words, the cylindro-conical hole shape is responsible for large portion of the measured propagation loss that amounts to about $\alpha_{\text{dB}} \approx 500 - 3000$ dB/cm depending on the frequency.

- **What can be done to improve the fabrication process?**
  The main effort in improving the technology should be directed to reduce the conical sidewalls in the upper part (to a depth of about 1.1 $\mu$m) of the hole rather than to increase the hole-depth or the smoothness of the sidewalls (chapter 6).

- **Is there a PhC waveguide design that has lower intrinsic propagation losses?**
  The W1-$a/2$ PhC waveguide is the design that has the smallest magnitude of the spatial Fourier component of the Bloch mode above the background-line. A propagation loss of $\alpha_{\text{dB}} \approx 80$ dB/cm is expected for a W1-$a/2$ PhC
waveguide design for a core layer thickness $d_{\text{core}} = 522$ nm, top-cladding thickness $d_{\text{clad}} = 300$ nm and a radius $r = 0.34a$ (chapter 7). We could further show that the propagation losses of the W$1-a/2$ PhC waveguide are currently limited by fabrication imperfections, i.e., the cylinbro-conical hole shape (chapter 6).

- Is there an alternative design that can provide both, ultra low propagation losses and vertical electrical current injection?

We proposed a PhC waveguide design that is essentially a membrane-type PhC waveguide with two narrow vertical contacting channels. The idea behind the design is to shift the background-line – given by the fundamental TM mode of the vertical slab waveguide – above all spatial Fourier components of the Bloch wave. Numerical simulations predicted propagation losses of $\alpha_{dB} < 20$ dB/cm for a frequency range of $\Delta \omega/2\pi c = 0.0022$. The proposed design is suitable for in-plane active PhC semiconductor optical amplifiers.

9.3 Outlook

The main obstacles for the successful implementation of electrically pumped active PhC waveguides are a) the lack of efficient carrier injection for membrane-type PhCs and b) the large propagation losses of substrate-type PhC waveguides. The large propagation losses of substrate-type PhC waveguides make it impossible to implement efficient single-mode line-defect PhC waveguides. Within the last decade, no significant improvement has been made to reduce the propagation losses to a level that would enable a net gain. We measured propagation losses of about $\alpha_{dB} \approx 50 - 100$ dB/cm for the W$3$ PhC waveguide. However, the smallest substrate-type line-defect PhC lasers are about $w = 1.4 \mu m$ wide, i.e., W$4$ and W$5$ PhC waveguides. Therefore, the propagation losses have to be lower than $\alpha_{dB} < 50$ dB/cm for a net gain. Experimentally measured propagation losses of $\alpha_{dB} = 154$ dB/cm are still a factor of three larger than the anticipated minimum requirements. Nevertheless, our simulations show that propagation losses as low as $\alpha_{dB} \approx 80$ dB/cm should be feasible experimentally for single-mode line-defect PhC waveguides. Even tough a discrepancy of roughly a factor of two remains, the implementation of an electrically driven single-mode active PhC waveguide has to be reconsidered. The missing factor of two may be obtained by further optimizations, such as increasing the number of quantum wells. The alternative approach of the proposed PhC waveguide design (cf. chapter 8) is promising but very challenging for a reliable fabrication. One reason is that the etch-rates of a selective wet etching process is not expected to be similar for the top and the bottom cladding, due to dynamics in the etching-solution and due to different doping concentrations in the top and bottom cladding.

The next steps are

- Manufacture waveguides that combine the optimized layer stack with the new hole shape resulting from the two new post-etch processes. Furthermore, it would be promising to optimize the vertical layer stack for the en-
engineered hole shape (after the mass transport and the selective wet-etching process).

- Increase the radius in the substrate layer further by using the selective wet-etch process. Our simulation results suggest that the propagation losses decrease for the lower frequency regime if the radius of holes in the substrate is enlarged.

- Manufacture the W1-\(\alpha/2\) waveguide proposed by Kuang et al. [141] (cf. Sec. 7.2) to demonstrate the low propagation losses experimentally. The cylindro-concial holes add a large propagation loss contribution due to fabrication imperfections. However, our results suggest that we are very close to an ideal cylindrical hole shape. Therefore, it is promising to fabricate the W1-\(\alpha/2\) waveguide using the new post-etch processes. If the simulated propagation loss of \(\alpha_{dB} \approx 80\) dB/cm could be verified experimentally, it would signify an improvement by one order of magnitude with respect to the state-of-the-art [271, 274, 260].

