Doctoral Thesis

The development of a fabrication process for passive photonic crystal devices in InP / InGaAsP

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The Development of a Fabrication Process for Passive Photonic Crystal Devices in InP/InGaAsP

A dissertation submitted to the SWISS FEDERAL INSTITUTE OF TECHNOLOGY ZURICH for the degree of Doctor of Technical Sciences ETH Zurich

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2008
To my family
Abstract

Photonic crystals (PhCs) – metamaterials with a periodic modulation of the refractive index in the order of the lights wavelength – provide an excellent control over the flow of light. Proper choice of the PhC design parameters allows to adapt the dispersion relation according to the researcher’s demand and even a photonic bandgap (PBG) – a frequency region where light propagation in the PhC is completely forbidden – may be opened. Their design flexibility makes them promising for enhancing the performance of optical devices like semiconductor lasers or integrated optical signal processing. A quite common and well-proven approach to make use of the unique properties of PhCs is the use of planar 2D-PhC. Thereby the periodic refractive index modulation is restricted to the horizontal plane, and light guiding in the vertical direction is achieved by a conventional slab waveguide. Usually the horizontal refractive index is spatially modulated by etching an array of air-holes into a background semiconductor substrate. For active telecom applications at $\lambda=1550\text{nm}$, the fabrication of such structures require advanced fabrication methods like nanometer-scale lithography or high aspect-ratio etching of indium phosphide (InP). Such fabrication methods are still beyond state-of-the-art semiconductor processing. Our research group started an activity to explore the capabilities of PhCs for integrated optics at $\lambda=1550\text{nm}$. This dissertation lays a cornerstone for the required fabrication and measurement technology. After an introduction to the research field, in the first part of this work the fabrication technology for PhCs is presented. Special emphasis on the semiconductor etching process is given here. In the subsequent chapters, we present and characterize our measurement setup. With the help of this equipment the transmission data of the PhC devices, which are presented at the end of this work, is measured.

The diameter and aspect-ratio of PhC holes which are required in this work are challenging for fabrication. At a diameter of around 200nm and etch depths larger than 2$\mu$m must be achieved. One challenging part for the fabrication is the patterning and fabrication of a suitable hard-mask for semiconductor etching. This step was discussed in-depth in the dissertation of R. Wüest [1]. Here we present the patterning of the semiconductor by inductively coupled plasma reactive ion etching (dry-etching). The used chlorine-based plasma has proven to be capable to achieve hole depths of 4.2$\mu$m, 3.8$\mu$m and 2.9$\mu$m for hole diameters of 417nm, 310nm and 180nm, respectively. Such depths are comparable with best literature values. The aggressive chlorine in the plasma leads to mask undercut due to lateral chemical etching. Therefore nitrogen was added to the plasma to passivate the hole sidewall. Its content in the plasma chemistry must be balanced carefully, as nitrogen not only prevents the undercut, but also makes the holes more rough and conical.

Characterization of the etched PhC holes by scanning electron microscopy (SEM) is straight-forward. Hole depth and shape can be fast and easily measured from the SEM micrographs of cross-sections through the holes. However, the surface roughness and carrier lifetime (CL) inside the PhC are not obtained this way. To obtain quantitative roughness measurements inside the holes of the surface roughness, we use conven-
tional AFM scanning of hole cross-sections in combination with a new scanning data processing method. Thereby, the existence of an optimal trade-off in respect to the nitrogen content of the etching plasma could be confirmed. The issue of the CL inside a PhC is also addressed in this work by employing pump-probe measurement. Different PhC design parameters and etching processes were investigated. The strongest influence on the CL comes from the sidewall density of the structure. By optimized processing, the CL can be enhanced. The optimum (longest carrier lifetime) is measured for the same process for which we also observe the smallest sidewall roughness by AFM scanning, and where the lowest surface roughness is seen by scanning electron microscope micrographs.

Not only the fabrication of PhC devices, but also their measurement requires effort in technology development. The very tiny PhC structures (seldom more than a few tens of micrometers in length) require an optical connection to an external light source and a power meter for the measurement. In this work, we use port-to-port measurements to characterize our devices. Light from a tunable laser source is coupled from one cleaved facet of the chip into an auxiliary waveguide. The light is then guided by this waveguides to the other side of the chip, while also passing the PhC device. Its intensity is measured on the other side by a power meter. The design and fabrication of these waveguides is discussed. In the dissertation of R. Wüest [1], a process is presented to fabricate single-mode ridge waveguides to access the PhC structures. Here, we simplify this process towards much faster fabrication time (roughly 2 days instead of 3 week’s work), at the expense of multi-mode photonic wire waveguides.

The suitability of the developed fabrication technology and the measurement setup is demonstrated at the end of the work. The quality of the holes has various consequences on the properties of PhCs. Losses are very pronounced in the bulk-material system, because (i) the PBG is located below the light line, and (ii) the fabrication of PhCs is very challenging and therefore fabrication imperfections (sidewall roughness, limited hole depth, non-cylindrical hole shape) are pronounced. Loss measurement of a single-mode PhC waveguide by the cutback method demonstrated losses down to 500dB/cm. Such values are indeed state-of-the art for this type of waveguide. This waveguide is further used to design a 60°-bend and a directional power splitter. An enhanced transmission (over 99% transmission) and a broad operation bandwidth (up to 40% of the PBG) were obtained by adjusting the location of the two holes at the bend apex. Waveguides and bends are the basic building blocks for dense integrated optics. A more complex functionality is a directional waveguide coupler. Two closely spaced PhC waveguides allow splitting the optical power into two branches. By changing the length of the device, any splitting ratio can be obtained. Topology optimization by varying the hole sizes around the waveguides allowed us to shorten the coupling length of the directional coupler drastically while maintaining a broad operation bandwidth. By changing the size of the holes between the waveguide, a short device length can be traded-off against the splitter bandwidth.

In a short outlook at the end, the most important results are summarized, and the pitfalls for an extension of our technology towards active devices (lasers, semiconductor optical amplifiers) and membrane-type PhCs is discussed.
Zusammenfassung


Der Durchmesser und die Tiefe der Löcher, die für diese Arbeit hergestellt werden müssen, sind eine Herausforderung für die Fabrikation. Ein Durchmesser von etwa 200 nm bei einer Tiefe von mehr als 2 μm muss erreicht werden. Eine Knacknuss dabei ist das Strukturieren einer geeigneten Hartmaske für den eigentlichen Halbleiter-Ätzschritt. Dieser Teil wurde ausgiebig in der Dissertation von R. Wüest [1] diskutiert. Hier präsentieren wir das Strukturieren des Halbleiters selbst mittels „inductively coupled plasma reactive ion etching ICP-RIE“ (Trockenätzen). Das verwendete, chlorbasierte Plasma ermöglichte es, Löcher mit einer Tiefe von 4.2 μm, 3.8 μm oder 2.9 μm für die Durchmesser von 417 nm, 310 nm oder 180 nm, herzustellen. Solche Werte sind vergleichbar mit dem, was in der Literatur publiziert wurde. Das aggressive Chlor führt jedoch zu einem lateralen chemischen Unterätzen der Maske. Daher wurde dem Plasma Stickstoff beigefügt, um die Seitenwände der Löcher zu...
Zusammenfassung

...schützen. Der genaue Anteil von Stickstoff muss sorgfältig optimiert werden, da zu viel Stickstoff zu konischen Löchern mit hoher Oberflächenrauhigkeit führt.


plexeres Device ist der Wellenleiterkoppler, basierend auf zwei nahe zusammenliegenden parallelen Wellenleitern. Dieser erlaubt das Aufteilen der Leistung in beliebigem Verhältnis. Die Optimierung des Designs durch das Ändern der Löchergrösse um die Wellenleiter herum erlaubt es, die benötigte Länge eines solchen Kopplers drastisch zu reduzieren.

In einem kurzen Ausblick am Ende dieser Arbeit werden die wichtigsten Ergebnisse zusammengefasst und die möglichen Probleme für die Erweiterung dieser Technologie Richtung aktive Bauelemente (Verstärker, Laser) oder in Richtung einer membranbasierten Technologie aufgezeigt.
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Chapter 1

Introduction to photonic crystals

“It's a magical world, Hobbes ol' buddy. Let's go exploring!”
Bill Watterson

1.1. Introduction

With increasing popularity, speed and availability of the internet, new applications for the data-network (e.g. video-conferences, high-resolution imaging, internet TV, VoIP) become more and more important in our daily life. As a consequence, huge amounts of data are stored on servers worldwide and sent around half the globe via data highways. The traffic on the worldwide network therefore grows tremendously. With the ongoing industrialization of developing countries, there is no end of this growth in sight. So far, electronic devices could cope with the increasing requirement on the amount and the speed of data transmission and processing by technological innovations. However, their improvement is traded-off by complex fabrication processes and miniaturization. With smaller dimensions other undesired effects become more important and might set a limit to further miniaturization. A fundamental change in the principle of data transmission and more important the development of advanced processing for integrated optical circuits (IOC) is expected to solve this issue.

With the invention of lasers, photo detectors and glass fibers, the era of optical data transmission and processing has started years ago. Photons are used as data carriers instead of electrons. The low transmission losses, speed and capacity of optical transmission cannot be beaten by metallic transmission lines and electronics [2]. Starting from first long-haul data transmission using light waves years ago, the fiber to the
home starts now to become standard in daily life. Glass fibers provide all the bandwidth required at present. However, with the triumphal progression of optical data transmission, the requirement for smaller, cheaper and faster optical data processing has emerged. Indeed, the data processing at the beginning and end of the optical data highway is still performed by conventional electronics. All-optical devices are too expensive or simply not available and therefore can only slowly replace electronics. This creates a bottleneck in the optical data highways. As a logical consequence, the aim is to replace electronic components on a chip at the beginning and end of a glass fiber by so-called all-optical\(^1\) devices. This leads us to the field of dense integrated optics. Only fully optical data processing on a small chip area can provide high speed and high fabrication yield at low cost. Unfortunately, mastering the challenges of all-optical data processing is much more complex than the relatively simple data transmission via optical fibers.

Although photons are very advantageous for data transmission, there are also serious drawbacks making all-optical data processing difficult: Photons do not interact with each other, and the interaction of them with matter is very weak compared to the electron-matter interaction. As a consequence, the development of new all-optical devices is confronted with two major challenges:

- **Photons do not like to be trapped.** Therefore they cannot be easily guided or stored on the nanometer scale. Typical dimensions of optical devices are therefore in the order of millimeters, orders of magnitudes larger than integrated electronics. Such a technology is far away from dense integrated optics.

- **Photons do not like to interact.** Light-light interaction is excluded by the linearity of Maxwell’s equations (see Chapter 2). Light-matter interaction which is necessary for optical data processing and light switching is rather weak. As a consequence, to obtain enough cumulative interaction of light with matter, the size of conventional optical chips needs to be huge. This is detrimental for dense integrated optics.

To overcome these limitations, new light guiding concepts to achieve dense integrated optics are necessary. In 1987, E. Yablonovitch [3] and S. John [4] discovered the unique optical properties of a medium whose refractive index is spatially periodically varied. These so-called photonic crystals (PhC) may overcome the above-mentioned restrictions, close the gap between electronics and photonics and provide a key technology for dense integrated optics. PhCs offer valuable features for the development of compact devices. Their properties and impacts will be now discussed in the next sections.

---

\(^1\) For the discerning reader, it should be mentioned that all-optical devices do not exist. They would require the interaction of light with itself, which is theoretically excluded by the linearity of the Maxwell equations. All light-light interaction has to be taking place by means of matter and often involve transitions of electrons between different states in the atom. Therefore, in this work we define all-optical devices that no macroscopic current flow or macroscopic charges are involved.
1.2. Photonic crystals

Over 20 years ago, E. Yablonovitch [3] and S. John [4] discovered the unique optical properties of photonic crystals [3-5]. By varying periodically the refractive index, the photons can interfere constructively or destructively with each other, and novel propagation behavior can be achieved which was impossible inside a homogenous material. The periodicity can be developed in one, two or all three spatial dimensions, as shown in Figure 1. Although normally not referred as such, a Bragg grating represents a simple one-dimensional PhC. Bragg grating fabrication is relatively simple, either by etching grooves into a background material (horizontal Bragg grating), or by epitaxial growth (vertical Bragg grating) as commonly applied for mirrors of vertical cavity surface emitting lasers [6] (VCSEL). However, a simple Bragg grating does not offer the possibility for the fabrication of compact PhC devices based on bandgap waveguiding. Only nature is able to grow full 3D PhC (e.g. opal, butterfly wings) [7], but with a lot of defects. The technological difficulties to fabricate PhCs rise from the following two facts:

- The most interesting properties of PhCs are achieved when the spatial periodicity of the modulation has approximately the same length as the wavelength of the light. With focus on telecom applications, which work typically at a $\lambda=1550\text{nm}$, this requires sub-micron fabrication technology [8, 9] which has only emerged recently.

- Full 3D PhCs (Figure 1c) exhibit the periodicity of the refractive index modulation in all three directions. Combined with the above-mentioned requirement for the length-scale of the periodicity, the fabrication challenges of full 3D PhCs makes commercial/practical applications currently almost impossible.

![Figure 1](image)

**Figure 1**: Schematic drawing of a one dimensional (a), two dimensional (b) and three dimensional (c) photonic crystal. The different colors represent materials with different refractive indices.

As a consequence of these challenges, only few reports are found on 3D PhC, such as e.g. the so-called woodpile structure [10, 11], autocloning techniques [12] or the (inverse) opal type [13-15].
A more promising concept for a successful application in dense integrated optics is the planar ("2½D") PhC. The periodicity is limited to the horizontal plane, whereas vertical light guiding is achieved by a conventional slab waveguide (Figure 2). This concept has numerous advantages compared to normal PhCs presented in Figure 1:

- The concept is compatible with (dense) integrated planar optics and allows for the integration of conventional and PhC devices.
- The fabrication of such structures for telecom applications is compatible with standard semiconductor processing. The fabrication process is commonly separated in two main steps,
  1. The growth of the vertical layer structure by planar epitaxy, usually by metal-organic vapor phase epitaxy (Chapter 8.4 in [8]) or molecular beam epitaxy (Chapter 8.6 in [8]).
  2. The etching of a periodic structure into the layer stack by dry-etching [9].

All the required technologies are standard in semiconductor processing, and therefore normal equipment and technology can be used.

As already mentioned, the concept of planar PhC has such striking advantages with respect to fabrication over full 3D PhC that currently almost only such crystals are considered for practical devices.

For the rest of this work, only planar PhCs will be discussed. The research on PhCs is driven by the demand of the telecom industry for smaller, faster and cheaper optical devices and OICs. Some possible applications for PhCs are presented in the following section. The theory of PhCs is presented in-detail in Chapter 2 of this work, whereas the fabrication is discussed in-depth in Chapter 3.

**Figure 2:** Schematic drawing of the “2½”-dimensional photonic crystal. The periodicity is limited to the horizontal plane, whereas the light is guided vertically by a conventional slab-waveguide. The different colors represent materials with different refractive indices.

1.3. **Application of photonic crystals for real devices**

Up to 2001, PhCs were believed to be the solution for all problems of dense-integrated optic. Since this hype has cooled down, the expectations of PhCs have become more realistic. PhCs provide valuable contributions to integrated optics, either by allowing shrinking the size of functionalities or by even providing novel functionalities that are not achievable by conventional waveguides. There are a variety of applications for industry which depend on these unique properties of the PhCs:
Photonic bandgaps. The most pronounced feature of photonic crystals – suitable design of the periodicity assumed – is the photonic bandgap (PBG) [16]. For a range of frequencies, the propagation of light is forbidden in the crystal. This gap of forbidden frequencies is similar to the bandgap of forbidden energies of electrons in a semiconductor. For the frequencies inside the PBG, the PhC acts as a mirror. Depending on the type of periodicity, the bandgap might exist for one or both polarizations TE and TM (Table 2).

Dispersion tailoring. A photonic crystal offers much more design degrees of freedom (e.g. lattice constant, lattice type, hole diameter, local defects) and a more complex dispersion relation than a classical ridge waveguide. Therefore they are promising for tailoring the dispersion relation (e.g. number of modes, group velocity, group dispersion) to the requirements of a specific application.

Cavities and waveguides. Similar to semiconductors, simple cavities or waveguides in a PhC can be achieved by defect “doping” the crystal. PhCs can be doped by locally disturbing the periodicity, which creates additional localized states. If such a state lies inside the PBG, it creates a high-Q cavity [17, 18]. Very high Q-factors up to $10^4$-$10^5$ are reported for such cavities. Connecting single cavities in a line, waveguides (defect lines) within a PhC are created [19], which can provide structures to be used as ultra-short pulse compression lines [20] or allow for extremely-low group velocities [21, 22]. These line-defect waveguides guide light by the PBG properties (“guiding by the gap”) and not on total internal reflection, thus bends with a very small bending radius are realizable [23, 24].

Filters. By spatially locally changing the hole pattern, efficient wavelength filters can be fabricated. Filter are based either on the creation of cavities in or next to the waveguide [25, 26], or by coupling light into a different waveguide [27, 28] using wavelength-dependant coupling properties.

Negative refractive index. A unique feature in PhCs not found in homogenous materials is the negative refractive index [29-31]. The negative refractive index raises from the complex band structure of the PhC. It is not found in natural materials. Materials with negative refractive index show special properties:

- Snell’s law is still valid, but the diffracted beam propagates towards the same side as the incident beam.
- The pointing vector is antiparallel to the phase velocity. The light pulse is propagating in the opposite direction to the phase propagation of the light.

Negative refractive index materials may have many applications for practical devices. Ultra compact polarization splitters, based on the property that only one polarization possesses negative refraction [29] and imaging systems with resolution below the diffraction limit (superlens) [31] can be fabricated.

Distributed feedback lasers. Second-order PhC lasers, operated at the band edge, can provide vertical lasing with a low threshold and a small device size [32, 33]. In these devices two grating orders exist; the first couples out the laser light perpendicular to the planar PhC, the second provides in-plane feedback for lasing.
“Slow-light modes” for enhanced light-matter interaction. PhC waveguide modes exhibit a strong nonlinear dispersion. In the region where the dispersion curves become flat \((d\omega/dk \approx 0)\), the group velocity \(v_{gr}\) of a propagating pulse becomes very slow \([21, 22]\). Slow-down factors of the light of up to \(v_{gr}=c/300\) have already been demonstrated \([21]\). The slow light propagation enhances the time of the pulse spent in the waveguide, and/or enhances the field strength and the light-matter interaction. However, a still unsolved problem is the broadband incoupling of the light from a fast-propagating mode into a slow-light mode \([34]\).

Table 1: Comparison of the effects found in ridge waveguiding, photonic wire (section 1.6.2) waveguiding and PhCs.