- Improve the wet-etching processes for the accurate control of the selective-etching of the InP layers in order to fabricate the narrow contact channel of the proposed cross-hair design (cf. chapter 8). If a PhC device with a net gain can be realized, then one can think of optimizing the dispersion of the line-defect PhC waveguide mode to exhibit a slow light regime below the background-line of the vertical contacting channels. This would allow us to reduce the device length of a semiconductor optical amplifier substantially.
Appendix

A.1 Governing Maxwell’s Equations

The macroscopic Maxwell’s equations are

\[ \nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \]  
(A.1)
\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \]  
(A.2)
\[ \nabla \cdot \mathbf{D} = \rho \]  
(A.3)
\[ \nabla \cdot \mathbf{B} = 0, \]  
(A.4)

where \( \mathbf{E} \) and \( \mathbf{H} \) are the electric and magnetic fields, \( \mathbf{D} \) is the displacement field and \( \mathbf{B} \) is the magnetic induction field and \( \rho \) and \( \mathbf{J} \) are the free electric charges and current density, respectively. We restrict us to piecewise homogeneous, lossless materials and to the absence of electric charges \( (\rho = 0) \) and currents \( (\mathbf{J} = \mathbf{0}) \). If we further assume a linear relation between the electric flux density and the electric fields \( \mathbf{D} = \varepsilon \varepsilon_0(\mathbf{r}) \mathbf{E} \) (this is an appropriate approximation for small field strengths), then the Maxwell’s equations simplify to

\[ \nabla \times \mathbf{H} = \varepsilon(\mathbf{r})\varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \]  
(A.5)
\[ \nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t} \]  
(A.6)
\[ \nabla \cdot \varepsilon(\mathbf{r}) \mathbf{E} = 0 \]  
(A.7)
\[ \nabla \cdot \mathbf{H} = 0. \]  
(A.8)

The magnetic and electric field components can be decoupled by applying the \( \nabla \times \) operator on both sides of the first two Maxwell’s equations (Eq. A.5 and Eq. A.6) followed by a substitution of \( \nabla \times \mathbf{E} \) by Eq. A.6 and of \( \nabla \times \mathbf{H} \) by Eq. A.5.
\[
\n\nabla \times \left[ \frac{1}{\varepsilon(r)} \nabla \times H \right] = -\mu_0 \varepsilon_0 \frac{\partial^2}{\partial t^2} H \tag{A.9}
\]

\[
\nabla \times \nabla \times E = -\mu_0 \varepsilon_0 \frac{\partial^2}{\partial t^2} E \tag{A.10}
\]

An equation for the electric field \(E\) only (Eq. A.10) and an equation for only the magnetic field \(H\) (Eq. A.9) are obtained. The two equations are equivalent, i.e., it is sufficient to solve only for one field component by using one of the equations. The other, complementary field component can then be derived from the solution by using either \(\nabla \times E\) (Eq. A.6) or \(\nabla \times H\) (Eq. A.5). In case of a periodic permittivity \(\varepsilon(r) = \varepsilon(r + a)\), where \(a\) is a translation vector, the differential equation of the magnetic field is the preferred equation, because of the hermiticity\(^1\) of the operator \(-\nabla \times \left[ \frac{1}{\varepsilon(r)} \nabla \times \right]\). This equation is referred to as the **master equation** [104].

By using the vector identity \(\Delta v := \nabla \cdot \nabla \cdot v - \nabla \times \nabla \times v\) and by using \(\nabla \cdot E = 0\) (Eq. A.7) and \(\nabla \cdot H = 0\) (Eq. A.8) the equations can be written as [172]

\[
\Delta E(r, t) + \varepsilon(r) \frac{1}{c^2} \frac{\partial^2}{\partial t^2} E(r, t) = -\nabla \left[ \nabla \left( \ln(\varepsilon(r)) \right) \right] E \tag{A.11}
\]

\[
\Delta H(r, t) + \frac{1}{c^2} \frac{\partial^2}{\partial t^2} H(r, t) = -\nabla(\ln(\varepsilon(r))) \times \nabla \times H. \tag{A.12}
\]

If only homogeneous materials are considered, then the right hand sides of Eq. A.11 and Eq. A.12 vanish and the following two wave equations are obtained

\[
\Delta E(r, t) + \varepsilon(r) \frac{1}{c^2} \frac{\partial^2}{\partial t^2} E(r, t) = 0 \tag{A.13}
\]

\[
\Delta H(r, t) + \frac{1}{c^2} \frac{\partial^2}{\partial t^2} H(r, t) = 0. \tag{A.14}
\]

For time-invariant dielectric systems, time-harmonic fields (i.e., a sinusoidal time-dependence of the fields \(e^{i\omega t}\)) can be assumed since any smooth signal can be represented by a superposition of harmonic components. For time-harmonic fields, the wave equation simplify to the so-called Helmholtz equations

\[
\Delta E(r, t) - \varepsilon(r) \frac{\omega^2}{c^2} E(r, t) = 0 \tag{A.15}
\]

\[
\Delta H(r, t) - \frac{\omega^2}{c^2} H(r, t) = 0. \tag{A.16}
\]

These equations are the governing equations for many practical electromagnetic problems, such as the asymmetric slab waveguide presented in Sec. 2.1.2.