<table>
<thead>
<tr>
<th>Feature</th>
<th>Ridge waveguide (low (\Delta n)-technology)</th>
<th>Photonic wires (high (\Delta n)-technology)</th>
<th>PhC technology</th>
</tr>
</thead>
<tbody>
<tr>
<td>Waveguides (mode characteristics)</td>
<td>• Single-mode (low losses)</td>
<td>• Single-mode (high losses) • Multi-mode (low losses)</td>
<td>• Single-mode (high losses) • Multi-mode (lower losses)</td>
</tr>
<tr>
<td>Guiding scheme</td>
<td>Total internal reflection</td>
<td>Total internal reflection</td>
<td>PBG guiding</td>
</tr>
<tr>
<td>Waveguide bends</td>
<td>Large bend radius</td>
<td>Sharp bends ((-\lambda))</td>
<td>Sharp bends ((-\lambda))</td>
</tr>
<tr>
<td>Special features</td>
<td>• Very low losses • Technology established</td>
<td>• Simple structures • Technology for research established</td>
<td>• PBG • Slow light • Negative refraction • Superprism effect</td>
</tr>
</tbody>
</table>

1.4. State-of-the-art photonic crystals

PhCs have been already widely explored by many research groups. However, the underlying material systems and vertical confinement mechanisms differ strongly. Depending on the application, different approaches provide the best solution. In this section, the different material systems and vertical confinement schemes are discussed and their suitability for specific applications is highlighted.

1.4.1. Hole-type and rod-type photonic crystals

The common fabrication technology for PhCs to achieve the refractive index modulation is the removal of material from a slab waveguide. The modulation of the refractive index is then created by the contrast between material and air. For the telecom wavelength, the periodicity of the modulation has sub-micrometer dimension and needs to be fabricated with advanced semiconductor processing technologies. Limited lateral resolution and the smoothing of sharp edges during material removal require a pattern based on preferably round structures. Apart from different diameters or lattice constants, two distinct basic concepts of PhCs can be realized, which are presented in Figure 3. The hole-type PhC consists of an array of air-filled holes in a background material. The inverse structure is normally denoted as rod-type PhC. Additionally,
either square-lattice or triangular-lattice arrangement of the holes/rods is practical. The advantages and disadvantages of these designs are listed in Table 2.

<table>
<thead>
<tr>
<th>Rod-type</th>
<th>Triangular lattice</th>
<th>Square lattice</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hole-type</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **Triangular lattice**
  - Large TE-bandgap for a reasonable hole size (radius ~0.25a-0.5a).
  - Small TM-bandgap (radius ~0.4a-0.5a), which are hard to fabricate due to the small interhole distance.
  - Very small complete bandgap.

- **Square lattice**
  - Bad vertical light confinement in defect waveguides based on missing rows of rods.
  - Very small TE-bandgap (radius ~0.3a-0.4a), which are hard to fabricate due to the small interhole distance.
  - Large TM-bandgap for a large radius range of ~0.1a-0.35a. The rods are, however, very thin in this region and thus the vertical confinement is bad.

- **Hole-type**
  - Small TE-bandgap for relatively large holes (radius ~0.4a), which are hard to fabricate due to the small interhole distance.
  - Large TM-bandgap for overlapping holes (radius ~0.5a-0.6a), outside the fabrication capabilities.

<table>
<thead>
<tr>
<th>Rod-type</th>
<th>Triangular lattice</th>
<th>Square lattice</th>
</tr>
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<tbody>
<tr>
<td>Hole-type</td>
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- **Triangular lattice**
  - Bad vertical light confinement in defect waveguides based on missing rows of rods.
  - Very small TE-bandgap (radius ~0.3a-0.4a), which are hard to fabricate due to the small interhole distance.
  - Large TM-bandgap for a large radius range of ~0.1a-0.35a. The rods are, however, very thin in this region and thus the vertical confinement is bad.

- **Square lattice**
  - Only TM-bandgap for thin rods (radius ~0.1a-0.3a).


More complex arrangement of the holes, e.g. the hexagonal honeycomb lattice [5, 35], are also investigated and can exhibit large TM bandgaps.

---

2 Easy to fabricate
1. Introduction to photonic crystals

**Figure 3**: Two different classes of PhCs. The periodic pattern can either be formed by an array of air holes in the background material, or by an array of sticks in air.

1.4.2. Material systems

The concept of planar PhCs can be realized within a large variety of material systems. Targeting $\lambda=1550\text{nm}$, the semiconductors silicon (Si) and indiumphosphide (InP) are the materials of choice. Both are transparent at the desired wavelength and fabrication technologies to structure the material at submicron length-scale are established. The choice between silicon and InP depends on the application.

- **Silicon** is widely used in the industry, and the technology has matured and is cheap. Therefore the use of silicon is easy and cheap, however using it as an active material providing optical gain is yet far from realization. Furthermore, a lattice-matched (strainless) compound with a different refractive index for vertical confinement is missing. Therefore passive membrane-type PhC are usually realized within silicon, either suspended in air or supported by a dielectric layer (SOI, Figure 4c).

- **InP** still only occupies a niche compared to mainstream silicon electronics. It is more expensive, brittle, more difficult to structure and the processing technology is less mature. However, lattice-matched quaternary compounds InGaAsP for the slab waveguide and the fabrication of quantum wells or quantum dots for gain combined with current pumping are available. Due to the missing capability to provide optical gain of Si, InP is the state-of-the-art material for active devices.

Within the class of III-V-compound semiconductors, also other compounds like

- Galliumarsenide (GaAs, lattice constant of 5.65Å [36], electronic gap 1.4eV (0.89μm) [36]) or
- Galliumnitride (GaN, lattice constant 3.19Å [37], electronic bandgap 3.4eV (0.37μm) [38]) [39, 40]

are under investigation. However, these materials are suited for the generation of other wavelengths than $\lambda=1550\text{nm}$ and therefore out of the focus of this work.
1.4.3. Vertical light guiding systems

For planar PhCs, a vertical confinement scheme based on a refractive-index contrast $\Delta n$ is possible. Two different concepts have emerged in research. They are presented in Figure 4.

- **The bulk-type (substrate-type) PhC** confines the light in a core layer, with a semiconductor cladding of lower refractive index above and below. Such devices are normally realized for the InP and GaAs material system, as lattice-matched quaternary compounds with different refractive index are only provided by these materials. However, only a limited narrow range of refractive indices are available within lattice matched materials. Therefore the refractive index contrast $\Delta n$ is low ($\Delta n/n<6\%$). Modes spread out deeply into the substrate, requiring the patterning of high-aspect ratio holes or rods, as the pattern in refractive index modulation needs to cover the whole vertical mode cross-section. Bulk-type PhCs with thick top-claddings offer simple concepts for electrical contacting and provide mechanically stable structures.

![Figure 4: Different fabrication schemes for the vertical confinement. (a) Bulk-type PhC with semiconductor core and cladding. (b) Suspended membrane PhC with air below and above the core. (c) Supported-membrane PhC.](image)

- **Membrane-type PhCs** confine the light in a high refractive index core. The semiconductor core is either suspended in air or supported by a low-refractive index material (e.g. SiNx, SiOx, polymers). The patterning of a membrane-type PhC is simple compared to a bulk-type PhC. No high-aspect-ratio structures need to be fabricated by a challenging etching process. Due to the strong mode confinement, the pattern needs only etched in the core, and the claddings are homogenous. Although the patterning of membranes is simple, the fabrication of the membrane adds other complexity to the fabrication.
  
  - Selective wet etching is required for suspended membranes. Such structures are quite fragile, as the thin membrane is free-standing.
  - Wafer bonding or selective wet oxidation is required for supported membranes. Instead of air, a low-refractive-index material is placed below the semiconductor membrane. Mostly a dielectric or an organic material is used.
Very complex issues in membrane-type PhCs technologies are bottom and top contacts for active electrically-pumped devices and the stability of suspended membranes.

1.4.4. Selection of the PhC type

In the preceding subsections, different classes of PhCs have been introduced. In this thesis, we focus on passive photonic crystals, but with emphasize on a possible extension towards electrically-pumped active PhC devices for telecom applications. The choice for InP-based bulk-type PhC fulfills the requirements for electrically pumped active devices. Complex conceptional and fabrication issues like gain in silicon or electrical contacting of membranes are avoided; however at the price of high-aspect-ratio etching of InP structures. The PhC devices in this work will be based on an air-hole-type triangular PhC for several reasons:

- Any airhole-type PhC confines the light better in the vertical direction than his rod-type counterpart. Light is only vertically guided in the semiconductor area. Hole-type PhCs consist mostly of semiconductor material (material filling factor > 50%), rod-type PhCs mostly of air (material filling factor < 50%).
- The incorporation of electrical contacts above and below the active core region is far easier for airhole-type PhCs.
- The triangular PhC exhibits a large photonic bandgap in the region within the feasible filling factors for the fabrication process (radius <0.4a, see Chapter 3). More complex patterns (e.g. honeycomb lattice of holes [35]) are not considered, as they are much less well understood by the research community than the simple triangular lattice.

The reasoning above leads to the focus of this work on InP bulk-type PhCs fabricated with a triangular lattice of airholes. Typically used filling factors are between r=0.30a and r=0.36a, whereas a is the lattice constant of the array of holes, and r the hole radius. Lower filling factors only provide a small bandgap, and higher filling factors are difficult to fabricate due to the narrow separation distance between adjacent holes. As discussed in detail in the next section, we will use a layer stack of undoped 300nm InP (upper cladding, n=3.17), 522nm InGaAsP (core layer, n=3.35) and InP substrate (lower cladding, n=3.17) through this work.

1.4.5. Vertical waveguide layer structure

The base substrate in this work is InP. The light confinement in the vertical direction is provided by a 3-layer slab waveguide based on InP-lattice-matched ternary or quaternary III-V semiconductor compounds. A core material with a higher refractive index than the surrounding claddings is required. From the full range of (Al, In, Ga)-(P, As, Sb)-compounds (see Figure 5), only InP-lattice matched materials are of interest. As this work does not focus on material development, we only consider the well-established InGaAsP-compounds as materials for the vertical slab waveguide. Sb-containing compounds require more elaborated epitaxy processes. Al-containing compounds may suffer from oxidation and low etching resistivity against HF.
In Figure 5, InP-lattice-matched $\text{In}_x\text{Ga}_{(1-x)}\text{As}_y\text{P}_{(1-y)}$ compounds (simply referred as InGaAsP for the rest of this work) are indicated with a thick red line. With increasing content of gallium, the semiconductor bandgap becomes smaller and will reach energies where light from our laser sources ($\lambda=1470\text{nm}-1630\text{nm}$) will be absorbed. Therefore not the full range of InGaAsP-compounds can be used for the passive transparent slab waveguide structure. InGaAsP has a higher refractive index than the cladding material InP ($n=3.17$). Values up to approximately $n=3.5$ can be reached, before the InGaAsP becomes opaque.

![Figure 5: Bandgap wavelength and lattice constants of III-V-compounds [36]. The InGaAsP-compounds on InP are of special interest in this work (blue-shaded area), especially lattice-matched to InP (thick red line). In the grey shaded area, the semiconductor absorbs the light from our laser sources. GaN with a lattice constant of 3.19Å [37] and a gap of 3.4eV (366nm) [38] cannot be grown lattice matched on InP.](image)

The exact choice of the vertical layer structure is based on earlier work [28]. Figure 6 presents the dimensions and refractive indices of the slab waveguide. The core layer consisting of $\text{Ga}_{0.21}\text{In}_{0.79}\text{P}_{0.57}\text{As}_{0.44}$ is lattice matched to InP. The index contrast $\Delta n$ between the InP and its quaternary layer is $\Delta n=0.18$. Therefore the light mode extends deeply into the substrate (still 10% intensity at 1μm below the surface). The slab waveguide only supports one vertical mode for each polarization (TE and TM, definitions see appendix E). The vertical layer structure is asymmetric and therefore the two polarizations are not completely decoupled [41]. However, the asymmetry (thin top cladding) is required due to the finite hole depth.
1. Introduction to photonic crystals

1.5. Motivation for this thesis

Photonic crystals are believed to advance the reduction of device size in integrated optics, and contribute novel functional features to the field of optics. Unfortunately, the exploration of such structures is demanding in terms of technology, characterization and simulation techniques. The development of PhCs devices needs to go through all steps presented in Figure 7:

1. First a sub-micrometer technology for the fabrication of such devices is necessary. This requires already a basic idea of how a final device will look like. Also modeling tools and a measurement environment must be available to characterize future devices.

2. When the technology is established, basic building blocks for integrated devices must be investigated. To compete with classical optical devices based on ridge waveguides, PhC devices must either be smaller and/or offer new, otherwise unachievable functionalities.

3. The combination of the basic building blocks with functional materials or technologies (e.g. all-optical switching [42, 43], hole infiltration [44, 45] or modulation by surface acoustic waves [46]) creates functionalities to actively influence light, like switching or modulation.

4. A simple functionality alone may not be a useful device for signal transmission or data processing. Only the combination of several (different) functionalities to a complete optical integrated device provides a useful device for the telecommunication with light.

Figure 7: The path to a product based on PhCs is long. Starting from the development of a technological environment for the research on PhCs, simple building blocks for basic light manipulation must be developed and a multitude of these blocks have to be assembled and integrated in order to create optical signal processing- and/or logic-units.
This work is supposed to lay the fundamen
t for the ongoing development towards
active electrically-pumped devices like PhC lasers or semiconductor optical amplifiers (SOA). Only the first two steps in the development (red boxes in Figure 7) are addressed here:

- The development and characterization of a fabrication process to etch deep holes into InP/InGaAsP, the basic element for a PhC. Due to the low vertical refractive index contrast, holes must be at least \( \sim 2.5 \mu m \) deep [47, 48] with a diameter of only a few 100nm.
- The development of a measurement environment to investigate fabricated PhC devices. This includes the setup itself as well as the fabrication and characterization of on-chip accessing-structures to the tiny PhC devices.
- The demonstration of the suitability of the fabrication process by the fabrication of benchmark building blocks of optical devices.

All investigations in this thesis are made with respect to passive PhC in the InP/InGaAsP bulk-type material system, with the focus on a possible further enhancement of the technology towards electrically pumped active PhC.

1.6. The competition: classical integrated optics

As it will become clear during this work, photonic crystals are much more complex with respect to theory, simulation, fabrication and measurement compared to “classical” integrated optics based on weakly guiding ridge waveguides (RW, Figure 8, left) or photonic wires (PW, Figure 8, middle). Thus one must ask the question whether it is worth to use PhCs or to stick to the “classical” concepts. In this section, we briefly review the figures of merit of the classical integrated optics, and set them in relation to the PhC technology. For that, we partly anticipate the results presented later in this work.

![Figure 8: The basic concepts of single-mode ridge waveguides, photonic wires and trench waveguides. The dimensions given are typical values for \( \lambda = 1550nm \). Ridge waveguides are normally covered by air, whereas photonic wires are embedded in or supported by a low-refractive-index material. Trench waveguides are a mix between ridge waveguides and photonic wires. They are called “trench waveguides”, as usually only a narrow trench is etched away on both sides of the waveguide, instead of removing all material.](image-url)
1.6.1. Ridge waveguides

Ridge waveguides are structures that guide light weakly in the lateral directions. Vertically, the light is confined by a slab waveguide, horizontally along a rib on the cladding (see Figure 8, left).

- **Propagation loss**: Extremely low propagation losses can be achieved with ridge waveguides (e.g. 0.7dB/cm in silicon [49]). Such low loss figures allow the use of ridge waveguides for long distance (on-chip, ~mm-cm-range) light guiding. Bulk-type PhCs are far away from reaching such low loss values. Even single-mode membrane-type PhC waveguides show losses one order of magnitude higher (GaAs W1: 7.6dB/cm [50], SOI W1 5dB/cm [51]).

- **Bending loss**: Due to the weak index contrast in a ridge waveguide, bends with acceptable low losses (0.001dB/bend for radius=600μm [49]) can only be achieved with huge (100μm-1mm) bending radii. Therefore ridge waveguides are not suited for dense integrated optics. The densification is limited by the bending loss.

- **Active devices**: The weak index contrast around the waveguide core ensures that the light mode penetrates into the substrate is far away from the air surface. Thus, it is easy to place electrodes for electrical pumping on top of the waveguide without introducing high propagation loss caused by the electrical contacts. The fabrication of lasers based on ridge waveguides is well-established [52].

1.6.2. Photonic wires

Photonic wire waveguides consist of a thin, normally of rectangular cross-section (dimensions well below 1μm), “wire” of a high-refractive-index material (Si, InP, GaAs), embedded in or supported by a low-refractive-index material (Air, BCB, SiOx, SiNx) (see Figure 8, middle).

- **Propagation loss**: Although the spatial dimensions of PWs are small, the fabrication is not especially challenging, as only shallow etching through the membrane is required. Propagation losses of 2.6dB/cm [53] or 2.4dB/cm [54] are reported in SOI based PWs. Membrane-type PhC waveguides show losses in the same order of magnitude (GaAs W1: 7.6dB/cm [50], SOI W1 5dB/cm [51]), but do not outperform the PW losses. Bulk-type PhCs, however, are far away from reaching such values.

- **Bending loss**: The bending loss of hard-confined PWs are small. For bending radii of 5μm, only -0.004dB/bend are reported [53]. Such properties are very competitive for dense integrated optics, and photonic crystals will not substantially reduce these values.

- **Active devices**: Due to the missing cladding – the PW only consists of a core, – and the high refractive-index contrast, the light mode “fills” the whole waveguide volume. Therefore electrical pumping of a PW is not feasible, as metal contacts will unavoidably come in contact with the light mode and
absorb the optical energy. As a consequence, most PW structures are realized on SOI, as the InP and GaAs semiconductors provide no benefit.

- **Light confinement**: Photonic wires allow tight light confinement in all spatial directions perpendicular to the propagation direction, thanks to the high refractive index contrast.

- **Power splitters and multimode interferometric devices (MMI)**: Using the concept of PW, 1x2 MMIs (used as power splitter) can be realized on a footprint of 3x7.6\(\mu\)m with a measured insertion loss of below 1dB [53]. Y-splitters also provide losses in the same order of magnitude (1.5dB) [53].

- **Mach-Zehnder interferometer (MZI)**: A delay length up to 1mm with an extinction ratio of 25dB is achieved [53].

### 1.6.3. Trench waveguides

Trench waveguides (see Figure 8, right) take an intermediate position between the RW and the PW. They confine the light by a weak refractive index contrast (\(\Delta n \sim 0.2\)) in the horizontal and by a strong refractive index contrast (\(\Delta n \sim 2.2\)) in the lateral direction. They are called “trench waveguides” because usually only a narrow trench is etched away on both sides of the waveguide, instead of removing all material except the waveguide, to save electron-beam lithography writing time (see section ). The trench is wide enough to suppress the lateral coupling of the light out of the waveguide.

- **Optical losses**: Wide multi-mode trench waveguides have comparable losses to ridge waveguides (~5dB/cm), narrow single-mode trench waveguides show huge losses (see Chapter 5). To guide the light over large distances (mm), single-mode trench waveguides are not suitable.

- **Bends**: Due to the large lateral index contrast, bends with lossless radii below 1\(\mu\)m can be easily fabricated.

- **Compatibility with the PhC technology**: The fabrication of trench waveguides is completely compatible with the bulk-type PhC fabrication. The same mask layer and etching step can be used to fabricate PhCs and trench waveguides together, thus simplifying the fabrication (Chapter 3).

The compatibility of the trench waveguides with the PhC fabrication technology is the deciding argument for their use in this work. A detailed discussion of their fabrication can be found in section 3.5.2 and their optical characterization in Chapter 5.