\(^1\)The proof of the hermiticity of the operator \(-\nabla \times \left[ \frac{1}{\varepsilon(r)} \nabla \times \right]\) is given in [104, pp. 10-12]
A.2  Remark on the Power Flux of a Superposition of Modes

Any of the obtained modes in Sec. 2.1.2 share the property, that its Poynting vectors are directed in propagation direction \( e_x \) exclusively. Because the discrete set of guided modes and the continuous set of radiation modes form a complete set of basis functions [164], any possible field pattern excited by an initial field \( A_z(x = 0) \) can be expanded in this set. It is argued, that the modes of the complete set, whose Poynting vectors are only directed in propagation direction \( e_x \), cannot in its sum express a radiation phenomenon with Poynting vectors pointing away from the waveguide. We will show in this section that this objection is not justified. We start with the time-averaged Poynting vector for time-harmonic fields defined as

\[
\langle \mathbf{S} \rangle_t = \frac{1}{2} \Re \left\{ \mathbf{E} \times \mathbf{H}^* \right\}.
\]

(A.17)

In case of TE modes \( \mathbf{E} = (0, E_{y,0}) \) and \( \mathbf{H} = (H_x, 0, H_z) \) we obtain

\[
\langle \mathbf{S} \rangle_t = \frac{1}{2} \Re \left\{ \begin{pmatrix} 0 & H_x^* \\ E_y & 0 \end{pmatrix} \times \begin{pmatrix} H_x^* \\ 0 \end{pmatrix} \right\} = \frac{1}{2} \Re \left\{ \begin{pmatrix} E_y H_x^* \\ -E_y H_x^* \end{pmatrix} \right\}.
\]

(A.18)

Thus TE modes have a power flow in propagation direction \( e_x \) but also in transverse direction \( e_z \). First, we consider a single TE mode. The Poynting vector component \( S_z \) in transverse direction \( e_z \) is

\[
2 \cdot \langle S_z \rangle_t = \Re \{ -E_y H_x^* \} = \Re \left\{ E_y e^{-i\beta_x x} \frac{-i}{\omega \mu_0} E_y e^{i\beta_x x} \right\} = \Re \left\{ \frac{-i}{\omega \mu_0} E_y^2 \right\} = 0,
\]

(A.19)

where we used \( H_x = \frac{i}{\omega \mu_0} \frac{\partial}{\partial z} E_y \) and \( H_z = -\beta_x E_y \). The power flow in transverse direction \( z \) of a single mode always cancel, because \( H_z \) is purely imaginary (Eq. 2.9: \( H_x = \frac{i}{\omega \mu_0} \frac{\partial}{\partial z} E_y \) and \( H_z = \beta_x E_y \) for \( E_y \in \mathbb{R} \). Thus the power flux of a single mode always exclusively directs in propagation direction \( e_x \). But, the sum of two radiation modes, however, results always in a non-zero power flux in transverse direction \( e_z \). Consider the sum of two radiation modes \( \mathcal{E}_1 \) and \( \mathcal{E}_2 \)

\[
E_y(x) = C_1(x) \mathcal{E}_1 e^{-i\beta_{x1} x} + C_2(x) \mathcal{E}_2 e^{-i\beta_{x2} x}
\]

(A.20)

where \( C_{1,2}(x) \) are two real coefficients that weight the radiation modes \( \mathcal{E}_1 \) and \( \mathcal{E}_2 \) and \( \beta_{x1}/\beta_{x2} \) are the propagation constants of the two radiation modes. By using Eq. 2.9 and Eq. 2.10 we obtain

\[
H_x(x) = \frac{i \kappa_1(z)}{\omega \mu_0} C_1(x) \mathcal{E}_1 e^{-i\beta_{x1} x} + \frac{i \kappa_2(z)}{\omega \mu_0} C_2(x) \mathcal{E}_2 e^{-i\beta_{x2} x}
\]

(A.21)

\[
H_z(x) = \frac{-\beta_{x1}}{\omega \mu_0} C_1(x) \mathcal{E}_1 e^{-i\beta_{x1} x} - \frac{\beta_{x2}}{\omega \mu_0} C_2(x) \mathcal{E}_2 e^{-i\beta_{x2} x}
\]

(A.22)

where \( \kappa_{1,2} \) is either \( \rho_{1,2}, \sigma_{1,2} \) or \( \Delta_{1,2} \) (cf. Sec. 2.1.2.4) dependent on transverse
position $z$. The power flux component in transverse direction $e_z$ is computed according to Eq. A.18

$$\langle S_z \rangle_t = \frac{1}{2} \Re\left( E_y H_z^* \right)$$

$$= \frac{1}{2} \Re \left\{ \left( C_1(x) E_1 e^{-i\beta_{x_1} x} + C_2(x) E_2 e^{-i\beta_{x_2} x} \right) \cdot \left( \frac{-i\kappa_1(z)}{\omega\mu_0} C_1(x) E_1 e^{i\beta_{x_1} x} + \frac{-i\kappa_2(z)}{\omega\mu_0} C_2(x) E_2 e^{i\beta_{x_2} x} \right) \right\}$$

$$= \frac{1}{2\omega\mu_0} C_1(x) C_2(x) E_1 E_2 (\kappa_1(z) - \kappa_2(z)) \sin((\beta_{x_1} - \beta_{x_2}) x) \quad (A.23)$$

The transverse component of the Poynting vector would only cancel in case that either $\kappa_1(z) = \kappa_2(z)$ or $\beta_{x_1} = \beta_{x_2}$. In other words, the transverse component of the Poynting vector only cancels if the two radiation modes $E_1$ and $E_2$ are the same ($E_1 = E_2$), i.e., only one radiation mode would propagate.

### A.3 Reciprocal Lattice Vectors for a 2D Photonic Crystal

In case of planar 2D PhC, the explicit formula for the reciprocal lattice vectors $b_1$ and $b_2$ for given lattice vectors $a_1$ and $a_2$ can be derived from Eq. 2.38 by requiring

$$b_i \cdot a_j = 2\pi \delta_{ij} \quad (A.24)$$

for all $N \in \mathbb{N}$, where $\delta_{ij}$ is the Kronecker delta function ($\delta_{ij} = 1$ if $i = j$, otherwise $\delta_{ij} = 0$). This equation is detailed as

$$a_1 \cdot a_1 = 2\pi \quad (A.25)$$

$$a_1 \cdot a_2 = 0 \quad (A.26)$$

$$a_2 \cdot a_1 = 0 \quad (A.27)$$

$$a_2 \cdot a_2 = 2\pi \quad (A.28)$$

using the components of $a_i = (a_{ix}, a_{iy})$ and $b_j = (b_{jx}, b_{jy})$ and solving the above linear system of equation the explicit formulas for the reciprocal lattice vectors $b_j$ are found

$$b_1 = \frac{2\pi}{\text{det}(a_1, a_2)} \begin{pmatrix} a_{2y} \\ -a_{2x} \end{pmatrix} \quad (A.29)$$

$$b_2 = \frac{2\pi}{\text{det}(a_1, a_2)} \begin{pmatrix} a_{1y} \\ -a_{1x} \end{pmatrix} \quad (A.30)$$

Two important properties can directly be derived from Eq. A.29 and Eq. A.30. First, the reciprocal lattice vectors $a_j$ are mutual perpendicular to their real space vectors $a_i$
Secondly, the magnitude of the reciprocal lattice vector $|b_{1,2}|$ is given by $|b_{1,2}| = (1/d_{1,2})$, where $d_{1,2}$ is the spacing of parallel lattice vectors $a_{2,1}$. It is hence possible to compute the reciprocal lattice vectors by means of geometrical drawing.

### A.4 Plane Wave Expansion

This section provides the detailed calculation of the plane wave expansion presented in Sec. 2.2.3.2. The starting point is the master equation as given in Eq. 2.51

$$- \nabla \times \left[ \frac{1}{\varepsilon(x)} \nabla \times H_{k_x,z}(x) \right] + \frac{\omega^2}{c^2} H_{k_x,z}(x) = 0. \quad (A.33)$$

By substituting $H_{k_x,z}$ by its plane wave expansion Eq. 2.50 we obtain

$$\left( \begin{array}{ccc} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{array} \right) \times \left[ \frac{1}{\varepsilon(x)} \left( \begin{array}{ccc} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{array} \right) \times \sum_m w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} e_z \right] +$$

$$\frac{\omega^2}{c^2} \sum_m w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} e_z = 0. \quad (A.34)$$

Because of the invariance in y-direction and z-direction, the partial derivatives in y and z vanish ($\frac{\partial}{\partial y} = 0$ and $\frac{\partial}{\partial z} = 0$). Therefore, the $x$- and $z$-component of the magnetic field become zero after the computation of the first rotation operator

$$\left( \begin{array}{ccc} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{array} \right) \times \left[ \frac{1}{\varepsilon(x)} \left( \begin{array}{ccc} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{array} \right) \times \sum_m w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} \right] +$$

$$\frac{\omega^2}{c^2} \sum_m w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} e_z = 0. \quad (A.35)$$

Next, the substitution of the periodic permittivity $\frac{1}{\varepsilon(x)}$ by its plane wave decomposition

$$\frac{1}{\varepsilon(x)} = \sum_l v_l e^{i \frac{2\pi}{\alpha} x} \quad (A.36)$$

is required to compute the remaining rotation operator and a scalar equation
for the \( z \)-component of the magnetic field is obtained

\[
\frac{\partial}{\partial x} \left[ \sum_l \nu_l e^{i \frac{2\pi}{a} x} \cdot \sum_m i (\hat{k}_x + m \frac{2\pi}{a}) \cdot w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} \right] + \frac{\omega^2}{c^2} \sum_m w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} = 0. \tag{A.37}
\]