### 1.6.4. Conclusion

The optical properties with respect to losses and extinction ratios of the classical (and optimized for this purpose) integrated optic devices are very hard to beat by using PhCs. So far, PhC cannot outperform them, and we believe that this will also be the case in the (near) future. Thus, there is no justification for PhCs to simply replace “normal” optical devices, due to their higher complexity in fabrication and their infe-
rior optical losses. Still, PhC devices can be competitive and very useful in the following fields:

- **Dispersion tailoring and control**: The dispersion of a PhC waveguide can be exactly tailored. It is much more complex than a simple waveguide. Using the degrees of freedom to design a hole-type PhC device (lattice constant, hole diameter, lattice type, modification of hole diameter or position next to the waveguide [e.g. used in section 6.3], waveguide type), the dispersion relation can be designed according to the demands for the desired optical devices.

- **Slow-light (see section 2.1.3.5)**: The waveguide modes in a PhC exhibit frequency ranges where the group velocity \( v_g \) of a pulse is very small, and theoretically it may reach zero. Such a waveguide has several useful properties: (i) due to the low group velocity, the device can be used to delay signal pulses and/or to enhance the interaction time of the pulse with the (nonlinear/gain) material. (ii) The reduction in pulse speed leads also to a field enhancement in the waveguide, which then enhances nonlinear interactions with the material.

- **Light confinement**: Photonic crystals allow tight light confinement in all spatial directions perpendicular to the propagation direction (for membrane-type PhCs at least). Furthermore, using slow-light, the electric/magnetic field can even more be enhanced due to the pulse compression.

- **Cavity-based devices (e.g. add-drop-coupler)**: Using membrane-type PhCs, extremely high Q-factors (theoretically up to \( 24 \cdot 10^6 \) \cite{55}, experimentally demonstrated up to \( 1 \cdot 10^5 \) \cite{18}) can be achieved.  

In this work, the focus lies on much simpler devices than the suggested applications mentioned above. However, such basic components – although not competitive with classical integrated optics – are required for the understanding of PhCs and for the later integration of active devices.

1.7. **Achievements of this work**

The following sections will list the content of the different chapters of this thesis and present the main achievements made within this work:

**Chapter 2 “The physics of photonic crystal devices”**. This chapter introduces the basic theory of PhC. Starting from the Maxwell equations, the assumption of periodicity in the refractive index of the material leads to the prediction of interesting PhC properties like the existence of a bandgap, strong confinement PBG waveguiding, or dispersion engineering for “slow light”.

The researcher’s intuition, which allows often a quite precise prediction of the behavior of a “classical” device, unfortunately often fails due to the complex structure and highly sensitive functionality of a PhC. Therefore 2D and 3D simulation tools are necessary to cope with the complexity of the structure. The tools used in this work are presented, and their requirements and limits are discussed.

**Chapter 3 “Etching of deep holes in InP for photonic crystals”**. Etching of deep holes of sub-\( \mu \)m diameter in a semiconductor material is a challenge beyond state-of-
1.7 Achievements of this work

The-art semiconductor processing. So many different requirements have to be considered that trade-offs and optimized compromises are unavoidable. During this work, the following achievements have been accomplished:

- The development of a fabrication process for the etching of deep holes in InP/InGaAsP/InP, arranged in a dense array.
- Furthermore, the impact of the different process parameters was explored to expand the understanding of the plasma etching process beyond just the view as a “black-box”.

Our developed fabrication process is capable to meet the requirement for PhC device fabrication and can compete with state-of-the-art fabrication technologies of PhCs.

Chapter 4 “Hole characterization”. The fabrication process may have a considerable impact on active PhC devices gain and optical propagation losses. Therefore careful characterization with respect to the fabrication process is required. Next to employing state-of-the-art characterization (etch-rates, lag effects), the following methods have been developed:

- A method to scan the surface roughness of the inner side of a PhC hole by a conventional atomic force microscopy (AFM) has been developed. As the surface of a hole is curved, direct extraction of a roughness value from an AFM scan is not possible. The development of a data processing routine however allowed the quantitative comparison of sidewall roughness between different processes.
- The carrier lifetime inside the active core region is critical for active devices, as it influences directly the lasing threshold or pump efficiency. The surface recombination on the hole sidewalls drastically lowers the carrier lifetime. The impact of processing on the surface recombination velocity and thus the carrier lifetime was investigated in this work. Not unexpectedly the highest carrier lifetime was obtained for the process where the holes are closest to the ideal shape and exhibit the lowest surface roughness.

Chapter 5 “Integration of photonic crystal devices for port-to-port measurements”. PhC devices are normally very tiny, seldom longer than a few tens of micrometers. All measurement equipment (laser sources, fibers, lenses, detectors) is huge in comparison to them. This size difference complicates the measurement process. In this chapter, all aspects of measurement of PhC devices with an external light source and detector are discussed. This involves the

- fabrication of access-waveguides on the chip to guide light to the PhC.
- development and characterization of a setup to measure PhC devices, including the discussion of the impact of the access structures on the overall measurement result.

Chapter 6 “Photonic crystal devices”. The performance of a fabrication process is not measured by beautiful holes in InP, but by the performance of an optical function-
ality. Therefore we present here three basic optical devices realized using our PhC fabrication process:

- **Waveguiding** is the most basic function that needs to be realized for integrated optics. With the cutback-method, we measured state-of-the-art propagation losses for our PhC waveguides.

- **Low loss and low reflection bending** of the light on a chip is a cumbersome task. Classical integrated optics needs a large device area for this function due to the low refractive index contrast $\Delta n$ of ridge waveguides. The use of PhCs shrinks the needed space by orders of magnitude. However, reflections at the apex of the bend become an issue. By careful and systematic optimization, it was possible to bring the reflection under control and design a bend with a large bandwidth and high transmission.

- **Power splitting** is a key feature for integrated optics, needed for many applications. Although a simple Y-branch realized within PhC shows excellent performance [28], it is very sensitive to fabrication fluctuations. Furthermore, the realization of splitting ratio other than 1:1 is hardly achievable in a controlled way. By using ultra short directional couplers, power splitters at any desired coupling ratio are demonstrated.

Chapter 7 “Summary, conclusions and outlook”. The focus of this work lies on passive photonic crystal devices. However, for the decision of the material system and during the development of the fabrication process, the ultimate goal of active PhC devices was never out of focus.
Chapter 2

The physics of photonic crystal devices

“I’M SIGNIFICANT! ...screamed the dust speck.”
Bill Watterson

In this chapter, the concepts and mathematical framework of photonic crystals are presented. The focus lies on the concepts and models needed to understand later results of our work, rather than in the detailed derivation of the formulation and models. The interested reader can find an excellent and detailed discussion of the mathematics of electromagnetism in general in [56] and of photonic crystals in particular in [5].

2.1. Fundamentals of photonic crystals

Maxwell’s equations are found to be generally valid to describe the propagation behavior of light in free space or within matter. Thus, they also govern the behavior of photonic crystals (PhCs). In this section, we briefly derive a mathematical description of PhCs.

2.1.1. The Maxwell equations

The natural starting point for the mathematical treatment of electromagnetic fields are the four Maxwell’s equations [56], which describe the interaction of the electric \( \mathbf{E}(\mathbf{r},t) \) and the magnetic field \( \mathbf{H}(\mathbf{r},t) \) with matter. Including macroscopic current and charges, they are:

\[
\nabla \cdot \mathbf{D}(\mathbf{r},t) = \rho(\mathbf{r},t) \quad (2.1a)
\]
2. The physics of photonic crystal devices

- Gauss' law for magnetism  \( \nabla \cdot \vec{B}(\vec{r}, t) = 0 \)  

- Faraday's law of induction:  \( \nabla \times \vec{E}(\vec{r}, t) = \partial_t \vec{B}(\vec{r}, t) \)  

- Ampère's Law  \( \nabla \times \vec{H}(\vec{r}, t) = \vec{J}(\vec{r}, t) - \partial_t \vec{D}(\vec{r}, t) \) 

For the treatment of passive PhCs, it is appropriate to simplify the equations and to assume the following:

- No free current or electric charges  \( \rho(\vec{r}, t) = 0, \quad \vec{J}(\vec{r}, t) = 0 \)  

- Linear, instantaneous, isotropic and lossless material response to the electric field  \( \vec{D}(\vec{r}, t) = \varepsilon(\vec{r}) \cdot \varepsilon_0 \cdot \vec{E}(\vec{r}, t) \)  

- Transparent materials: \( \varepsilon(\vec{r}) \) is real and positive [5].

- Linear, instantaneous, isotropic and lossless material response to the magnetic field, with the assumption that the material’s magnetic permeability is very close to 1 (weak magnetic response of the material)  

\[
\vec{B}(\vec{r}, t) = \mu(\vec{r}) \cdot \mu_0 \cdot \vec{H}(\vec{r}, t) \approx \mu_0 \vec{H}(\vec{r}, t)
\]

The assumption of linear, instantaneous and lossless materials simplifies the model, but is sufficient to understand the basic properties of PhCs. With these assumptions, Maxwell’s equations can be simplified as:

- Gauss' law:  \( \nabla \cdot (\varepsilon(\vec{r}) \cdot \varepsilon_0 \cdot \vec{E}(\vec{r}, t)) = 0 \)  

- Gauss' law for magnetism  \( \nabla \cdot \vec{H}(\vec{r}, t) = 0 \)  

- Faraday's law of induction:  \( \nabla \times \vec{E}(\vec{r}, t) = \mu_0 \cdot \partial_t \vec{H}(\vec{r}, t) \)  

- Ampère's Law  \( \nabla \times \vec{H}(\vec{r}, t) = \varepsilon(\vec{r}) \cdot \varepsilon_0 \cdot \partial_t \vec{E}(\vec{r}, t) \)

In general, the fields are complex functions in time and space. However, for harmonic fields, we can separate the temporal and spatial part of the functions by defining:

\[
\vec{E}(\vec{r}, t) = \Re \left( \vec{E}_m(\vec{r}) \cdot e^{j\omega t} \right) \\
\vec{H}(\vec{r}, t) = \Re \left( \vec{H}_m(\vec{r}) \cdot e^{j\omega t} \right)
\]

This “Ansatz”, together with the Faraday's law and Ampère's Law (substituting \( \nabla \times \vec{E}(\vec{r}, t) \) in Faraday’s law of induction, equation 2.2c), leads us to the so-called master equation for the field \( \vec{H}_m(\vec{r}) \). The master equation is an eigenvector-equation with eigenvectors \( \vec{H}_m(\vec{r}) \) and eigenvalues \( \omega \).

\[
\nabla \times \left( \frac{1}{\varepsilon(\vec{r})} \nabla \times \vec{H}_m(\vec{r}) \right) = \omega^2 \cdot \mu_0 \cdot \varepsilon_0 \cdot \vec{H}_m(\vec{r}) = \frac{\omega^2}{\varepsilon} \cdot \vec{H}_m(\vec{r})
\]
From the master equation for $\tilde{H}_n(\vec{r})$, we can obtain the electrical field by equation (2.4).

$$\tilde{E}_n(\vec{r}) = \frac{i}{\omega \cdot \varepsilon_0 \cdot \varepsilon(\vec{r})} \nabla \times \tilde{H}_n(\vec{r})$$

The speed of light in vacuum, $c = \left(\sqrt{\varepsilon_0 \cdot \mu_0}\right)^{-1}$, is defined by the electric permittivity and the magnetic permeability. It is common to solve the master equation for $\tilde{H}_n(\vec{r})$ and calculate $\tilde{E}_n(\vec{r})$ from $\tilde{H}_n(\vec{r})$. In principle, the opposite approach would also be possible, but leads to a more complicated master equation for $\tilde{E}_n(\vec{r})$ (a so-called generalized eigenvalues problem [5]), which have mathematical operators on both sides of the equation.

$$\nabla \times \nabla \times \tilde{E}_n(\vec{r}) = \frac{\omega^2}{c^2} \cdot \varepsilon(\vec{r}) \cdot \tilde{E}_n(\vec{r})$$

Such an equation is more complicated to solve. Also the use of $\tilde{D}_n(\vec{r})$ instead $\tilde{E}_n(\vec{r})$ does not simplify the problem. Although simpler because we have only operators on one side, the operator is not hermitian anymore. Thus, the solution via $\tilde{H}_n(\vec{r})$ is preferred, as it delivers the simplest mathematical description for the problem.

Each solution $\tilde{H}_n(\vec{r})$ of the eigenvalue-problem (2.3) for the spatial field represents an eigenmode for a lightwave of frequency $\omega$. Any solution of the system can be decomposed into a superposition of its eigenmodes, as the eigenmodes form a basis for the solution space.

For a homogenous, isotropic media ($\varepsilon(\vec{r}) = \varepsilon$ is spatially constant) plane waves of the form $e^{i\tilde{k} \cdot \vec{x} - i\omega t}$ solve the differential equations, with $\tilde{k}$ being the wave number of the solution (representing the momentum of a plane wave). The solution is distinct, only one solution exists for each $\tilde{k}$. The relation between the wave number $\tilde{k}$ and the eigenvalue $\omega(\tilde{k})$ (representing the frequency of the plane wave) is called the dispersion relation. In a homogenous media (and as a special case of it, in vacuum), it is a linear relationship $\omega(\tilde{k}) = c \cdot |\tilde{k}| / \sqrt{\varepsilon}$. By defining the refractive index $n$ of a medium as $n := \sqrt{\varepsilon}$, we can rewrite the dispersion relation as $\omega(\tilde{k}) = c \cdot |\tilde{k}| / n$.

### 2.1.2. The solution of the master equation for a periodic media

A periodic media $\varepsilon(\vec{r})$ can be described by base lattice vectors $\vec{a}_1$ and $\vec{a}_2$, which span the unit cell of the lattice, and the distribution of the dielectric material $\varepsilon(\vec{r})$ in the unit cell. Figure 9(a) presents the definitions for the different quantities in the lattice. A lattice in real space defines a reciprocal lattice (as show in Figure 9(b)).
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The reciprocal lattice is spanned by the reciprocal base lattice vectors \( \mathbf{b}_1 \) and \( \mathbf{b}_2 \), which must fulfill the relation \( e^{i \mathbf{a} \cdot \mathbf{b}_i} = 0 \) for any base vector of the real space. For a more detailed description of the reciprocal space, the reader should refer to textbook on solid state physics, e.g. [57].

We now focus on solutions of the master equation for PhCs which show a periodic spatial modulation in the refractive index \( \varepsilon(\mathbf{r}) = \varepsilon(\mathbf{r} + m \cdot \mathbf{a}) \) or \( n(\mathbf{r}) = n(\mathbf{r} + m \cdot \mathbf{a}) \) for \( m \) being an integer number.

We shall restrict the discussion on 2D photonic crystals with a triangular periodic array of holes in a semiconductor material, as this is the PhC concept we have chosen in this work. The mathematics does not change for other types of lattices, and can be readily generalized for the consideration of 3D PhCs.

\[ \begin{align*}
\begin{array}{c}
\text{(a) Direct lattice} \\
\text{(b) Reciprocal lattice}
\end{array}
\end{align*} \]

**Figure 9**: Lattice and reciprocal lattice of a triangular photonic crystal. The photonic crystal is defined by its base vectors \( \mathbf{a}_1, \mathbf{a}_2 \) (both of length \( a \)) and the refractive indices of the holes and the background material.

The periodicity further allows us to separate the solutions of the master equation (2.3) according to the Bloch’s theorem [5] in the form

\[ \tilde{H}_{k,\omega}(\mathbf{r},t) = \Re \left( e^{i \mathbf{k} \cdot \mathbf{r}} \cdot u_{k}(\mathbf{r}) \cdot e^{i \omega(t)} \right), \]

where \( u_{k}(\mathbf{r}) \) is a periodic spatial function with the same periodicity as \( \varepsilon(\mathbf{r}) \). The proof of the Bloch theorem can be found in the literature [5]. From equation (2.4), we can draw the following conclusions:

- The solutions \( \tilde{H}_{k,\omega}(\mathbf{r},t) \) of the master equation (2.3) are plane waves with wave vector \( \mathbf{k} \), but modulated by a periodic function \( u_{k}(\mathbf{r}) \).
- The solutions are periodic in the reciprocal space with the periodicity \( 2\pi/a \) of the reciprocal lattice vectors. Therefore the solution space of \( k \) can be
restricted to the first Brillouin zone (“unit cell” of the reciprocal lattice [5], Figure 9b) with no loss of generality. Solutions in other Brillouin zones are identical to the solutions in the first zone from a physical point of view.

- The simple linear dispersion relationship \( \omega(k) = c \cdot |\mathbf{k}| / n \) (as in the case of a plane wave in a homogenous medium) no longer holds.

The solutions of the master equation are usually called Bloch modes. The dispersion relation (Figure 10) gives important insights in the properties of the PhC like band-gaps, mode gaps or group or phase velocities, without the detailed knowledge of the field distribution. These features will be described in the next section.

### 2.1.3. Photonic crystal properties

The periodicity of the dielectric material changes the dispersion relation drastically compared to a homogenous media. The normally linear relation between \( k \) and \( \omega \) changes to a complex nonlinear relation \( \omega(k) \) exhibiting special features not observed in a homogenous material. The following section presents some of the most important properties of PhCs, which will be used in the subsequent chapters.

A planar PhC, in which air-holes in a the semiconductor slab waveguide form the periodic modulation, is fully described by the lattice type, the lattice constant \( a \) and the ratio \( r/a \) of the hole radius \( r \) to the lattice constant \( a \) (air filling factor)\(^3\).

#### 2.1.3.1. Polarization

The PhC modes are strongly dependant on the polarization of the field. This work follows the convention used in [5] for the two polarization states (appendix E).

- Transversal electric (TE) polarization: The H-field is perpendicular to the slab waveguide plane, \( \vec{H} = H \cdot \hat{e}_z \) and \( \vec{E} \cdot \hat{e}_z = 0 \).

- Transversal magnetic (TM) polarization: The E-field is perpendicular to the slab waveguide plane, \( \vec{E} = E \cdot \hat{e}_z \) and \( \vec{H} \cdot \hat{e}_z = 0 \).

The reader should be aware that different definitions for the polarization TE and TM are found in literature. Note that the separation of the modes in two independent polarizations is only valid for a symmetric slab waveguide. In the asymmetric case, one can still separate between TE-like and TM-like modes, but they are not completely decoupled [41].

#### 2.1.3.2. Scalability

In Maxwell's equations, no fundamental scale is introduced. Therefore in non-dispersive media, all quantities scale with the lattice constant of the underlying lattice. If we

\[^3\] Alternatively the air filling factor \( ff \) can be defined as the amount of space occupied by holes, for a triangular lattice \( ff = \frac{2\pi \left( \frac{r}{a} \right)^2}{\sqrt{3} \left( \frac{r}{a} \right) \frac{\text{Hole area}}{\text{Cell area}}} = \frac{\text{Hole area}}{\text{Cell area}} \). In this work, the relation between radius and lattice constant is defined as filling factor.
scale the lattice constant with an arbitrary real number s, the following scaling laws hold (normalization):

- Lattice constant, hole radius \( a \rightarrow s \cdot a \) and \( r \rightarrow s \cdot r \)
- Wavelength \( \lambda \rightarrow s \cdot \lambda \)
- (Angular) Frequency \( \omega \rightarrow \frac{\omega}{s} \)

The scalability of all quantities allows us formally to introduce reduced frequency units \( u \), as only the relation of the wavelength to the lattice constant is relevant for the properties of a PhC.