By applying the chain rule the partial derivative \( \partial / \partial x \) can be computed

\[
\left[ \sum_l i l \frac{2\pi}{a} \cdot \nu_l e^{i \frac{2\pi}{a} x} \cdot \sum_m i (\hat{k}_x + m \frac{2\pi}{a}) \cdot w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} - \sum_l \nu_l e^{i \frac{2\pi}{a} x} \cdot \sum_m (\hat{k}_x + m \frac{2\pi}{a})^2 \cdot w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} \right] + \frac{\omega^2}{c^2} \sum_m w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} = 0. \tag{A.38}
\]

In the following, a careful rearranging of the sum terms is required to simplify the equation. First we make use of the rule that applies to the product of two summations \( \sum_n a_n \cdot \sum_m b_m = \sum_n (\sum_m a_n b_m) \)

\[
\left[ - \sum_m \{ \sum_l (\hat{k}_x + m \frac{2\pi}{a}) \cdot w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} l \frac{2\pi}{a} \cdot \nu_l e^{i \frac{2\pi}{a} x} \} - \sum_m \{ \sum_l (\hat{k}_x + m \frac{2\pi}{a})^2 \cdot w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} \cdot \nu_l e^{i \frac{2\pi}{a} x} \} \right] + \frac{\omega^2}{c^2} \sum_m w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} = 0. \tag{A.39}
\]

In a second step we can exploit the addition of two summations according to

\[
\sum_n a_n + \sum_n b_n = \sum_n a_n + b_n
\]

\[
- \sum_m \{ \sum_l (\hat{k}_x + m \frac{2\pi}{a}) \cdot w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} l \frac{2\pi}{a} \cdot \nu_l e^{i \frac{2\pi}{a} x} + \sum_l (\hat{k}_x + m \frac{2\pi}{a})^2 \cdot w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} \cdot \nu_l e^{i \frac{2\pi}{a} x} e^{imKx} \} + \frac{\omega^2}{c^2} \sum_m w_{k_x,m} H_0 e^{i(k_x + m \frac{2\pi}{a}) x} = 0. \tag{A.40}
\]

Then, by applying \( \sum_n a_n + \sum_n b_n = \sum_n a_n + b_n \) again we obtain
\[
\sum_m \left\{ \sum_l \left( (\hat{k}_x + (m + l)\frac{2\pi}{a}) \cdot w_{k_x,m} H_0 e^{i(\hat{k}_x + (m + l)\frac{2\pi}{a})x} \cdot v_l \right) \right\} - \\
\frac{\omega^2}{c^2} \sum_n w_{k_x,m} H_0 e^{i(\hat{k}_x + m\frac{2\pi}{a})x} = 0. \quad (A.41)
\]

This equation has to hold for all values of \(x\), i.e., it has to hold for each summand of the summation over \(m\). Technically, both sides are multiplied by an orthogonal function \(f(x) = e^{-i(\hat{k}_x + p\frac{2\pi}{a})x}, p \in \mathbb{Z}\) and then integrated over the unit cell \(\int_{-a/2}^{a/2} dx\). An eigenvalue equation is obtained for \(m = p - l\)

\[
\sum_l \left( (\hat{k}_x + p\frac{2\pi}{a}) \cdot (\hat{k}_x + (p - l)\frac{2\pi}{a}) \cdot w_{k_x,p-l} v_l \right) = \frac{\omega^2}{c^2} w_{k_x,p} \quad (A.42)
\]

### A.5 Analysis of Lattice Disorder and Radius Variations in our PhC Waveguides

Disorder in the lattice can be introduced at various positions in the fabrication process. R. Wuest [294, Chapter 3] developed a proximity effect correction algorithm dedicated to reduce the variations of the radius of the holes due to proximity effects, such as forward scattering and slow secondary electrons and electron backscattering. A standard deviation of roughly 2.8 % is achieved by using the PEC software instead 6.3 % formerly. In Fig. A.1 the analysis of the image processing is shown for one PhC sample. The image processing algorithm essentially consists of a fitting procedure, that fits a circular shape to the SEM images of holes taken at the top surface of the etched PhC structures. From the data of the fitted circles the

![Figure A.1: A: SEM micro-graph cutout of a typical PhC. The red circles represent the fitted circles. From the data of the center of the fitted circles, the lattice constant can be determined by computing the distance between the centers of the circles. B: The histogram of the lattice constant. C: The histogram of the computed radii. Both histograms can be fitted to a Gaussian distribution to determine the mean and the variance.](image-url)
radius and the distance between the circles can be computed. The histogram of the radius and the lattice constant is shown in Fig. A.1 (center, right) for the shown SEM micro-graph in Fig. A.1 (left).

Figure A.2 shows the analysis of the lattice constant and the radii for an array of PhCs with different lattice constants $a$ and different radii $r$. The variance of the lattice constant $\sigma_a$ shown in the left plot of Fig. A.2 reveals an outliers in the standard deviation of lattice constants between 400 nm and 450 nm. Even so, the mean value of the standard deviation $\sigma_a/a$ steadily decreases with increasing lattice constant $a$. The plot on the rights of Fig. A.2 shows the standard deviation $\sigma_r/r$ of the hole radius and the fit to a $1/r$-dependence.