- Reduced frequency: \( u = \frac{a}{\lambda} = \frac{a \cdot \nu}{c} \)

with \( c \) equals the vacuum speed of light and \( \nu \) the real frequency.

The scaling properties and the introduction of reduced units allow us to virtually “broaden” the bandwidth of the probing source. The same device with the same filling factor but different lattice constants \( a \) is fabricated on the chip. For each measurement, a different reduced frequency range \( u = a / \lambda \) is probed. The full spectrum is then composed from the spectra of the individual devices. This method is commonly referred as lithographic tuning [58].

However, the scaling possibilities of the PhC are limited in this work for three reasons:

- Material dispersion
- As it will be shown later (section 4.1.1), the outcome of the fabrication processes for etching of deep holes is dependent on the diameter of the holes. While changing the lattice constant, the hole diameter must also be scaled, to maintain a constant filling factor. This however results in holes with different roughness and shape between tuning steps, and therefore different device properties – especially the device loss.
- By using 2D planar PhC, the periodicity in the third dimension is broken and replaced by a non-periodic slab waveguide. Therefore a fundamental length (e.g. core thickness, cladding thickness) is introduced, and the scalability is lost (layer thicknesses are absolute values and cannot be scaled easily with the wavelength on a single chip). As a consequence,
  - the lattice constant has to be specified for 3D simulations (relative to the dimensions of the vertical layer stack) which also contain the vertical layer stack.
  - The effective refractive index \( (n_{\text{eff}}) \) represents the layer stack in 2D simulations. It is dependent on the frequency (see section 2.3.1). By specifying \( n_{\text{eff}} \), the frequency is absolutely defined and cannot be scaled with the lattice constant. Thus, \( n_{\text{eff}} \) indirectly introduces a fundamental length.
The missing scalability prevents a perfect overlap between the piecewise measurement of a spectra by means of lithographic tuning, and can also be seen in exact 3D simulations of the lithographic tuning process [59]. However, the error (gap) is small compared to the transmission features of a PhC measurement.

### 2.1.3.3. Bandgap

The most prominent feature of a PhC is the existence of the so-called photonic bandgap (PBG). A PBG is a frequency range where no modes can propagate. For these frequencies a PhC acts as a mirror. Figure 10 presents an example for a simulated dispersion relation (lowest three modes) of a 2D PhC exhibiting a PBG. It is common to plot the dispersion relation only along the symmetries axis. Although not guaranteed for all structures, it is very often – and especially for the structures considered in this work – the case that the minima and maxima of the bands are located on the zone edges or even in the corners. [5]. For r/a≈0.31 between u=0.23 and u=0.31, there is no light mode present and light of these frequencies cannot exist within the crystal.

![Dispersion diagram of the TE polarization of a triangular photonic crystal with filling factor r/a=0.31. It is common to only show the dispersion relation along the symmetry axis of the crystal (Γ-M-K-Γ).](image)

The existence and position of the bandgap depends on the background material, the filling factor and the polarization. If a PBG opens for only one polarization, it is referred to a TE or TM bandgap, if both polarizations show overlapping PBG, the union of the PBGs is referred to a complete PBG. Detailed PBG maps for all basic design concept considered in this work can be found in Table 2 [5]. For the triangular air-hole design, a PBG opens for r/a between r/a≈0.2 and r/a≈0.5 for the TE polarization and for the TM polarization from r/a≈0.4 to r/a≈0.55. The PBG of the two polarizations are only partly overlapping.

### 2.1.3.4. Photonic crystal waveguides

Similar to semiconductors, additional modes can be introduced in the band diagram by “doping” the crystal. Doping is achieved by locally modifying the perfect lattice of the PhC. Although many different types of doping are imaginable, e.g. changing the
size, shape or refractive index of a hole, the most common dopant is simply omitting a hole.

We will reconsider now the triangular PhC of section 2.1.3.3. Omitting a single or several holes in the otherwise perfect lattice creates a single, spatially localized defect mode in the crystal [17, 18, 60] (Figure 11A and B). Such cavities can exhibit very high Q-values. Coupling these cavities along a line, a structure that guides light [19] is formed (Figure 11C). Removing a complete row of holes, we obtain a W1 waveguide (Figure 11D consisting of a single row of omitted hole) and the W3 waveguide (Figure 11E, consisting of three rows of omitted holes). These two basic types of waveguides are mostly used in planar PhCs.

![Figure 11](image-url):
Different resonators and waveguides created inside a PhC: (A) Cavity by modifying a hole diameter, (B) cavity by omitting a hole, (C) coupled cavity waveguide, (D) W1 waveguide and (E) W3 waveguide. The dashed circles indicate omitted holes.

![Figure 12](image-url):
Dispersion diagram computed in 2D using MPB [61, 62] of the TE polarization of a W1 waveguide with r/a=0.31 in the direction of the waveguide. The grey regions indicate the presence of modes of the undisturbed PhC, where no guiding by the PBG-properties can be achieved. The two colored modes correspond to the guided modes of the waveguide, commonly referred as the odd (red) and even (blue) mode (corresponding to their symmetry in respect to the center of the waveguide). The light lines are drawn in green (upper: for air; lower: for InP, n=3.14). For a discussion of the light line, we refer to section 2.2.1.
Figure 12 presents the dispersion diagram for a W1 waveguide for the propagation direction of the waveguide. The grey regions indicate the modes of the undisturbed PhC. As stated above, within the PBG additional modes have appeared which belong to guided modes (k-vector along the defect) in the waveguide. Two different modes are distinguished: the odd and even mode. The nomination of the modes is in relation to the symmetry of the mode with respect to the symmetry axis of the waveguide. For k-vectors outside the propagation direction, also additional modes may occur in the PBG. These modes belong to cavity modes, formed by the (1-dimensional) cavity perpendicular to the waveguide (Figure 13, right).

![Waveguide and Cavity Diagram](image)

**Figure 13**: A row of defects (e.g. a simple W1 waveguide) acts as a waveguide for k-vectors with a propagation direction along the defect (left), or as a cavity for k-vectors perpendicular to the waveguide (right).

The W1 waveguide is of great interest in research, as it has wide ranges where it is single-moded. However, it is very lossy (compare Table 3). Also used for PhC devices are multi-mode W3 waveguides. They show much lower losses, but are multi-moded.

2.1.3.5. Group velocity and slow light

The speed of light traveling inside a PhC differs significantly to that in a ridge waveguide. Inside a PhC, light can exhibit a dispersion relation (Figure 12) very distinct from the ridge waveguide dispersion, which gives rise to e.g. pulse propagation with a very low group velocity (slow-light) [21, 22]. In this section, the light propagation inside a W1 waveguide is discussed and important features for PhCs are highlighted.

The characteristic figures of the propagation speed of a mode are its phase and group velocity. They are calculated as

- **Phase velocity** \( v_{ph} = \frac{\omega}{k} \) \hspace{1cm} (2.6)

  The phase velocity defines the speed of the phase of the wave (e.g. of a maximum of the field oscillation).

- **Group velocity** \( v_{gr} = \frac{\partial \omega}{\partial k} \) \hspace{1cm} (2.7)

  The group velocity is the speed of the envelope of a light pulse. The group velocity corresponds to the *slope* in the dispersion diagram. Within a PhC
2. The physics of photonic crystal devices

waveguide, the dispersion curves can become flat and show therefore a low group velocity ($v_{gr} \ll c$).

Of special interest are slow-light modes, where the group velocity is slowed by orders of magnitude [21, 22, 63] relative to the light speed $c$. The low group velocity offer advantageous properties for devices:

- The propagation of a light pulse is slowed down, allowing the use of such a waveguide as an optical delay line or data storage line. Also, the interaction time of the pulse with the medium is prolonged, enhancing the effect of the material on the light. Gain and unfortunately losses are both enhanced within such waveguides.

- Due to the slow light propagation, the intensity of the field within the waveguide is enhanced [63]. This allows stronger light-matter interaction and enhances the nonlinear effects of the material, e.g. for all optical switches.

Slow-light promises smaller devices and stronger non-linear effects. However, an yet unsolved problem in the PhC community is the incoupling from “fast” waveguides of light into slow light modes [34]. This problem is an ongoing research area, which must be solved before the realization of practical applications of slow light (e.g. using spatial tapers [64] or lattice-constant tapering (lattice parameter tuning) [65, 66]).

2.2. Optical losses as a figure of merit

2.2.1. The light-line

Modes of a PhC (waveguide) can be classified according to their position with respect to the light line\(^4\) \(\omega_R = c \frac{|\vec{k}_R|}{n_R}\) (green lines in Figure 12). Their position in the \(\omega\)-\(k\)-space is relevant for the possibility to couple to radiative (non-guided) modes in the upper (normally air) or lower cladding (in our case the InP substrate). In the following, the subscript $R$ in the equations denotes the radiative modes in the air / substrate. $n_R$ refers to the refractive index of the media in which these modes propagate (commonly air above the core, $n_R = 1$, and below the core layer, air for membranes, $n_R = 1$; SiN$_x$O$_y$ for supported membranes $n_R \approx 1.5$-2; InP for bulk-type PhCs, $n_R = 3.14$). A radiative mode of frequency $\omega_r$ has a k-vector of the length $\omega_r n_R / c$, oriented in any arbitrary spatial direction. To be able to couple a PhC mode to such a radiative mode, the following conditions must be fulfilled (compare Figure 14):

- Energy conservation (frequency conservation) \(\omega_R = \omega_{\text{PhC}}\) (2.8)

- Parallel impulse conservation \(\vec{k}_R \cdot \vec{e}_x = k_{\text{PhC}}\) (2.9)

- The overlap-integral (which is proportional to the coupling efficiency) must be non-vanishing.

\(^4\) The light line is the dispersion relation of a plane wave propagating in a homogenous media of the same refractive index as the upper or lower cladding.
2.2 Optical losses as a figure of merit

$\mathbf{e}_x$ stands for the unity vector in the propagation direction of the guided mode ($\mathbf{k}_{\text{PhC}}$).
Equation (2.9) can only be fulfilled, if $k_{\text{PhC}} \leq c \cdot \omega_{\text{PhC}} / n_R$. In this case, both the energy conservation (equation 2.8) and the impulse conservation (equation 2.9) can be fulfilled and coupling to a radiative mode is possible (Figure 14, red arrow). Commonly, this situation is referred to be “above the light line”. In the opposite case, when $k_{\text{PhC}} > c \cdot \omega_{\text{PhC}} / n_R$, there is no possibility to couple to a free-space radiative mode, as the impulse conservation (equation 2.9) cannot be fulfilled (Figure 14, blue arrow). This case is commonly referred to be “below the light line”.

\[
\left| k_R \right| = \frac{\omega_R \cdot n_R}{c}
\]

Figure 14: The possibility of a PhC mode to couple to a free-space mode depends on the length of its k-vector. If it is short enough, it can couple to a free-space mode, while energy conservation (equation 2.5) and impulse conservation (equation 2.6) is fulfilled (red arrows). If the k-vector of the Bloch mode is too big, no coupling is possible.

Only for membrane-type PhCs, operation of a waveguide below the light line is possible. In the case of the substrate-type PhC, the light line of the substrate (lower green line in Figure 12) lies completely below the PBG, inside which the guided modes are located, and thus coupling to the radiative modes in the substrate is always possible for waveguide modes in the PBG.

Equations 2.8 and 2.9 are only a required condition, but comprise no information about the strength of the modal coupling. To calculate the coupling strength (and in the following the propagation loss), the overlap integral of (all) the radiative modes with the guided mode must be calculated. With the currently available computational resources, this undertaking is not feasible due to the size and complexity of the computational domain. Even using an approximation of the radiative modes with undisturbed plane waves still requires the calculation of an infinite number of integrals (for the infinite spatial directions of relevant plane wave). Therefore such a calculation is far beyond the scope of this work, and remains also unsolved in the literature. Therefore it is not clear if out-of-plane losses are a relevant loss mechanisms. However, we believe from comparing the losses of a membrane-type PhC waveguide operated below and above the light line (reference [67] in Table 3) that the loss mechanism is indeed relevant.
2.2.2. The different loss mechanisms

Next to very practical issues for fabrication, like single chip processing time, reproducibility of the fabrication, yield and fabrication tolerances\(^5\), the optical propagation losses of the final device are the figures of merit of the technology.

Light in PhCs can be attenuated through three distinct loss channels. It can either be absorbed by the medium (e.g. the semiconductor itself, or metal contacts on top of the waveguides), be reflected by an interface or coupled to other (non-confined) light modes. Almost all loss mechanisms are based on mode coupling of the guided mode to non-guided modes with different coupling strength.

In literature, loss is usually characterized by two different figures of merit:

- For the propagation of light through a planar PhC, the losses can be modeled in 2D by a formal imaginary dielectric constant \( \varepsilon'' \) [68, 69]. In the 2D model representing the PhC, \( \varepsilon'' \) is added to the dielectric constant of the holes \( \varepsilon_{\text{hole}} = 1 - i \cdot \varepsilon'' \). The \( \varepsilon'' \)-model substitutes the mode coupling to non-guided mode by a light-absorbing medium in the holes. The \( \varepsilon'' = \varepsilon''_{\text{int}} + \varepsilon''_{\text{fab}} \) is composed of an intrinsic contribution \( \varepsilon''_{\text{int}} \) (coupling to radiative mode without any distortion of the PhC structure) and a contribution from imperfect hole shape \( \varepsilon''_{\text{fab}} \).

The total imaginary dielectric constant \( \varepsilon'' \) is determined either by fitting 2D-simulated transmission spectra to transmission measurements or by simple models, e.g. as proposed by Benisti et.al for the intrinsic contribution [59, 69] (section 2.2.2.1) and for finite (but still cylindrical) hole depth [59] or for the contribution of a non-cylindrical hole shape by Ferrini et.al. [68, 70] (section 2.2.2.2).

![Figure 15: Sources of losses in a PhC device (e.g. PhC waveguide bend). A) Material absorption, B) Out-of-plane scattering (also into the substrate, not shown in the picture) due to intrinsic coupling to radiative modes, or enhanced coupling to radiative modes due to imperfect hole fabrication (hole depth, hole shape, roughness, disorder), C) Radiation leakage, D) Insufficient guiding by the PBG caused by TE-like and TM-like mode-coupling due to the slab asymmetry, E) Interface-losses (e.g. reflections or out-of-plane-scattering).](image)

\(^5\) Minimal hole size, minimal hole distance, hole placement accuracy, hole diameter accuracy
2.2 Optical losses as a figure of merit

- In waveguides-based devices, losses are specified in dB/cm or dB/mm. Transmission measurements are usually performed to obtain the waveguide loss figure. In the case of high losses in the PhC waveguide, the cutback-method may be applied. If low-loss PhC waveguides are investigated, the use of the fringe-contrast method is more convenient [71]. This method uses the fringes of the “cavity” created by the waveguide between two cleaved facets to determine the loss (see Appendix 3 for a mathematical description of the method).

Losses arising from the PhC can be separated into three different categories:

2.2.2.1. Intrinsic losses

Intrinsic losses even occur in the perfect crystal where the fabricated chip corresponds exactly to the desired structure. They represent therefore a lower limit for the achievable loss.

- Light absorption by the semiconductor is considered to be negligible, as long as the electronic bandgap $E_g > \hbar \omega$.

- For active, electrically pumped PhC devices, a metal contact on top of the upper cladding is required. The mode penetrates into the metallic layer, and is absorbed. Depending on the thickness of the cladding and the width and position of the metal contact, losses due to light absorption can be in the order of several 1000dB/cm [72].

- Even perfect planar PhCs suffer from out-of-plane scattering due to the presence of the holes, when the mode lies below the light-line [5]. In this case, non-vanishing coupling to radiative modes can occur (see section 2.2.1). Benisti et.al [69] explain the intrinsic losses by radiative dipoles in the hole. They provide an equation to estimate the strength of the losses by $\epsilon_{\text{int}}^*$:

$$\epsilon_{\text{int}}^* = \frac{\pi^2}{6} \frac{V}{(\lambda / 2n_{\text{clad}})^3} \left( \frac{\Delta \epsilon}{\eta} \right)^2 \eta \Gamma,$$

where $V$ is the volume of the hole in the core $V = \pi r^2 \cdot d_{\text{core}}$, $\Gamma$ the confinement factor of the (vertical) mode in the slab waveguide core and $\eta$ the extraction efficiency of the dipole radiation. Their model assumes the possibility to separate the spatial dependence of the refractive index into the horizontal plane and the vertical slab waveguide according to $\epsilon_{3D}(x, y, z) \approx \epsilon_{\text{plane}}(x, y) + \epsilon_{\text{slab}}(z)$. This simplification of the spatial distribution of the refractive index allows to separate the electromagnetic fields into $E(x, y, z) \approx \psi(x, y) \cdot \zeta(z)$. The difference between the real structure $\epsilon_{3D}(x, y, z)$ and the approximation $\epsilon_{\text{plane}}(x, y) + \epsilon_{\text{slab}}(z)$ is considered as a radiative dipole (first Born approximation [73]), located in each hole. This dipole emits light out-of-plane and is therefore responsible for the optical losses. The radiation by the dipoles in the PhC is assumed to be incoherent in the model. For a detailed analysis
and explanation of this equation and all factors, the reader may consult the reference [69]. Also the subsequent extension of this model for extrinsic losses (section 2.2.2.2) are based on the same model and treat the deviation from the “ideal” hole as radiative dipole. Here only the red terms are of importance. They let us conclude that

- \( \varepsilon_{\text{int}}^{\ast} \) scales with \( \Delta \varepsilon^2 \cdot \Gamma \). This index contrast \( \Delta \varepsilon \) and the confinement factor \( \Gamma \) are rather small in our case, compared to membrane-type PhCs. With respect to intrinsic out-of-plane scattering, the bulk-type material system is thus superior\(^6\) to the membrane-type material systems [69] (Figure 15B). Of course, the situation becomes different as soon as we consider the extrinsic losses (see section 2.2.2.2).

- \( \varepsilon_{\text{int}}^{\ast} \) scales with \( n_{\text{clad}} \). Therefore the cladding (upper or lower) with the highest refractive index contributes most to the losses.

The intrinsic scattering – despite the regular PhC patterning – is assumed to be incoherent [69]. Theoretical values for \( \varepsilon_{\text{int}}^{\ast} \) from equation 2.10 between 0.024 and 0.048 are realistic [59].

### 2.2.2.2. Extrinsic losses

Extrinsic losses arise from fabrication imperfections. Real holes have angled sidewalls, rough sidewall surfaces and the depth is limited by the selectivity of the fabrication process against the mask. These imperfections give rise for extrinsic losses:

- **Limited hole depth** and **angled hole sidewalls** are both sources of extrinsic losses, as addressed by Benisty et.al. [59] (truncated holes) and Ferrini et.al. [68, 70] (angled hole sidewalls). Thereby the difference between the truncated/angled hole and the infinitely deep cylindrical hole is viewed as a perturbation (leading to a dipole moment) for the Bloch modes, and thus couple them to the radiative modes. For truncated holes, the losses scale with the overlap-integral of the vertical light mode and the filled part of the holes (equation 2.11),

\[
\varepsilon_{\text{fab}}^{\ast} \sim \int_{-\infty}^{\text{hole depth}} \zeta(z) \, dz, \tag{2.11}
\]

where \( \zeta(z) \) is the vertical mode profile, and thus depend also on the index contrast between core and cladding, the core thickness and to a lesser extend on the cladding thickness [68].

For angled sidewalls, Figure 16 (from [70]) shows the values for the \( \varepsilon_{\text{fab}}^{\ast} \)-parameter for a filling factor of 50% and an upper hole diameter of 460nm. Depending on the relation between sidewall angle of the holes and the hole

---

\(^6\) This is of course only valid above the light line. Below the light line, there are no modes to couple to, and thus the intrinsic losses must vanish.
depth, the losses due to non-ideal hole shape are either dominated by the finite hole depth or the sloped sidewalls.

**Figure 16**: $\varepsilon_{\text{fab}}''$-parameter as a function of hole depth and hole shape for a filling factor of 50% and an upper hole diameter of 460nm. Both angles sidewalls and finite hole depth give a contribution to $\varepsilon_{\text{fab}}''$. d denotes the hole depth.


- **Sidewall roughness** creates scattering centers, which lead to out-of-plane losses. Bogaerts et.al. [74] treat roughness as a small dipoles located at the sidewalls, and calculate their impact on light scattering. Different shapes of the dipole and recapturing of the scattered light into the waveguide is considered in their model. In terms of sidewall roughness, membrane-type PhC exhibit lower losses than bulk-type PhC with the same surface roughness [74]. However, their model is simplified, and they do not relate their roughness loss figure to other loss mechanisms. Addressing the loss by brute-force simulations instead of a mathematical description fails on the fine (~1nm) structure of roughness, orders of magnitude smaller than typical dimensions (~100nm) of the undisturbed hole pattern. Thus, meshing and simulation of such a structure goes normally beyond the scope of current available computational power, even for the finite element method (see section 2.3.3) with its adaptable grid size. Therefore the question of the relative strength of the roughness-induced losses to other loss mechanisms remains currently unanswered.

- **Disorder-induced losses** arise from varying hole size, non circular hole shape or non-periodic placement of the holes. Ferrini et.al. [75] addresses this topic again with the $\varepsilon''$-model. Within the model, the disorder-induced losses contribute to the total losses as $\varepsilon'' = \varepsilon''_{\text{int}} + \varepsilon''_{\text{fab}} + \varepsilon''_{\text{dis}}$. The same description of the deviation between real and fabricated hole as radiative dipole – analogue to the surface roughness or the hole-shape calculation – is used.

The relevance of disorder-induced losses depends on the confinement scheme. In substrate-type PhCs, disorder-induced losses are negligible compared to those caused by intrinsic coupling to radiating modes, if disorder does not exceed values of $\sigma(\delta x)/r < 6\%$ and $\sigma(\delta r)/r < 3\%$ for position and hole radius dis-
order, respectively [1] (where \( r \) is the hole radius, \( \delta x \) is the deviation in hole centre placement and \( \delta r \) the deviation in hole radius, respectively). These limits are well fulfilled for our fabrication process [1], and thus these losses are not further considered. For membrane-type PhC, however, the guiding below the light line is theoretically lossless, and every distortion adds additional losses. Therefore disorder-induced losses must be considered for membrane-type PhCs [1].

Realistic values for measured \( \varepsilon'' \) for PhCs in the low-refractive index contrast material system are typically one order of magnitude larger than the intrinsic values [68]. Thus we conclude that indeed the fabrication imperfections are responsible for the reported high losses (Table 3).

2.2.2.3. Structural losses

Structural losses arise from the design of the device.

- To this category, we assign e.g. losses at interfaces. They arise from a transmission through the interface smaller than 100%.

- In a PhC waveguide, light is laterally confined by the PhC. The confinement is perfect for an infinite crystal. In reality, the PhC is finite. To speed up the electron beam lithography writing during fabrication, only a few rows of holes along the waveguide are written (~6-12 rows). Therefore we do not have “perfect” lateral confinement and energy is radiated laterally away from the waveguide (radiation leakage). Radiation leakage was theoretically found to be negligible when using more than 6 rows on each side of the PhC device are etched [1].

- Also in this category belong losses due to the asymmetric waveguide design. The separation between TE and TM-polarization is only valid for a symmetric slab waveguide structure. If the symmetry is broken, we only can categorize the modes into TE-like and TM-like [41]. The two polarizations can now couple. Because the triangular lattice of air-holes has only a PBG for the TE polarization (within reasonable filling-factors), the PBG-property is not completely fulfilled, and light-guiding by the PBG becomes lossy [41].

2.2.2.4. The relative strength of the loss mechanisms

To the best of our knowledge, no publication so far compared theoretically or experimentally the relative strengths of all these loss mechanisms. As the presented models all are based on different assumptions, it is not possible to relate them directly. However, as it is well known that for bulk-type PhCs, losses are much higher than for membrane-type PhC. Therefore, we conclude that the extrinsic effects clearly dominate the intrinsic effects, as extrinsic effects predict significant higher losses for bulk-type PhCs. As such losses are caused by fabrication imperfections, it is mandatory to reduce them by an advanced fabrication technology.
2.2 Optical losses as a figure of merit

2.2.3. State-of-the-art losses in photonic crystal waveguides

The critical figure of merit for light propagation in a PhC waveguide is the propagation loss. These values are widely published within the community. However, to put the loss values in perspective, one must distinguish between different types of implementation of realistic PhC devices (waveguide type, vertical confinement type, position of the mode relative to the light line). Table 3 provides an overview of different experimental loss values found in literature.

<table>
<thead>
<tr>
<th>Type</th>
<th>Material</th>
<th>Vertical confinement</th>
<th>Reported Loss value</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>W1</td>
<td>SOI</td>
<td>Membrane below the light line</td>
<td>24dB/cm</td>
<td>[67]</td>
</tr>
<tr>
<td>W1</td>
<td>SOI</td>
<td>Membrane above the light line</td>
<td>400-1300dB/cm</td>
<td>[67]</td>
</tr>
<tr>
<td>W1</td>
<td>GaAs</td>
<td>Membrane below the light line</td>
<td>7.6dB/cm</td>
<td>[50]</td>
</tr>
<tr>
<td>W1</td>
<td>SOI</td>
<td>Membrane below the light line</td>
<td>40dB/cm</td>
<td>[76]</td>
</tr>
<tr>
<td>W1</td>
<td>SOI</td>
<td>Membrane below the light line</td>
<td>5dB/cm</td>
<td>[51]</td>
</tr>
<tr>
<td>W1</td>
<td>InP</td>
<td>Bulk above the light line</td>
<td>1800dB/cm</td>
<td>[77]</td>
</tr>
<tr>
<td>W1</td>
<td>InP</td>
<td>Bulk above the light line</td>
<td>600dB/cm-1000dB/cm</td>
<td>[78]</td>
</tr>
<tr>
<td>W2</td>
<td>InP</td>
<td>Bulk above the light line</td>
<td>40dB/cm</td>
<td>[79]</td>
</tr>
<tr>
<td>W3</td>
<td>InP</td>
<td>Bulk above the light line</td>
<td>15dB/cm</td>
<td>[79]</td>
</tr>
<tr>
<td>W3</td>
<td>SOI</td>
<td>Membrane below the light line</td>
<td>260dB/cm</td>
<td>[80]</td>
</tr>
<tr>
<td>W3</td>
<td>InP</td>
<td>Bulk above the light line</td>
<td>18dB/cm</td>
<td>[81]</td>
</tr>
<tr>
<td>W3</td>
<td>GaAs</td>
<td>Bulk above the light line</td>
<td>&lt;200dB/cm</td>
<td>[82]</td>
</tr>
<tr>
<td>W3</td>
<td>InP</td>
<td>Bulk above the light line</td>
<td>100dB/cm</td>
<td>[83]</td>
</tr>
</tbody>
</table>

Table 3: Measured loss values for different material systems and waveguide types reported in literature. Loss measurements obtained for our material system are highlighted in bold. Bulk-systems are always operated above the light line.

The span of the values is huge, reaching from 5dB/cm to 1800dB/cm. Generally, we can separate the reported values into three different operation regimes of the PhC waveguide:

- **W1 (or W3) waveguides below the light line**: Membrane-type PhCs have the advantage to have a frequency region where the W1 waveguide is operated below the light line. Also the fabrication process is much less demanding, as only shallow holes (<1μm) are required. Therefore low losses (<50dB/cm) can be achieved with this type of PhC waveguides. However, electrical contacting for active devices is unfeasible for these structures.

- **W1 waveguides above the light line**: Above the light line, losses increase due to out-of-plane scattering. As soon as we operate a W1 waveguide above the light line, losses drastically increase (≥100dB/cm). Such high loss values are also reported for a membrane type PhC waveguide operated above the light line [67], and for all bulk-type PhC W1 waveguides [77, 78]. To best of our knowledge, no report of low-loss PhC W1 waveguides operated above the light line is available. Huge losses (1280dB/cm [84], 3D FDTD) in this type of structures are also confirmed theoretically. These first simulations of 3D losses are close to experimental values.
2. The physics of photonic crystal devices

- **W3 waveguides above the light line**: For a W3 waveguide, loss (< 100dB/cm) is considerably lower than for a W1 waveguide.

W1 waveguides in the bulk-type PhCs would be the most promising candidate for future active devices, as they are single-mode and can be pumped electrically. Unfortunately, even with an advanced fabrication technology, we do not expect loss value which can compete with the membrane-type PhCs or with conventional ridge waveguides.

### 2.2.3.1. Application of the $\varepsilon''$ model to waveguides

The $\varepsilon''$ model was initially developed to include losses of Bloch modes inside the photonic crystal bends [69]. However, it is also applied to include propagation loss in PhC waveguide simulations [28]. Figure 17 presents the simulated propagation loss of a W1 waveguide ($r/a=0.31$) for different hole refractive indices $\varepsilon_{\text{hole}}=1-i \cdot \varepsilon''$. The values for $\varepsilon''$ vary from 0.00 to 0.3 for the even and 0.2 for the odd mode, respectively. The loss value is extracted from the attenuation of the power density flux.

**Even mode**: The simulation of the even mode, using the $\varepsilon''$ model, predicted the correct qualitative frequency behavior of the propagation loss. The obtained loss values in the slow-light region close to the even mode cutoff increases strongly for constant $\varepsilon''$, compared to the linear dispersion regime of a W1 waveguide. This is due to the higher lateral extension of the slow-light mode (compare with e.g. Figure 79) and the resulting the higher overlap of the mode with the area of a finite $\varepsilon''$ value (holes). The even mode cutoff is correctly predicted by the simulation, independent of the $\varepsilon''$. The whole simulated frequency range is single-moded, as the odd mode is not excited due to the symmetry of the source.

**Odd mode**: The odd mode has a node in the middle of the waveguide, and therefore the electrical field is high in the area of a finite $\varepsilon''$ value (holes). Therefore the same $\varepsilon''$ leads to a much higher propagation loss value for the odd mode than for the even mode. The obtained propagation loss value depends on the excited odd mode. The frequency range supported by the odd mode is not completely odd-single-moded. Therefore the propagation loss for the same $\varepsilon''$ is irregular over the frequency range.

In conclusion, Figure 17 shows that the $\varepsilon''$-model can be used to include loss in a 2D simulation. However, the obtained propagation loss as a function of $\varepsilon''$ depends on the overlap of the field with the holes and not on the physical properties of the mode. Therefore, the model parameter $\varepsilon''$ is only used as an empirical fit parameter in the simulation.
2.3 Simulation methods

Simulation tools are indispensable for the understanding and optimizing of PhC devices. They can predict the transmission properties of a device prior to its time-consuming fabrication and characterization, and assist in understanding complex measurement results. However, the simulation of a PhC itself is challenging, because of the competition between accuracy (the complex PhC structures require a fine spatial resolution) and computational efficiency. “Exact” computational models are seldom feasible, as one is typically limited by computational power. To mitigate this, one use approximations (e.g. 2D instead of 3D models, coarser grid), which introduce numeric errors, or with physical approximations (e.g. losses represented by a complex dielectric constant [68, 69]). One must carefully select and evaluate approximations in order to make a problem tractable, without introducing significant errors.

In this work, simulations are used to optimize designs and to understand the optical measurements of the devices which are presented in Chapter 6. The plane-wave expansion (PWE) method using MPB\(^8\) [61, 62] is used to calculate dispersion relations of PhCs and PhC waveguides, whereas complete and complex devices were simulated using the finite element (FE) method with COMSOL \[85\]. The following sections give an overview over the employed methods and their limitations.

---

7 3D, with a very fine grid to resolve all features
8 MIT Photonic Bands
2. The physics of photonic crystal devices

2.3.1. Effective refractive-index determination

All of the simulation methods we used are based on a discrete approximation of the continuous distribution of material within the computational domain. The resolution of the discretization grid determines the accuracy of the simulation result. However, the number of spatial grid points scales by a power of 3 with the grid resolution in three dimensions (3D), which can lead to excessively large computational memory and processor requirement. Due to computational power restrictions, the simulations in this work have been performed in 2 dimensions, by reducing the inhomogeneous vertical layer stack of the vertical slab waveguide in the third dimension to a scalar effective refractive index. Compared to full 3D simulations, two-dimensional (2D) simulations are fast and systematic device optimization becomes possible, but it must be verify that no important physical effects are lost (e.g. out-of-plane losses).

![Effective refractive index](image)

**Figure 18**: Simulated effective refractive index ($n_{eff}$) for the different modes in the standard slab waveguide used in this work. The waveguide supports single TE (white) and TM (blue) modes above 1.35 μm. Below this wavelength, second order modes with significantly lower $n_{eff}$ are present in the slab waveguide. Within the tunable range of our laser sources, the waveguide is single-mode.

The effective refractive index ($n_{eff}$) is determined by the propagation constant of a light mode in an undisturbed slab waveguide. Calculation of $n_{eff}$ is performed analytically by computing the 3-layer slab waveguide mode in the vertical direction [86]. Using 2D simulations together with $n_{eff}$ suggests that the full 3D solution of the master equation can be separated in first order into a horizontal and vertical contribution according to equation (2.12) [69], where $\zeta(z)$ is the vertical guided mode profile. The solution strategy is to first determine $\zeta(z)$ and $n_{eff}$. Afterwards, the horizontal 2D problem for $\vec{H}_{k,\omega}^{2D}(x,y,t)$ is solved using the previous determined $n_{eff}$.

$$\vec{H}_{k,\omega}^{2D}(x,y,z,t) = \vec{H}_{k,\omega}^{2D}(x,y,t) \cdot \zeta(z)$$ (2.12)

The mode profile $\zeta(z)$ in the vertical direction depends on the frequency. Therefore, the $n_{eff}$ of the slab waveguide depends on the frequency. This frequency dependence of $n_{eff}$ is shown in Figure 18 for our material system. Within the range of the tunable
laser sources (Chapter 5, $\lambda=1470\text{nm}-1630\text{nm}$), the slab waveguide only supports one mode for each polarization, with a decreasing $n_{\text{eff}}$ for higher wavelengths. Below $\lambda=1.35\mu\text{m}$, the slab waveguide becomes multimode. We approximated the effective refractive index according to $n_{\text{eff}} = -0.0633\mu\text{m}^{-1}\cdot\lambda + 3.3571$ for our simulations.

Another source of dispersion is the material dispersion of the semiconductor itself. Between 1460nm and 1650nm it reduces from $n=3.178$ to $n=3.156$ [87].

The effective refractive index approach has, however, its limitation. It is only valid for low index contrast structures. This condition is almost fulfilled in the vertical direction (contrasts as small as $\Delta n=0.18$, <6%, except for the InP-air interface). In the horizontal direction, however, the modulation between the semiconductor background material and the holes is too strong to assume the strict validity of the $n_{\text{eff}}$-approach. Despite the inaccuracy of the $n_{\text{eff}}$-model, it was applied in the 2D simulations. No better models for 2D simulations are available, and an optimization in full 3D is normally beyond available computational resources.

### 2.3.2. Plane-wave expansion method

The publically available plane-wave expansion (PWE) software MPB [61, 62] was used in this work to calculate the dispersion diagrams of various structures. MPB is designed to calculate the fields and the dispersion relation $\omega(k)$ of the modes in a periodic medium in either 2D or 3D based on the dielectric function in the unit cell for any given $k$. In this section, we introduce briefly the principles of this simulation method and its limitations.

To determine the dispersion relation $\omega(k)$, the dielectric function $1/\varepsilon(\vec{r})$ and the fields $\vec{E}_{n,k}(\vec{r})$ and $\vec{H}_{n,k}(\vec{r})$ are decomposed into Fourier series. The sum of the Fourier series extends over all inverse lattice vectors. For calculation reasons, the series are, however, truncated. The number of considered plane waves depends on the desired accuracy. Substituting the Fourier series into the master equation gives

$$\nabla \times \left( \sum_F \varepsilon_F e^{i\vec{F} \cdot \vec{r}} \nabla \times \sum_G \vec{H}_G e^{i\vec{G} \cdot \vec{r}} - e^{i\vec{k} \cdot \vec{r}} \right) = \frac{\omega^2}{\varepsilon_0} \sum_G \vec{H}_G e^{i\vec{G} \cdot \vec{r}} e^{i\vec{k} \cdot \vec{r}},$$

(2.13)

where $\vec{F}$ and $\vec{G}$ are inverse lattice vectors, and $\varepsilon_F$ and $\vec{H}_G$ the Fourier components of the dielectric function $\varepsilon(\vec{r})$ and the magnetic field $\vec{H}(\vec{r})$, respectively. In this equation, the cross product can be calculated and the result sorted according to the base functions $e^{i\vec{F} \cdot \vec{r}}$. We obtain a set of linear equations (one equation for each basis function), representing an eigenvector problem for the eigenvalue $\omega$. Such an equation system can be solved by standard numeric methods. The plane-wave expansion method relies on the periodicity of the material. For each given $k$, the eigenvalues $\omega(k)$ are calculated simultaneously.

The main disadvantage of the PWE method is the inability to consider dispersive effects and the restriction of the method to strictly periodic media. PWE determines...
the frequencies $\omega$ as a function of $\vec{k}$, and thus $n(\omega)$ cannot be set prior to the simulation. Both limitations can partly be circumvented.

Figure 19: Periodic boundary conditions (for 2D). In the case of a simple crystal, the unit cell contains one hole. The PWE software then continues the unit cell in all 4 directions (arrows). To simulate a W1 waveguide – which breaks the periodicity of the structure in the lateral direction to the waveguide – the supercell approach is used. The supercell includes several rows of holes adjacent to the missing hole of the waveguide.

- For non-periodic structures, like a W1 waveguide or a cavity, the supercell approach is a common technique to make the structure periodic (Figure 19). The basic idea is to enlarge the simple unit cell into a supercell of $n \times m$ unit cells, and place the non-periodic structure in the middle of the supercell. The PWE then applies periodic boundary conditions to this supercell, resulting in an array of parallel waveguides or cavities. One needs to ensure that parasitic coupling between the multiple waveguides does not occur, by adding enough undisturbed rows of unit cells (holes) along the PhC waveguide. Previous investigations have shown that lateral coupling can be neglected if more than 6 rows of holes are introduced between adjacent waveguides [1]. In this work, supercell simulations of waveguides or coupled waveguides (Chapter 6) are simulated with at least 12 separating hole rows.