For the benchmark PhC waveguide presented in chapter 5 and chapter 6, a typical standard deviation of the lattice constant of about $\sigma_a/a = 0.01 - 0.012$ and extreme values up to $\sigma_a/a = 0.02$ are found. The typical standard deviation of the hole radius is $\sigma_r/r = 0.01 - 0.02$ for a radius of 148 nm.

### A.6 Free Carrier Absorption Models

The doping of a semiconductor results in a strong increase of free carriers, i.e., free electrons or free holes located in the conduction band of the semiconductor. Photons can be absorbed by exciting a free carrier to an unoccupied, higher energy level in the same conduction band. Free-carrier absorption is proportional to the carrier densities of the doped semiconductor materials. A non-zero absorption coefficient always leads to a change in the real part of the refractive index due to the Kramers-Kronig relation. Using the Drude model [304], the change of the complex refractive index $\tilde{n} = n + i\kappa$ due to free carriers is given by

$$\tilde{n}(\lambda, n, p) = n + i\kappa = n_{ref} - \alpha_c \left( \frac{e}{m_n} + \frac{h}{m_p} \right) + i \cdot \frac{\lambda}{4\pi} (\alpha_n e + \alpha_p h) \quad (A.43)$$

where
Table A.1: Used parameters for the free-carrier absorption model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>InP</th>
<th>(\text{In}<em>{0.53}\text{Ga}</em>{0.47}\text{As} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electron mobility (\mu_e)</td>
<td>5400 [cm(^2) V(^{-1}) s(^{-1})]</td>
<td>12000 [cm(^2) V(^{-1}) s(^{-1})]</td>
</tr>
<tr>
<td>Hole mobility (\mu_h)</td>
<td>200 [cm(^2) V(^{-1}) s(^{-1})]</td>
<td>300 [cm(^2) V(^{-1}) s(^{-1})]</td>
</tr>
<tr>
<td>Electron Effective Mass (m_e)</td>
<td>0.08 (\cdot) (m_0)</td>
<td>0.041 (\cdot) (m_0)</td>
</tr>
<tr>
<td>Hole Effective Mass (m_h)</td>
<td>0.6 (\cdot) (m_0)</td>
<td>0.45 (\cdot) (m_0)</td>
</tr>
<tr>
<td>refractive index (n_{ref}(\lambda))</td>
<td>Palik</td>
<td>Sellmeier</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
\alpha_c &= \frac{q^2 \lambda^2}{8\pi^2 c^2 \varepsilon_0 n_0} \\ 
\alpha_n &= \frac{q^3 \lambda^2}{4\pi^2 c^3 \varepsilon_0 n_{ref} \mu_e m_e^2} \\ 
\alpha_p &= \frac{q^3 \lambda^2}{4\pi^2 c^3 \varepsilon_0 n_{ref} \mu_h m_h^2}
\end{align*}
\quad (A.44) (A.45) (A.46)
\]

\(\alpha_c\) and \(\alpha_n\) are the extinction coefficient and the real part of the refractive index respectively, and \(q\) is the elementary charge, \(\lambda\) is the wavelength, \(c\) is the speed of light and \(\varepsilon_0\) is the vacuum permittivity. \(e\) and \(h\) are the carrier densities of the electrons and the holes, respectively. The material specific parameters are listed in Table A.1. A further increase the intricacy represents, the frequency dependence of the refractive index \(n_{ref}\) of the undoped materials. For InP, we used measured data [210]. The refractive index of the ternary \(\text{InGaAs}\) layer depends on the composition and thus we used the Sellmeier model [205] for the \(\text{InGaAs}\) layer:

\[
n_{\text{InGaAs}}(\lambda) = \sqrt{A + \frac{B}{1 - \frac{C \cdot E_{g, GaAs}}{\lambda^2 E_g(\lambda)^2}}} \
\quad (A.47)
\]

where \(E_{g, GaAs}\) is the band gap energy of \(GaAs\) and \(E_g(x)\) is the band gap energy of \(In_xGa_{1-x}As\). \(A, B\) and \(C\) are fitting parameters of the Sellmeier model. All used parameters are given in Table A.2.

Table A.2: The used Sellmeier parameters for \(\text{InGaAs}\) [205].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>(\text{In}<em>{0.53}\text{Ga}</em>{0.47}\text{As} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(E_{g, GaAs})</td>
<td>1.424</td>
</tr>
<tr>
<td>(E_g(x))</td>
<td>(E_g(x) = E_{g, GaAs} - x \cdot 1.501 + x^2 \cdot 0.436)</td>
</tr>
<tr>
<td>A</td>
<td>8.95</td>
</tr>
<tr>
<td>B</td>
<td>2.054</td>
</tr>
<tr>
<td>C</td>
<td>0.6245</td>
</tr>
</tbody>
</table>
n-doping: free electrons

![Graph showing absorption coefficient as a function of wavelength for free electrons.]