- To consider dispersion, the frequency range of interest can be separated into discrete intervals (Figure 20). For each frequency interval, $n_{\text{eff}}$ is determined and the full dispersion diagram is calculated. The results of the different simulations are then concatenated by taking the dispersion diagram only in frequency intervals for which $n_{\text{eff}}$ was calculated, and composing the whole dispersion diagram. This procedure is, however, inefficient, as many diagrams have to be calculated to cover the whole frequency range.

- In the case where we are only interested in the location of a single frequency feature (e.g. cut-off frequency, PBG), an iterative approximation of the correct location is pursued, as presented in Figure 21. The solution $\omega(k)$ is iteratively approximated by alternately calculating the band diagram and $n_{\text{eff}}$. The
enhancement of the accuracy in the location of a frequency feature is about 1-3%, and typically 2-3 iterations are necessary for convergence.

![Composition of the dispersion diagram including waveguide dispersion.](image)

**Figure 20**: Composition of the dispersion diagram including waveguide dispersion. Each color represents a dispersion diagram calculated with an $n_{\text{eff}}$ based on the frequency in the middle of the corresponding slice (red box). Between the slices, the dispersion is not exactly continuous.

![Algorithm to calculate $\omega(k)$ including dispersion using PWE.](image)

**Figure 21**: Algorithm to calculate $\omega(k)$ including dispersion using PWE. The time-consuming step is the simulation. The time required for the simulation linearly scales with the number of iterations.

All approaches require additional computational power, as the computational domain is enlarged or the whole simulation has to be performed several times. However, as long as we restrict ourselves to 2D simulations, the computational time is still acceptable (only a few hours).

### 2.3.3. Finite elements method

Finite element methods (FEM) were first developed in the 1940s. Commercial use began in the 1950s with its application to aircraft design [88]. In 1968, it was applied to electromagnetic (EM) problems [88, 89] for the first time. Today, it is applied to a wide range of physical problems. In this section, we give a brief introduction into the basic ideas of FEM and their limitations.
FEM solve boundary value problems (BVP). The BVP is given by a differential equation for the unknown function \( \Phi \) in the computational domain and fixed function values for \( \Phi \) and \( \partial \Phi \) along the boundary of the computational domain. The method is based on discretization of the solution \( \Phi \). For that purpose, the computational domain is divided into smaller elements. In 2D triangles are the most commonly used element. This division process is called meshing. The mesh can have different densities at different locations, depending on the expected field distribution (based on experience) and on material properties (high density of elements for nonlinearities or inhomogeneities), as well as the boundary shape. Within an element of the mesh, the function \( \Phi \) is approximated by functions \( \Phi^e \), For which the simplest approximation (in 2D) is the linear equation \( \Phi^e = a \cdot x + b \cdot y + c \) (plane). Instead of having \( a \), \( b \) and \( c \) as free parameters, it is preferable to compose the linear element functions \( \Phi^e \) from 3 linearly independent shape functions \( \phi_x \), \( \phi_y \), and \( \phi_z \), according to \( \Phi^e = \phi_x^e \cdot N_x^e + \phi_y^e \cdot N_y^e + \phi_z^e \cdot N_z^e \). The solution \( \Phi \) is then the union of all element approximation functions \( \Phi \approx \bigcup_{\text{elements}} \Phi^e \). By inserting the approximate solution \( \Phi \) into the master equation (2.3) in the integral form, an equation system for the weight variables \( \phi^e \) is obtained.

The exact mathematical procedures of FEM are complex and beyond the scope of this introduction. A detailed introduction the FEM is given in [88]. In the next part of this section, we discuss some details about FEM which is relevant to this work. Although FEM is also capable to calculate the time evolution of the system, we only used the simpler and faster static (no time evolution) simulations in this work.

**Dispersion.** As the solution is calculated for each frequency separately, the introduction of any type of dispersion is straightforward, as the refractive index can be changed between each frequency simulation.

**Detector principles and reflections.** FEM calculates the complete electric / magnetic field distribution. To determine the transmission \( T \) (equation 2.14) through a device, the power flux must be extracted by placing detectors at the in- and output of the device.

\[
T = \frac{\text{transmitted power after the device}}{\text{injected power in the device}}
\]  
(2.14)

For our 2D device simulations, it is assumed that the light can only pass through the device, or is reflected by the device (Figure 22a). Out-of-plane losses (not possible to be directly included in 2D), absorption (lossless material) and radiation leakage (sufficient rows of holes within the simulation domain along the waveguide) are neglected (energy conservation over all channels). Two different detector types are used in this work.

---

9 First spatial derivation
2.3 Simulation methods

Figure 22: a) In lossless 2D simulations of a 2-port device, the input light can only propagate through the device, or be reflected (energy conservation). b) FEM-flux detectors (integration of the pointing vector across the waveguide) before and after the device. The input detector before the device only measures the difference between input and reflected flux. Only a time-resolved simulation (which would take longer and is more complicated) could discriminate between the two fluxes. c) Power-density detectors before and after the device. The input detector before the device measures the sum of the input and reflected power.

- **Power flux detectors** (Figure 22b) measure the power flux through a boundary inside or at the edge of the computational domain by integrating the pointing vector across this boundary. The transmission \( t^{10} \) is calculated according to \( t = \frac{p_{\text{output}}}{p_{\text{input}}} \), where \( p_{\text{input}} \) and \( p_{\text{output}} \) are the power fluxes through the detector in the input and output waveguide, respectively.

The flux detector implementation in COMSOL cannot discriminate the direction of the flux, therefore the input detector (Figure 22a) measures \( p_{\text{input}} = p_{\text{source}} - p_{\text{reflected}} = p_{\text{transmitted}} \) and the obtained transmission is always equal to 1. To use flux detectors, it must be prevented that light is not reflected back into the input flux detector. This is e.g. the case for simulations with lossy materials or 3D simulations which include out-of-plane scattering, but not for the devices presented in Chapter 6.

A method to overcome the reflection problem is to use time-resolved simulation of a pulse propagating through the device, to discriminate with time windows between the source pulse and the reflected pulse.

- For simulations featuring single-mode input- and output-waveguides of the device, **energy density detectors** (Figure 22c) are used. The energy density \( \rho \) over the same area across the input and the output waveguide is integrated according to

\[
E_{\text{input/output}} = \int_{\text{Detector area (2D)}} \int_{\text{Detector volume (3D)}} \rho_{\text{input/output}}
\]

\( 10 \) To clarify the notation, small letters are used in combination with the power-flux detector method, whereas upper letters are used when the energy density integration method is used.
The power flux through this area is proportional to the integrated energy density $p_{\text{input,output}} = r \cdot E_{\text{input,output}}$ (with an unknown proportional constant $r$), whereas the contributions of the source wave and the reflected wave are added in the input waveguide. A proof of this relation can be found in the appendix A.

From these two detectors, we can extract the transmission as follows:

$$ T = \frac{2 \cdot p_{\text{output}}}{p_{\text{input}} + p_{\text{output}}} = \frac{2 \cdot r \cdot E_{\text{output}}}{r \cdot E_{\text{input}} + r \cdot E_{\text{output}}} $$ (2.16)

The equation (2.16) is derived in the appendix A. This method accounts correctly for reflections in lossless waveguides. However, we should not conceal the limitations of this method:

- The method fails in the case of multimode waveguides, as the mode beating of the coupled modes becomes larger than the integration area, leading to unphysical results which strongly depend on detector positions and size.

- In the case of lossy waveguides, the energy conservation relation $p_{\text{source}} - p_{\text{reflected}} = p_{\text{transmitted}}$ does not hold anymore, and the method becomes inaccurate. The calculation of the transmission must be enhanced with a loss term to account for the energy conservation.

$$ T = \frac{2 \cdot p_{\text{output}}}{p_{\text{input}} + p_{\text{output}} + p_{\text{losses}}} $$ (2.17)

The error introduced by the losses depends on the relative strength of the lost power compared to the other power values. Only as long as relation is small, the method is approximately correct.

- The calculation scheme relies on the assumption that the integrated energy density is proportional to the power flux: $p_{\text{input,output}} = r \cdot E_{\text{input,output}}$. The proportional constant $r$ must not be known, as in the case of physically identical waveguide in the input and output branch. The factor $r$ is cancelled when calculating the transmission.

2.3.4. Comparison of PWE und FEM

Table 4 lists the advantages and disadvantages of the different simulation methods used in this work.
2.3 Simulation methods

<table>
<thead>
<tr>
<th></th>
<th>PWE</th>
<th>FEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Input</td>
<td>• k-vector</td>
<td>• Frequency</td>
</tr>
<tr>
<td></td>
<td>• Unit cell</td>
<td>• Design</td>
</tr>
<tr>
<td>Output</td>
<td>• Band diagram</td>
<td>• Total field plot</td>
</tr>
<tr>
<td></td>
<td>• Field plot</td>
<td></td>
</tr>
<tr>
<td>Restrictions</td>
<td>• Only periodic structures</td>
<td>• Not widely used for PhCs</td>
</tr>
<tr>
<td></td>
<td>• No material/waveguide dispersion</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• No losses</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Static solutions (no time dependence)</td>
<td></td>
</tr>
<tr>
<td>Advantages</td>
<td>• Well established for PhCs</td>
<td>• Very flexible</td>
</tr>
<tr>
<td></td>
<td>• Straight forward simulation tool</td>
<td>• Time-dependence possible (but not used in this work)</td>
</tr>
</tbody>
</table>

Table 4: Comparison between PWE and FE.

- PWE is the method of choice for obtaining dispersion diagrams. It is however restricted to infinite periodic structures, and cannot handle dispersion without additional effort. From the simulation, field patterns and dispersion relations are obtained without further data processing. Losses cannot be included in the simulation.

- FEM can handle a wider variety of designs than PWE. It is used to simulate complex devices. It is the method of choice if larger, non-periodic structures need to be simulated. Dispersion is included. From the simulation, field patterns and transmission spectra can be obtained without further data processing. Losses can either be directly included by 3D simulations (simulations including out-of-plane losses), or by using an complex refractive index (\( \varepsilon'' \)-model [69]).

2.3.5. Mode solver to determine waveguide cross-section modes

In this work, the mode solver from Lumerical [90] is used to calculate the spatial mode fields, the polarization and the effective refractive indexes of the modes of the trench waveguides. The software uses a full-vectorial frequency-domain solver to find the modes of the waveguides. It is used in Chapter 5 to calculate the following data:

- The single-mode width of the accessing trench waveguide is determined by the calculation of the numbers of modes as a function of the waveguide width. Thereby it was ensured that all modes (of both polarizations) are found by the software.

- The coupling efficiency from the exciting light beam (approximated as a Gaussian beam) to the trench waveguide modes is estimated by calculating the mode overlap integral (OL) according to [90]:

\[
OL = \Re \left( \frac{\int \mathbf{E}_1 \times \mathbf{H}_2^* \cdot ds \cdot \int \mathbf{E}_2 \times \mathbf{H}_1^* \cdot ds}{\int \mathbf{E}_1 \times \mathbf{H}_1^* \cdot ds} \right) \frac{1}{\Re \left( \int \mathbf{E}_2 \times \mathbf{H}_2^* \cdot ds \right)} \quad (2.18)
\]
where \( E_1, H_1 \) is the waveguide mode of interest, and \( E_2, H_2 \) the field of the Gaussian beam. Equation 2.18 only accounts for the mode overlap, and does not contain the optical losses caused by reflections at the air-semiconductor interface. The Gaussian beam is defined by its waist radius (between 2-5\( \mu \)m in our simulations) and the distance of the waist from the cleaved facet (always assumed to be 0 in our simulations).

### 2.4. Conclusions

The propagation of light in a photonic crystal is completely described by the Maxwell’s equations 2.2a-2.2d. The periodicity of PhCs allows simplifying the Maxwell’s equations to the Master equation 2.3 and leads to the general solution for a light mode inside a PhC of the form of a \textit{Bloch mode}

\[
\bar{H}_{k,\alpha}(\mathbf{r}, t) = \Re \left( e^{i\mathbf{k} \cdot \mathbf{r}} \cdot u_{k}(\mathbf{r}) \cdot e^{i\omega(t)} \right).
\]  

(2.5)

A PhC mode can exhibit interesting features like the scalability, a photonic bandgap or slow-light light propagation.

An analytic solution of the master equation 2.3 is almost impossible. Therefore the light behavior of PhC devices must be determined analytically. Simulation tools like MPB [61, 62] for dispersion characteristics and COMSOL [85] for complete device simulations are used in this work. These tools provide all required information for the device simulation and optimization presented in this work.

The loss of a PhC device will be the key property which decides about its practical applicability. Losses arising in a PhC can be categorized as \textit{intrinsic losses} (not to be influenced by the researcher), \textit{extrinsic losses} which can be reduced by fabrication technology improvement and \textit{structural losses} which can be reduced by clever device design. In bulk-type PhCs, no literature reports of propagation losses below 500dB/cm have been found. All these devices are operated below the substrate light line, and therefore the coupling to radiative modes is always possible. Therefore device miniaturization is very important, to avoid long propagation distances within the PhC.
Fabrication technology has a dominant influence on the PhC device performance. It determines the optical losses and the transmission spectra. Excellent control and reproducibility of the process parameters is mandatory, requiring detailed knowledge about the fabrication process to enable a stable and reliable etching of the photonic crystals (PhC).

In this chapter, the results related to the fabrication of deep and high aspect ratio holes in InP-based semiconductors are discussed. We start with a brief introduction into semiconductor processing in general and dry etching of semiconductors in particular. Then, each step for the fabrication of complete PhCs devices is discussed.

3.1. Introduction

As discussed in the previous chapters, photonic crystals (PhC) are promising structures to be used in future all-optical data transmission links. However, the drawback of these structures is their very challenging fabrication at the nanometer scale. Our focus on telecom applications imposes the following technological requirements for our fabrication technology: The use of InP and its quaternary compounds as a base material and the focus on the wavelength of $\lambda=1550\text{nm}$ (telecommunication bands). These choices have the following impact on the fabrication technology:
3. Etching of deep holes in InP for photonic crystals

- The lattice-matched InP/InGaAsP material system is limited to a low refractive index contrast $\Delta n = 0.18$. As a consequence, the vertical mode profile extends several micrometers deep into the semiconductor substrate [28, 91]. To fabricate low-loss photonic crystals, the hole pattern needs to extend through the major portion of the vertical mode profile. This leads to a required hole depth of over $\sim 2.5 \mu m$ [1, 92].

- Interesting photonic crystal features – bandgap or band edge – are located near the reduced frequency $u=0.3$ for our lattice type (triangular array of holes). This results in a lattice constant of around 450nm for the telecom wavelength, and a hole diameter between 250-315nm ($r/a=0.25-0.35$).

3.1.1. Fabrication challenges of photonic crystals

The requirement of etching holes with a very small diameter (200nm) in a dense array (lattice constant $\sim 400$nm) together with the required depth is beyond standard patterning technology used for electrical semiconductor devices. Only the combination of a complex patterning technology with an optimized dry-etching method allows the creation of such PhC structures. The fabrication challenges are in detail:

- Patterning of the submicron structures requires [93, 94] electron beam lithography (EBL). Conventional optical (or deep-UV) lithography with expensive mask sets fails to be practicable for the demands and required flexibility in PhC research.

- To achieve a homogeneous hole pattern, proximity effects arising during electron-beam writing have to be controlled and corrected [1, 93, 95].

- The low acceleration voltage of our EBL system of 30kV limits the PMMA resist thickness to $\sim 220$nm due to forward scattering of the impinging electrons [1]. Thicker resists cannot deliver the required resolution. Direct deep semiconductor etching with the very thin EBL resist as a mask is not feasible with Cl₂, as the resist show in general not enough plasma etching resistivity and thermal stability to withstand the harsh conditions in the semiconductor dry etching reactor. Therefore an intermediate anorganic so-called hard-mask has to be introduced [92] (2-layer resist process).

- The required depth of the holes of over $2.5 \mu m$ [47, 48] and the diameter of the holes in the order of 250-315nm translates therefore into an aspect ratio in etching of 1:10 and more. Such deep structures suffer from aspect-ratio dependent etching rates [96, 97] (“lag effects”, section 4.1.1). The holes must be

  (i) deep [47, 48],
  (ii) of cylindrical shape [68], and
  (iii) with smooth surfaces [74, 98].

Careful balancing and trading-off of the different goals during optimization is a necessary task [99].
We developed successfully a fabrication technology that is capable to produce holes suitable for the fabrication of PhC devices in the InP/InGaAsP material system. In this chapter, we present the results of the PhC fabrication technology.

### 3.1.2. State-of-the-art in photonic crystal hole fabrication

Many attempts (Table 5) have been made to etch deep holes for PhC structures into InP. Here we list the achieved hole depths from other research groups. The direct comparison of the results becomes difficult, as the hole depths are reported for different hole diameters.

<table>
<thead>
<tr>
<th>System</th>
<th>Chemistry</th>
<th>Results depth@diameter</th>
<th>Comments</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAIBE</td>
<td>Cl₂/Ar</td>
<td>2.5μm@170nm 3.4μm@250nm 4.0μm@300nm</td>
<td>Measured the bandgap with the internal light source [58] method: ε''=0.08 obtained</td>
<td>[100]</td>
</tr>
<tr>
<td>CAIBE</td>
<td>Cl₂/Ar</td>
<td>2.4μm@220nm</td>
<td></td>
<td>[48]</td>
</tr>
<tr>
<td>CAIBE</td>
<td>Cl₂/Ar</td>
<td>5.3μm@250nm</td>
<td>Record value</td>
<td>[81,101]</td>
</tr>
<tr>
<td>CAIBE</td>
<td>Cl₂/Ar</td>
<td>2.3μm@220nm 2.5μm@300nm</td>
<td></td>
<td>[83]</td>
</tr>
<tr>
<td>CAIBE</td>
<td>Cl₂/Ar</td>
<td>3.0μm@300nm</td>
<td></td>
<td>[102]</td>
</tr>
<tr>
<td>ECR-RIE</td>
<td>Cl₂/Ar</td>
<td>3.8μm@(250nm)</td>
<td>Hole diameter for that depth not stated in the reference, estimate from their published image.</td>
<td>[103]</td>
</tr>
<tr>
<td>ECR-RIE</td>
<td>Cl₂/Ar</td>
<td>3.2μm@200nm</td>
<td>Diameter not explicitly mentioned in the reference. It was calculated from the given aspect-ratio value.</td>
<td>[104]</td>
</tr>
<tr>
<td>ICP-RIE</td>
<td>HI/Xe</td>
<td>2.3μm@180nm</td>
<td></td>
<td>[105]</td>
</tr>
<tr>
<td>ICP-RIE</td>
<td>Cl₂/Ar/N₂</td>
<td>2.9μm@180nm 3.8μm@310nm 4.2μm@417nm</td>
<td>This work</td>
<td>[106]</td>
</tr>
<tr>
<td>ICP-RIE</td>
<td>Cl₂/O₂</td>
<td>3.4μm@240nm</td>
<td></td>
<td>[47]</td>
</tr>
<tr>
<td>ICP-RIE</td>
<td>SiCl₄</td>
<td>3.6μm@260nm 3.8μm@320nm</td>
<td>Diameter not explicitly mentioned in the reference. It was calculated from the given aspect-ratio value.</td>
<td>[107]</td>
</tr>
</tbody>
</table>

**Table 5:** State-of-the-art reported hole depths in InP from literature.

Except for the record value from Kotlyar *et.al.*, all reported values are of the same order of magnitude (~3μm). Our technology is therefore indeed state-of-the-art, especially for ICP-RIE systems. However, the record value obtained by CAIBE-etching [81] lets us conclude that CAIBE might be slightly superior to the other technologies with respect to PhC fabrication.
3. Etching of deep holes in InP for photonic crystals

![Figure 23](image)

**Figure 23**: The achieved hole depths in relation to the hole diameter: our results (red) and literature values (white).

### 3.2. III-V-semiconductor processing technology

Processing technology is a complex field because of the feature size of the fabricated structures, the demands in cleanliness and purity of the used substances and a relative lack of theory and simulation tools to model the processes. A lot of research is devoted to the structuring of semiconductors at nanometer scale, as the advancement of the whole computer industry depends on scaling towards miniaturization (Moore’s Law [108]). The physical processes involved in dry-etching (supply of etchants, reaction kinetics, desorption process and removal of reactants) are highly complex. Simple attempts to simulate the etching process have been made (e.g. in reference [109] for etching profiles and process latitudes in bombardment-induced reactive-etching processes.). However, a complete and general model of the reactive ion etching of InP and quaternary InGaAsP compounds – especially for high-aspect ratio structures – is still missing. Therefore conclusions are often based on assumptions and experiments. A theoretical model for large-area GaAs-etching with chemical assisted ion beam etching (CAIBE) can be found in reference [110] or [111]. However, these models are limited use for InP PhC etching, as they do not account for the special conditions of InP PhC etching, as e.g. the high aspect ratio, the high difference in mass between P (31u) und In (115u), and the low volatility of InP. For InP PhCs etching, a model is proposed in reference [112] by Berrier *et al.* The model is restricted to 1D (no lateral etching or changing hole diameter along the depth is considered) and includes

- the supply of etching gas to the bottom of the hole (molecular gas flow),
- the redeposition of etch products, the sputter yield of the In-compounds at the surface (InP and InClx, P is not considered in the model as it is sputtered away easily) and
- the coverage of the surface with these compounds.
Under this assumption, the rate of removal of the InP atoms is calculated. The model predicts qualitatively correctly the lag effects (subsection 4.1.1), and identifies the supply of etch species to the bottom of the hole and the desorption of the etch products as limiting factors. However, quantitative agreement cannot be expected by such a simple 1D approach and by so many unknown (or imprecisely known) model parameters. Although the model assumes a CAIBE system, the model also qualitatively agrees with lag effects observed in the ICP-RIE system.

In this section, we only give a very brief introduction into this field and limit ourselves to present only the basic knowledge necessary for the key fabrication steps for III-V compound semiconductor PhCs. A good introduction in processing in general is given by Sze [8]. The more interested reader is referred to the excellent textbooks of Sugawara [9].

Key fabrication steps for III-V-semiconductor with respect to PhC fabrication are:

- **Resist coating and patterning.** Only focused ion beam (FIB) [113] patterning is capable to directly (mask-less) structure a semiconductor. As this technique is not capable of fast and cheap patterning, the mostly-used patterning technique is *(deep-UV) optical or electron-beam lithography* (Figure 24 step C-F).

- **Deposition and patterning of dielectric.** Resists are usually organic materials, which provide not sufficiently etch-resistance to be used directly as a mask for the semiconductor etching. To overcome this deficiency, an intermediate, more resistive hard mask must be used, which is patterned by the resist and will be used as a mask to pattern the semiconductor subsequently. This intermediate hard mask consists in our case of silicon nitride, but silicon oxide is also often used.

- **Semiconductor etching.** The horizontal structuring of the semiconductor is normally achieved by etching, with the help of a patterned hard mask. The
3. Etching of deep holes in InP for photonic crystals

The etching process of semiconductors will be discussed in detail in section 3.2.2 (Figure 24, step H).

3.2.1. Electron-beam lithography

3.2.1.1. Advantages of electron-beam lithography

The vast majority of semiconductor devices are patterned by optical lithography, where a light-sensitive resist layer on top of the semiconductor is partly exposed to light (Figure 24 step C-F). The performance of any exposure method can be characterized by three parameters: Resolution, alignment precision and throughput. While optical lithography performs well with respect to throughput, it fails with respect to resolution and alignment precision at moderate costs because of the limiting wavelength of the light. This is a major handicap for PhC fabrication. Deep-UV lithography pushes the limit downwards, but remains still significantly higher than the achievable resolution of electron beam lithography.

The most flexible method of choice for PhC fabrication is therefore electron-beam lithography (EBL). Instead of photons with a large wavelength, high-energy electrons are used. The EBL writes the structures sequentially. A beam of accelerated electrons is focused directly towards the sample by electric and magnetic forces. Electrical fields extract the beam and steer it across the surface of the sample and draw the desired pattern directly in the resist, without a mask. EBL clearly beats the optical lithography in terms of resolution. The DeBroglie-wavelength \( \lambda_{DB} \) of electrons is orders of magnitudes smaller. Then, for our 30kV-EBL system, a single electron has a wavelength sufficient small for our purpose:

\[
\lambda_{DB} = \frac{h}{p_e} = \frac{\frac{h}{\sqrt{2m_eE_e}}} {\sqrt{\frac{m_e}{E_e}[\text{keV}]}} = 0.007\,\text{nm}
\]

with the Planck’s constant \( h=6.63\cdot10^{-34}\,\text{m}^2\cdot\text{kg/s} \) and \( p_e, m_e \) and \( E_e \) the impulse, mass and energy of the electron, respectively. Therefore the resolution of the EBL is not limited by the wavelength of the electrons, but by technical limitations of the EBL (~2nm for the used EBL system, caused by the minimal focused diameter of the electron beam). However, in terms of throughput, the EBL is not the method of choice. As the structures are written sequentially, exposure time for one single wafer ranges from a few minutes up to several days. Although this long time is acceptable for research, it is a major shortcoming that needs to be solved for industrial mass fabrication.

The physical process behind EBL is the modification of the resist by the electron irradiation. Some resists like PMMA consist normally of very long chains of organic base modules. Figure 25 for example presents the chemical composition of the resist PMMA (Polymethylmethacrylate, \( \text{C}_5\text{O}_2\text{H}_8\text{n} \)). The long chains are broken into smaller sections by the electron beam irradiation, which are now more easy soluble in the developer liquid than the unexposed long chains.
3.2.1.2. Proximity effect correction

The key requirement to achieve high accuracy with EBL is the control of proximity effects by proximity effect correction (PEC). PEC is discussed in depth in the literature [1, 93, 95] and only a brief explanation of the basics is given here. Proximity effects arise from additional exposure of the resist by backscattered electrons from the substrate. A point exposure at position $\bar{x}_0$ deposits energy ($forward$ exposure dose) in the resist in a pattern that is in the horizontal plane ideally a 2D-dirac delta function

$$E(\bar{x})^{ideal}_{forward} = \delta(\bar{x} - \bar{x}_0),$$

(3.2)

more realistically however a narrow gauss-shaped peak

$$E(\bar{x})_{forward} = a \cdot \exp \left( \left| \bar{x} - \bar{x}_0 \right|^2 / \alpha^2 \right)$$

(3.3)

with a full width at half maximum (FWHM) $\alpha$ of a few tens of a nanometer (Figure 26, blue).

The high-energy electrons are scattered in the resist (forward scattering) and the underlying substrate (backward scattering) and partly backscattered into the resist again. These additional backscattered electrons give rise to an spatially broadened energy deposition in the resist ($background$ exposure dose). The backscattered exposure pattern is again well approximated by a broad gauss-shaped function

$$E(\bar{x})_{backward} = b \cdot \exp \left( \left| \bar{x} - \bar{x}_0 \right|^2 / \beta^2 \right)$$

(3.5)

with a FWHM $\beta$ of several micrometers (Figure 26, red). More complex functions to describe the energy deposited by the backscattered electrons are presented in reference [93] or [114]. The total deposited energy dose is the sum of both contributions:
3. Etching of deep holes in InP for photonic crystals

\[ \text{E(} \bar{x} \text{)} = \text{E(} \bar{x} \text{)}_{\text{forward}} + \text{E(} \bar{x} \text{)}_{\text{backward}}. \]

If the deposited energy in the resist exceeds a threshold value (the clearing dose), it is dissolved during development and this location is exposed for further etching.

Now let’s consider a fixed point in the resist. The total deposited energy at this point is the convolution of the exposure dose pattern \( D(\bar{x}) \) with the energy distribution function \( E(\bar{x}) = E(\bar{x})_{\text{forward}} + E(\bar{x})_{\text{backward}} \), and is therefore also depending on the surrounding structures:

\[ E_{\text{deposited}}(\bar{x}) = \int D(\bar{y}) \cdot E(\bar{x} - \bar{y}) \, d\bar{y}. \] (3.6)

As a good approximation, the exposure of an array of circles can be treated as an array of point exposures located in the centers of the circles. The amount of energy deposited in these points directly influences the hole radius [1]. To achieve a homogeneous hole size over an array of holes,

- the parameters for the forward and backward scattering (a, b, α and β in the example above) have to be determined for the particular resist and substrate material system. Methods for that are presented in the literature [95].

- the exposure dose pattern \( D(\bar{x}) \) has to be found in order to achieve a homogeneous energy dose \( E(\bar{x}) \) at all holes. The solution for the exposure dose pattern \( D(\bar{x}) \) is usually found with complex software products, like the software nanoPECS [115], developed by the Electronics Laboratory, ETH Zurich, and Raith GmbH.

Mastering the two above-mentioned tasks enhances the accuracy of the nominal hole patterning significantly. An improvement in hole-diameter uniformity by PEC from 6.2% hole-size variation for an uncorrected generic design to as low as 1.4% for a PEC-corrected generic design can be achieved [1, 116].

### 3.2.1.3. Alternatives to electron beam lithography

Although of minor interest so far, other methods for the patterning of a semiconductor for PhCs should also be mentioned.

- **Optical interference lithography** [117] uses the interference of several coherent light beams to create a periodic (interference) pattern in a light-sensitive resist. This technique is fast, and allows for patterning of large areas. Introducing local changes in the pattern to create local functionalities (e.g. waveguides) is hardly possible.

- **Nano-imprint patterning** [40, 118, 119] uses a mold that is pressed into a soft resist layer to create patterns. The flexibility of this technique is however worse than that of EBL.

- **Focused ion beam milling** [113] (FIB) allows the direct fabrication of the PhC holes in the semiconductor and therefore the same flexibility as EBL. The
3.2 III-V-semiconductor processing technology

throughput of such an equipment is worse, as the hole milling is much slower than the hole exposure by EBL. As a consequence, it is rather used to post-process PhC devices by locally modify single holes in the final device.

- **Deep UV patterning** (DUV) is still not used for PhC at the telecom wavelength, as its resolution (~300nm for the equipment available in our lab) is still too high. However, by even reducing the wavelength further to extreme ultraviolet (EUV) [120], it might become possible in future to commercially expose PhC devices for mass-fabrication.

### 3.2.2. Plasma etching

Etching is the technology to pattern a semiconductor at the nanometer scale. The atoms of a semiconductor are selectively removed where they are not protected by an appropriate mask. In this section, a brief summary of plasma etching is given. For details, the reader is referred to [9].

Two different principles of etching are employed in the semiconductor industry: **wet etching** and **dry plasma etching**. Advantages and disadvantages are presented in Table 6. Photonic crystals are high-aspect ratio structures with a very small feature size, therefore only dry etching can be used to fabricate them. For the remaining part of this section, only dry- or plasma etching process is considered. Dry etching and plasma etching are used as synonyms in this work.

<table>
<thead>
<tr>
<th>Feature</th>
<th>Wet etching</th>
<th>Dry plasma etching</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material selectivity</td>
<td>High</td>
<td>Low</td>
</tr>
<tr>
<td>Anisotropy</td>
<td>Low&lt;sup&gt;11&lt;/sup&gt;</td>
<td>High</td>
</tr>
<tr>
<td>Minimal feature size</td>
<td>Large</td>
<td>Small</td>
</tr>
<tr>
<td>Surface quality</td>
<td>High</td>
<td>Low</td>
</tr>
<tr>
<td>Crystal damage</td>
<td>Low</td>
<td>High</td>
</tr>
<tr>
<td>Homogeneity</td>
<td>Low</td>
<td>High</td>
</tr>
<tr>
<td>Equipment</td>
<td>Simple, cheap</td>
<td>Complex, very expensive</td>
</tr>
<tr>
<td>Material removal</td>
<td>Chemical reaction with the liquid</td>
<td>Chemical reaction with ions, radicals and physical removal by ion bombardment</td>
</tr>
<tr>
<td>Etchants supplier</td>
<td>Liquid acid</td>
<td>Plasma and gas</td>
</tr>
</tbody>
</table>

**Table 6**: Differences between wet- and dry etching according to [121]. The key features for PhC fabrication are highlighted with bold fonts.

### 3.2.2.1. Plasma for dry-etching of semiconductors

A plasma is a partially ionized gas mixture consisting of equal numbers of electrons and ions, together with neutral particles. The free charges are created by high-frequency field discharge, created by a capacitor-electrode in the gas. Only every 1’000<sup>th</sup> to 10’000<sup>th</sup> atom is ionized in plasmas typically used for the etching of semiconductors [9].

<sup>11</sup> High anisotropy with wet etching can be achieved for crystal-orientation selective wet etching. However, such an approach is not considered for round PhC holes.
The plasma is ignited in the process chamber of the etching tool (Figure 27). The charged particles may come in contact with the metallic chamber walls and are neutralized (ions) or absorbed (electrons). Due to the much lower atomic weight, the negatively charged electrons move faster over longer distances and are absorbed more readily than ions are neutralized by the chamber wall. This creates a positively charged plasma in the center of the chamber and builds up a space-charge in the plasma and thus a voltage between the chamber walls and the plasma (the so-called DC-bias). As the plasma itself is a good conductor thanks to the free electrons, most of the voltage drops across the sheath region [121] close to the chamber walls, where the charge carriers are depleted. This voltage is typically in the order of several 100V, depending on the plasma conditions (mainly pressure and RF-power).

![Figure 27: Schematic of a plasma discharge. A neutral layer between the positively charged plasma and the chamber walls is built up by the plasma itself, referred as sheath.](image)

The electric field between the plasma and the chamber walls is responsible for accelerating the ionized atoms or molecules towards the sample. Due to the homogeneous electric field, they hit the surface at almost normal incidence.

### 3.2.2.2. Plasma etching of semiconductors

In plasma etching, the patterning of the semiconductor is achieved by partly covering the surface with a mask material that protects the underlying semiconductor from sputtering or chemical etching. Commonly used mask materials are (organic) resists, metals (e.g. chromium or nickel) or dielectrics (e.g. SiNₓ, SiOₓ, AlOₓ). The semiconductor together with the mask is exposed to the plasma, and in the unprotected parts, the semiconductor material is removed. After etching, the mask is normally removed by solvents (resists) or highly selective wet etching (metals, dielectrics). Good mask materials must fulfill the following properties:

- The mask material must be easy to pattern. For resists, this requirement is fulfilled in a straight-forward way. In the case of a metal mask, the patterning is usually achieved by a lift-off process [8], as a good chemistry to selectively dry-etch metals against a photoresist mask is hardly available.

Dielectric masks are themselves normally patterned with another dry-etching step and a resist mask (Figure 24 step G).
• The mask must *withstand the etching plasma* during the subsequent semiconductor etching (high selectivity of the plasma against the mask).

• The mask must be *easily removable after dry-etching*. Ideally, an acid that only attacks the mask (e.g. HF for dielectrics on InP/InGaAsP) but not the semiconductor must be available.

As shown in section 3.3.1, only dielectric masks are usable for our purpose. Resists are not stable enough to survive the harsh conditions in the plasma chamber, and metals get easily attacked by the chlorine present in the etching plasma.

During plasma etching, the masked surface of the semiconductor is exposed to a low-pressure neutral gas of molecules and radicals and to a bombardment of ionized atoms or molecules with almost vertical incidence. The combination of the neutral gas and the accelerated ions is responsible for the etching of the semiconductor. Different reactions with the semiconductor may occur (simultaneously) during etching:

A) *Physical sputtering*: The ions in the plasma are accelerated by the electric field in the sheath. They hit the semiconductor material at high kinetic energy (in the order of a few hundred electronvolts, \( E_{\text{kin}} = \text{ion charge} \cdot \text{DC-bias} \)), and can physically remove other atoms with low binding energy. Pure sputtering is rarely used, as this technique is slow, has low selectivity and sloped sidewalls due to sidewall shadowing (shielding of the non-perpendicular impinging ions by the sidewalls, preventing them to reach the bottom of the etched surface) [122].

B) *Pure chemical etching*: The plasma is able to deliver reactive species (atoms, molecules or radicals). They diffuse to the surface and react spontaneously with the semiconductor, to form a highly volatile product that is desorbed from the surface (e.g. \( \text{In}^3+3\cdot \text{Cl}^+ \rightarrow \text{InCl}_3-3e^- \)). The pure chemical etching – apart from crystal orientated etching – is isotropic. Because of the chemical reaction, the etching is however very selective against different materials (e.g. mask material, or different semiconductor quaternary layers).
C) *Ion enhanced energetic chemical etching:* Similar to pure chemical etching, the material removal is based on a chemical reaction with an etchant to form a volatile product. However, the reaction might not initiate spontaneously at sample temperature. Additional energy for the reaction has to be delivered from the kinetic energy (in the order of a few hundred electron volts, $E_{\text{kin}}=\text{ion charge} \cdot \text{DC-bias}$) of directed impinging ions. Therefore, in contrast to purely chemical etching, the etching is anisotropic. Because of the chemical reaction, the etching is very selective against different materials.

D) *Inhibitor driven ion assisted etching:* Etchants not only etch the semiconductor, but might also form a protective film on the surface (e.g. polymer-formation in a CH$_4$-containing plasma), either directly or after they undergo a reaction with the semiconductor. On horizontal surfaces, the film is continuously removed by kinetic ions. On steep sidewalls, however, the protective film remains, preventing lateral etching. Highly vertical sidewalls can be achieved by this sidewall passivation [99] by a delicate balance between etching and inhibition.

The contribution of each etching mechanism to the total removal of the semiconductor depends on the chemical composition of the plasma, the pressure, and the kinetic energy of the ions. By carefully balancing the contributions, vertical profiles and high selectivity against the mask can be achieved.

### 3.2.2.3. Plasma etching systems

Several different plasma etching systems have been reported and are currently used for the fabrication of PhCs:

- **Chemically assisted ion beam etching (CAIBE).**
  This method uses a parallel beam of ions accelerated towards the sample, together with a neutral gas, to etch the semiconductor. Several articles [83, 101, 102] report the use of the gas combinations Ar (ions) and Cl$_2$ (neutral gas). An excellent hole depth of around 4μm [101] was achieved.