Figure A.3: Left: the absorption coefficient as a function of the operation wavelength $\lambda$ for free electrons (top) and free holes (bottom) for InP. Center/Right: The real and imaginary part of the refractive index of InP as a function of the doping concentration for $\lambda_0 = 1550$ nm.

refractive index due to the higher mobility and lower effective mass with respect to the free holes.
Bibliography


278


[205] B. Optoelectronics”. Refractive index \( n \) of In\(_{x}\)Ga\(_{1-x}\)As alloys. URL http://www.batop.de/information/n_InGaAs.html (2012). (cited on page 263.)


Bibliography


Nomenclature

- \( \mathbf{a}_i \) lattice vectors
- \( a \) lattice constant
- \( \beta_x \) propagation constant in \( e_x \)-direction
- \( \mathbf{b}_i \) reciprocal lattice vectors
- BRWG buried rectangular wave guide
- \( c_0 \) speed of light
- \( \Delta \) transverse wave number in the top cladding layer
- \( d_{W1} \) width of the line-defect PhC waveguide (lateral separation distance between the PhC claddings)
- \( \mathcal{E} \) the solution of an eigenvalue equation, i.e., an optical mode
- \( \mathcal{E}(\rho) \) radiation mode with parameter \( \rho \)
- \( \mathcal{E}_B \) Bloch mode
- \( \mathcal{E}_n \) \( n \)-th guided mode
- \( \varepsilon(\mathbf{r}) \) permittivity
- \( \mathbf{E} \) electric field
- FDTD finite difference time domain method
- FEM finite element method
- FMM Fourier modal method
- \( g_0 \) gain coefficient
- GFT Green’s function tensor method
- GME guided mode expansion method
- \( \mathbf{H} \) magnetic field
- \( H \) heat generation rate
- \( h_{bot} \) thickness of the InP bottom cladding
- \( h_{top} \) thickness of the InP top cladding layer
- \( I_{op} \) drive current
- \( J \) current density
- \( J_0 \) material transparency current density
- \( J_{tr} \) transparency current density of the device
- \( \hat{k}_x \) principal wave vector / dominant Fourier component of the Bloch mode \( \mathcal{E}_B \)
- \( \hat{k} \) Bloch index
- \( \mathbf{k} \) wave vector of a plane wave
- \( k \) thermal conductivity
- \( k \) wave number of a plane wave
- \( k_0 \) vacuum wave number \( k_0 = \omega / c \)
**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ME</td>
<td>mode expansion method</td>
</tr>
<tr>
<td>MMP</td>
<td>multiple multipole method</td>
</tr>
<tr>
<td>$n_{\text{eff}}$</td>
<td>effective refractive index</td>
</tr>
<tr>
<td>$\psi_k$</td>
<td>Bloch wave / Bloch function</td>
</tr>
<tr>
<td>$\varphi_k(r)$</td>
<td>Bloch function</td>
</tr>
<tr>
<td>PBG</td>
<td>photonic band gap</td>
</tr>
<tr>
<td>PhC</td>
<td>photonic crystal</td>
</tr>
<tr>
<td>PWE</td>
<td>Plane wave expansion method</td>
</tr>
<tr>
<td>Si</td>
<td>silicon</td>
</tr>
<tr>
<td>$\rho$</td>
<td>transverse wave number in the bottom cladding layer</td>
</tr>
<tr>
<td>$r$</td>
<td>position vector</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>radius of the circular holes</td>
</tr>
<tr>
<td>$s_{y1}$</td>
<td>lateral shift of the first row of holes</td>
</tr>
<tr>
<td>$s_{y2}$</td>
<td>lateral shift of the first row of holes</td>
</tr>
<tr>
<td>SOA</td>
<td>semiconductor optical amplifier</td>
</tr>
<tr>
<td>$\theta_c$</td>
<td>critical angle</td>
</tr>
<tr>
<td>$T$</td>
<td>temperature</td>
</tr>
<tr>
<td>$t_{\text{core}}$</td>
<td>thickness of the InGaAsP core layer</td>
</tr>
<tr>
<td>$V_{\text{diode}}$</td>
<td>voltage across the diode terminal</td>
</tr>
<tr>
<td>$v_{gr}$</td>
<td>group velocity of a propagating wave packet</td>
</tr>
<tr>
<td>$v_{ph}$</td>
<td>phase velocity of a propagating wave</td>
</tr>
<tr>
<td>$w$</td>
<td>amplitude of the spatial Fourier components of the Bloch mode $\mathcal{E}_B$</td>
</tr>
<tr>
<td>$w$</td>
<td>width of the contacting channel</td>
</tr>
<tr>
<td>$w_{\text{eff}}$</td>
<td>effective (undepleted) width</td>
</tr>
<tr>
<td>$Z$</td>
<td>thermal impedance</td>
</tr>
</tbody>
</table>
Index

absorption, 178
  free carrier, 264
absorption loss, 103
acid
  citric, 224
  hydrochloric, 223
algebraic convergence rate, 88
background-line, 129
BCB, 224
benzocyclobutene, 224
Bloch index, 36, 38
Bloch mode, 113, 129
Bloch wave, 113, 235
Brillouin zone, 38, 61
  first, 38, 235
  irreducible, 38
  reduced, 38
citric acid, 224
coefficient of determination, 163
coupling losses, 180
cross-hair device, 232
current injection schemes, 232
cutback-method, 157
dB-scale, 163
defects in photonic crystals, 42
degree of freedom, 82
depletion width, 241
dispersion, 235
dispersion relation, 64
Effective Index Approximation, 54
evanescent radiation modes, 28
exponential convergence rate, 88
extrinsic propagation losses, 184
Fabry-Perot fringes, 166, 169
Fabry-Perot method, 157
finite difference method, 58
finite element method, 58
flux distribution method, 162
four wave mixing, 4
Fourier optics, 46
free carrier absorption, 264
Fresnel’s equation, 146
gain, 242
gap map, 39
goodness of fit, 163
grid resolution, 171
guided mode, 26
HCl, 223
heat conduction equation, 243
heat dissipation, 243
Helmholtz equation, 124, 258
hydrochloric acid, 223
interface losses, 180
intrinsic loss, 179
intrinsic propagation losses, 184
leaky wave, 104, 108, 113, 181
light-line, 23, 31, 130
line-defect
  PhC waveguide, 40
  photonic crystal waveguide, 42, 63
linear regression, 163
lithographic tuning, 222
loss
  absorption loss, 103
  interface, 180
  intrinsic, 179, 184
  leaky waves, 108
  mode coupling, 180
  out-of-plane, 179
  propagation loss, 108
  radiation leakage, 179
  scattering, 180
  surface scattering, 104
  volume scattering, 103
  waveguide, 107
loss channel, 181
master equation, 258
material absorption, 178
mesh resolution, 171
method
  finite differences, 58
  finite elements, 58
  multiple multipole, 58
  of auxiliary sources, 58
mini-stop bands, 45
mode
  3D line-defect PhC waveguide, 63
  Bloch, 113, 129
evanescent radiation mode, 28
  guided mode, 26
  photonic crystal mode, 38
planar slab waveguide modes, 31
  radiation mode, 26, 28
settling, 171
  slow light, 43
mode settling, 171
mode-maps, 66
multiple multipole method, 58
multiple reflections, 169
out-of-plane losses, 179
parity, 41, 64
photonic band gap, 39, 63
photonic crystal features
  defects, 42
  mini-stop band, 45
  photonic band gap, 39
slow light, 43
photonic crystal waveguide, 42
  polarization, 53
plane wave expansion, 58, 121
polarization
  2D line-defect PhC waveguide, 40, 234
  3D line-defect PhC waveguide, 53
  slab waveguide, 24, 234
primitive cell, 59
propagation loss, 108, 163
radiation leakage, 179, 188
radiation losses, 32
radiation mode, 26, 28
reciprocal lattice, 35, 38, 63
reflection coefficient, 160
scattering losses, 180
self-heating, 243
Sellmeier model, 265
separatrix, 130–132, 135–138, 235
slab-waveguide
  polarization, 24
slow light, 43
super-cell, 60
super-cell approach, 59, 60
surface scattering loss, 104
TE mode
  2D photonic crystal, 38
  slab waveguide, 24
thermal impedance, 245
TM mode
  2D photonic crystal, 38
  slab waveguide, 24, 235
transmission coefficient, 160
unit-cell, 59
volume scattering loss, 103
W-waveguide, 179
wave equation, 125, 258
waveguide loss, 107
Curriculum Vitae

Personal Information

Roman Kappeler
Born April 4, 1979 in Uzwil, Switzerland
Citizen of Schwyz SZ, Switzerland

Education

2006-2012 PhD studies in information technology and electrical engineering (Dr. sc.) at ETH Zurich, Switzerland
2000-2006 MSc studies in information technology and electrical engineering (MSc EEIT) at ETH Zurich, Switzerland
1999-2000 Swiss Army, Rank of a ‘Fourier’
1998-1999 Studies in électronique physique at the University of Neuchâtel, Switzerland
1994-1998 Gymnasium (Matura Typus C: Science) at Kantonsschule am Burggraben St.Gallen, Switzerland
1991-1994 Secondary school at Katholische Kantonsskundarschule St.Gallen, Switzerland
1986-1991 Primary school in Engelburg, Switzerland

Professional Experience and Projects

2006-2012 Research and teaching assistant at Electronics Laboratory, ETH Zurich, Switzerland
2006 Master project at the Institute of Optics, University of Rochester NY, USA and ETH Zurich
2004 Internship at ESTEC (European Space and Technology Centre of ESA) in Noordwijk, Netherlands
Publications

2012


2011


2010


2008


2007


2005

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Zurich, October 2012

ROMAN KAPPELER