- **Inductively coupled plasma reactive ion etching (ICP).**
  A whole range of different chemistries are reported for PhC etching:
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- SiCl₄ resulting in a hole depth of over 4.5 μm [107],
- SiCl₄ [107],
- Cl₂/O₂ [47],
- Cl₂/Xe [123] or
- Cl₂/Ar/N₂ [106]

Also methane-containing CH₄/Cl₂/H₂ [124] plasmas are used. Their application is however restricted to membrane-type PhCs, as deep hole etching is much more difficult than with chlorine based plasmas due to their high selectivity against quaternary materials and the strong tendency to form polymer films.

- Electron cyclotron resonance (ECR).
  This technique is also employed for PhC fabrication. For membrane PhC, a CH₄/H₂/Ar chemistry [125] can be used. For high aspect-ratio etching, the use of Cl₂/Ar is reported [103, 104].

Except for the record value from Kotlyar et al., [81, 101] all reported values are of similar depth (Table 5). However, the record value obtained by CAIBE-etching [81] let us conclude that CAIBE is slightly superior to the other systems with respect to PhC fabrication.

In our own case, we use an Oxford Plasmalab 100+ ICP-RIE system to pursue our goal to etch deep holes into the semiconductor. CAIBE and ECR-RIE were not available for our purpose. The number of suppliers for such a commercial ICP-RIE dry-etching systems is high[12]. However, the basic building blocks of are always the same:

- A vacuum chamber for the plasma, with a pump system and a pressure control. The reactants need to be removed from the chamber by continuous flushing the chamber with fresh gas.
- A (heatable) stage to hold the sample inside the chamber. Depending on the equipment, the stage comprises a heating and/or cooling system.
- A gas supply system with different gas sources.
- An RF-power generator to ignite and maintain the plasma in the chamber. A conventional plasma etching system (reactive ion etching system, RIE) couples the RF-power over a plate capacitor arrangement between stage and chamber walls into the plasma.
- More sophisticated inductively coupled plasma RIE (ICP-RIE) systems have an additional coil around the camber to couple power also inductively into the plasma. The additional power source allows adjusting the plasma density and the DC bias voltage independently and gives more flexibility during process optimization.

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3. Etching of deep holes in InP for photonic crystals

In this work, an ICP-RIE Oxford Instruments Plasma Technology System 100 with a head 180 is used. A sketch of the chamber system is shown in Figure 28. Our system is equipped as follows:

- Temperature controlled stage with a range from –150°C to 400°C for up to 4” wafers
- Available Gas sources:
  - For chemical etching: CH₄, H₂, Cl₂
  - For physical etching: Ar
  - For sidewall passivation: N₂
  - For chamber cleaning: SF₆, O₂
- A pumping system to achieve pressures down to 1mTorr during processing.
- RF power source: 500W at 13.56 MHz
- Inductively coupled plasma power source: 3000W at 13.56 MHz

This system is capable to etch InP and its quaternary material with etch-rates up to several micrometers per minute, with a high anisotropy on large-scale structures. For the etching of PhCs, a high aspect ratio process is required. Its development and characterization is presented in the next sections.

![Figure 28: Schematics of a plasma reactor used in this work.](image)

3.3. Mask fabrication for the etching of photonic crystals

This chapter summarizes the fabrication of the mask for the subsequent plasma etching. The detailed investigation about our hard-mask fabrication process can be found in reference [1].

3.3.1. Mask material

At the beginning of the development of a hard mask, the large number of different available mask materials must be restricted to promising candidates, based on experience and literature. Three categories of mask materials are available. They are listed together with their advantages and disadvantages below and in Table 7.
3.3 Mask fabrication for the etching of photonic crystals

- **Photoresists** and **electron beam resists** are very convenient mask materials, as they allow for direct patterning by lithography. Only electron beam lithography is suitable for high-resolution patterning. Optical lithography is limited by the wavelength of the exposure light. The drawback of these resist systems are the very low resistivity against etching plasmas and the instability at high temperatures.

- **Metals** as an etch mask are more suited for plasma reactors at high temperature (a few 100°C). Metals need be patterned either
  - by chemical etching. Not all metals allow for their chemical etching (e.g. gold). Others can be chemically etched, but suffer from a low resistivity against chlorine (e.g. titanium) which is used for semiconductor etching.
  - by physical sputtering in the plasma reactor, resulting in a low selectivity of the photoresist against the metal mask.
  - by lift-off techniques, what results in a challenging process. Very small pieces of metal need to be lifted off which results in a difficult mask patterning process.

This makes most metals unsuitable as a mask material for etching InP-related materials.

<table>
<thead>
<tr>
<th>Material system for the mask</th>
<th>Dielectrics</th>
<th>Metal</th>
<th>Photoresist</th>
<th>EBL resist</th>
</tr>
</thead>
<tbody>
<tr>
<td>Example</td>
<td>SiNₓ, SiOₓ</td>
<td>Cr, Ni</td>
<td>AZ series</td>
<td>PMMA, ZEP</td>
</tr>
<tr>
<td>Mask material deposition</td>
<td>PECVD (PVD)</td>
<td>PVD</td>
<td>Spin-coating</td>
<td></td>
</tr>
<tr>
<td>Pattern creation/writing</td>
<td>Indirect by dry-etching</td>
<td>Indirect by lift-off-technique or dry-etching</td>
<td>Direct exposure and development</td>
<td></td>
</tr>
<tr>
<td>Fabrication process for the patterning of the mask</td>
<td>Etching Lift-off</td>
<td>Mask aligner</td>
<td>Electron-beam lithography</td>
<td></td>
</tr>
</tbody>
</table>

| Small feature size | Yes | Yes | No | Yes |
| Resistivity against Cl₂ | Yes | No | No | No |
| Temperature stability | Yes | Yes | No | No |
| Selective removal against InP | Yes | Yes | Yes | Yes |

**Table 7**: Requirements for a mask for semiconductor etching, and degree of performance of different classes of mask materials with respect to these requirements.

---

13 PVD: Physical vapor deposition.
• **Dielectrics** fulfill all requirements for a hard-mask material for semiconductor etching using chlorine-based plasma. Dielectrics are stable up to high temperatures, and withstand chlorine relatively well. However, they need an additional patterning step either by dry etching or lift-off. Dielectrics are normally deposited by plasma-enhanced chemical vapor deposition (PECVD). As this technique deposits the material isotropically on the wafer surface, patterning by lift-off techniques is not possible.

No single mask material does fulfill all requirements for a mask for semiconductor patterning. Therefore only a combination of two mask materials will be a successful approach. Obviously, the best choice is a layer stack of an **electron beam resist** together with a **dielectric hard mask**. PMMA 950k was used as electron beam resist. With the available equipment in FIRST lab, silicon nitride (SiNₓ), silicon oxide (SiOₓ) or silicon oxinitride are candidates for a hard-mask. We have chosen silicon nitride (SiNₓ) as hard-mask material. Preliminary etch tests have shown that SiNₓ is slightly superior to SiOₓ with respect to stability against our used semiconductor etching plasma. In literature, both SiNₓ and SiOₓ are commonly used as mask materials, as there is no clear advantage of one of the dielectrics, and depending on the used semiconductor etching plasma, either of both might withstand the etching better.

SiNₓ is deposited by an Oxford Instruments Plasmalab PECVD System 80. As precursors, hydrosilicon SiH₄ and ammonia NH₃ are used. We performed a coarse optimization of the deposition conditions (sample temperature, plasma pressure, plasma power and chemical composition). Only a higher silane content than in the standard process in the plasma improves the etch resistivity against the semiconductor etching plasma. Therefore, only the silane flux was increased by 100% with respect to the machine’s standard deposition parameters and further optimization was not pursued. We have evidence that the higher silicon content of the SiNₓ enhances the resistivity of the dielectric against sputtering, as silicon has a higher atomic weight than nitrogen.

### 3.3.2. Resist patterning

In our work, a 210nm thick PMMA 950k (Polymethylmethacrylat, (C₅O₂H₈)n, Figure 25) layer is used [1]. The resist layer thickness is a trade-off between maximal thickness and patterning accuracy. The exposure of the holes is performed on our Raith150 EBL system, with a maximal 30kV acceleration voltage. The patterning accuracy is limited by increased forward scattering of the electron beam in thick resists [1]. This limitation can only be avoided by higher acceleration voltage (100kV). The design is proximity corrected [93] prior to writing. The proximity parameters have been determined using the doughnut method [95]. The resist is developed in methyl-isobutylketone (MIBK) and isopropyl alcohol 1:3 mixture at 21°C for 65sec. This mixture is known [126] to provide excellent resist contrast.

---

14 The standard process for SiNₓ was proposed by the equipment manufacturer.
The issue of PhC hole disorder-induced (random fluctuations of the hole position $\delta x$ and hole radius $\delta r$ around their target value) losses arises when patterning of the mask is discussed. Luckily, in substrate-type PhCs, disorder-induced losses are negligible compared to intrinsic losses, as long as the standard deviation of the disorder is below $\sigma(\delta x)/r<6\%$ and $\sigma(\delta r)/r<3\%$ for position and hole radius, respectively [1] (whereas $r$ is the hole radius, $\delta x$ is the deviation in hole centre placement and $\delta r$ the deviation in hole radius). These limits are well fulfilled for our fabrication process [1], and thus these losses must not further be considered.

### 3.3.3. Pattern transfer into the hard-mask

Pattern transfer from the PMMA resist-layer into the SiNx hard-mask is the last step prior to semiconductor ICP-RIE etching. Maximal etch selectivity between the resist mask and the SiNx and high pattern transfer fidelity is required. The process itself is described in-depth in the thesis of R. Wüest [1] and only summarized here. The basic etching steps are depicted in Figure 29.

The etching process described in [1] is capable of transferring holes with a diameter as low as 150nm from the 210nm PMMA resist into 400nm of silicon nitride. Lag effects (aspect-ratio dependant etch rates) [96] play an important role in dry etching. As a result, large openings (large holes) in the resist are substantially overetched. To achieve the desired aspect-ratio and selectivity, several improvements towards a standard etching recipe were necessary:

- Between the PMMA and the SiNx, an intermediate 30nm thick titanium (Ti) layer is introduced. This layer helps
  1) to avoid charging during EBL writing, and
  2) enhances the overall etching selectivity.

Although special care is taken to avoid the oxidation of the Ti surface, a thin TiOx layer is unavoidably formed. Such a layer is too inert for chemical etching. For removal, an initial argon sputtering step is therefore introduced (Figure 29, B). The bare Ti is then chemically removed by dry-etching with a SF6/N2 plasma (Figure 29, C). During this step, also most of the initial PMMA has been consumed by the plasma, however ideally a thin layer of PMMA still remains after the completion of the Ti etching step.

- The SiNx etching itself is a cyclic process based on a CHF3/O2 chemistry. An etching cycle typically lasts for 30sec. 90sec flushing time is introduced between two cycles (Figure 29, D). The flushing cycle gives time to the etchants and reactants sticking on the surface to evaporate and for the Ti to rebuild the hard TiO2 [92]. This procedure also avoids excess polymer formation. 14 cycles are typically required for a mask thickness of 400nm.
3. Etching of deep holes in InP for photonic crystals

All these steps are performed without opening the reactor chamber. The resulting mask holes are presented in Figure 30. Hole aspect ratios in the SiNx over 1:2.5 are obtained, which allows the etching of sufficiently small and deep holes to fabricate useful PhCs.

3.4. Hole etching for photonic crystals in InP/InGaAsP/InP*

Once the hard mask is patterned, the task of structuring the semiconductor can be tackled. The goal is obvious: Etching holes into the semiconductor that come as close as possible to perfect, infinitely deep cylinders. The array of holes has a typical lattice constant of 450nm and a hole diameter of 150-300nm. The hole depth must be more than 2.5μm to penetrate the whole vertical light mode profile over its vertical extend. To achieve the goal, the full range of process parameters of the etching system must be optimized.

3.4.1. Etching chemistry

3.4.1.1. Etching chemistry and sample temperature

It is striking that almost all research groups working on deep hole etching in InP use chlorine-based chemistries, in combination with a neutral (Ar or Xe) element (Table 5). The addition of methane is hardly used for PhC etching, although it is a standard
etching gas for InP [127]. The high selectivity of InGaAsP against InP when using methane makes the etching of the core-layer difficult (low selectivity against the hard-mask). Indeed, we measure a selectivity of 1:4 [128] when using CH$_4$/H$_2$/Ar, which makes high aspect-ratio etching very difficult. We therefore focus on the investigation of the Cl$_2$-based chemistry. As we will see later, the addition of nitrogen is mandatory to prevent undercutting by sidewall passivation. Table 8 lists the different contributions of the gases to the etching process.

<table>
<thead>
<tr>
<th>Material</th>
<th>Process</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorine (Cl$_2$)</td>
<td>Chemical etching</td>
<td>Removes In by forming InCl$_3$. InCl$_3$ is only volatile at elevated (&gt;100-200°C) temperatures.</td>
</tr>
<tr>
<td></td>
<td>Physical sputtering</td>
<td>Sputter yield of chlorine is nearly as good as Ar (same atomic weight)</td>
</tr>
<tr>
<td>Argon (Ar)</td>
<td>Physical sputtering</td>
<td>Reduces the selectivity</td>
</tr>
<tr>
<td>Nitrogen (N$_2$)</td>
<td>Surface passivation</td>
<td>Prevents undercutting below the mask</td>
</tr>
</tbody>
</table>

Table 8: Overview over the different reactions of the etching plasma with the substrate.

For chlorine-based etching, the most critical aspect is the desorption of InCl$_x$ from the InP surface, because it has a very low volatility due to a high melting point (583°C at normal pressure [129], 224°C around process pressure (1mTorr) [130]). For the efficient removal of the etching products, an elevated temperature of the sample is therefore required. To supply the sample surface with the required energy for InCl$_3$ evaporation, different heating methods can be considered:

- Most straightforward is a heating stage. A heating inside the stage delivers the required energy [83, 103, 131-134]. A special solution is an intense halogen lamp as a heating source [48].

- It is possible to supply the energy for the InCl$_x$ evaporation by the plasma itself. If thermal contact to the (cold) stage is weak, the ion bombardment by the plasma can sufficiently heat the surface. Although in this case the stage is reported to be at room temperature, the actual chip surface temperature is estimated to be several 100°C, sufficiently for the InCl$_x$ evaporation [104, 135]. However, the heating only by the plasma is not favorable:
  - The heating by the plasma requires a dense plasma and a high DC-bias voltage, to provide sufficient energy to the sample. This imposes limitations to the usable parameter space.
  - The heating is dependant on the process parameter and process duration, and cannot be controlled independently.
  - The heating is irreproducible, as the thermal contact between wafer and stage is not under control, and therefore different from run to run.

We have used a heating stage to study the influence of the substrate temperature on the morphology of the etched surface of the InP at different stage temperatures for a
Cl₂/CH₄/H₂ chemistry. The temperature is measured in-situ by a thermocouple in the stage under the carrier wafer. The chip backside has almost the same temperature as the stage, although some additional heating of the exposed wafer surface from the plasma occurs. Figure 31 presents the etch rate and the surface morphology for the same etching process at different stage temperatures. The higher etching rate at higher temperature comes along with a smoother surface, as less InClₓ remains on the surface and leads to micromasking. Aware of the difficulties to evaporate InClₓ, we conclude that the sample heating is indeed crucial for the etching process. The surface becomes smooth above about 180°C.

![Figure 31](image)

**Figure 31:** Etch rate and etched surface morphology of InP vs. temperature for large-area etching for a Cl₂/CH₄/H₂ chemistry. The temperature is measured by a thermocouple in the stage. The insets show the etched surface for the corresponding temperature. All images are of the same scale.

### 3.4.1.2. Sidewall passivation

As it will become evident later, sidewall passivation by e.g. nitrogen [106] or oxygen [47] addition is important when working with a „pure“ chlorine plasma without methane addition. The sidewalls of the holes need to be passivated from the aggressive chlorine gas, to avoid undesired undercut by chemical etching.

- **Methane** is a good passivation. It directly protects the surface by forming a polymer film [127] and preventing the chlorine molecules to react with the InP. The film is formed at the bottom and sidewalls of the etched areas as well as on the hard mask. On the InP surface, the polymer formation is in direct competition with etching of InP \((\text{In}^+3\cdot\text{CH}_3^+\rightarrow\text{In}((\text{CH}_3)_3^-\cdot3\cdot\text{e}^\cdot))\).

- **InCl₃** is also capable to form a passivation film, although its strength is strongly dependent on the sample temperature. The process window for the optimal temperature for passivation is unfortunately very small and therefore difficult to keep under control.
• **Nitrogen** is known to form N-P bonds with the phosphorous of the InP [136, 137]. This bonding can be used to prevent the In from reacting further with the chlorine and, therefore, to passivate the surface.

• **Oxygen** addition is reported by Carlström *et al.* [47] to be used to passivated the surface. However, they do not report about the mechanism for passivation. We speculate that the oxidation of the surface prevents lateral chemical etching.

Due to the high selectivity of methane against InP and the difficulties with the temperature control, we decided to use nitrogen as a passivation element in our etching plasma. It does not chemically react with the semiconductor. To avoid additional passivation by InCl₃, the temperature (200°C) is chosen above the vapor pressure of the InCl₃.

### 3.4.2. Experimental method for the coarse process optimization

We start this section with an introduction to the *design of experiment* method (DOE) proposed by Taguchi [138]. Originally developed for completely different applications, the method is also used to optimize the etching process. The interested reader is referred to reference [139], where the application of this method to process optimization is explained in detail. A short introduction to the basic idea of this method is given in the following section.

The generic problem of dry-etching process development is the optimization of a set of variable input parameters of the etching process (power, pressure, gas composition, temperature, etc.), so that the etched structure is optimized with respect to one or several¹⁵ quantitative figures of merit (e.g. hole depth, sidewall angle, surface roughness).

---

¹⁵ The method can only optimize for one figure of merit. If several figures of merit are of interest, one can either (i) optimize all parameters independently, and then manually trading-off the process (e.g. hole depth, hole shape, hole sidewall roughness), or (ii) calculate one “master figure of merit” from the individual figures of merit, if possible (e.g. “optical propagation loss” as a function of hole depth, hole shape, hole sidewall roughness).
3. Etching of deep holes in InP for photonic crystals

and minima and maxima might be missed. Right: The DOE method selects only a sub-sample of the data points from the discrete parameter space (middle), and constructs the missing results from statistical assumptions.

Input parameters are normally continuous parameters (or the spacing of the parameters is fine enough that they can be assumed to be continuous). To determine the complete relation between the input parameters and the figure of merit, an infinite number of experiments needs to be performed (Figure 32, left). As this is of course unpractical, only discrete (and often equidistant) parameter values for each input parameter are chosen. The brute-force method to optimize the fabrication process performs the experiments with all possible combinations of parameter values. However, trying out all these combinations systematically is still beyond the capacity of the plasma etching tool and its operator (Figure 32, middle). On the other hand, random selection of a (small) subset of experiments to reduce the effort don’t lead to the optimization goal either.

There the DOE method helps to reduce the number of necessary experiments systematically. The DOE uses statistical methods to select an optimal subset (Figure 32, right) from all different parameter combinations, which allow then to extrapolate or predict the result from the other parameter combinations. Only a brief introduction into the basics is given here; the interested reader may refer to [138, 139]. To find a representative subset is complicated, but luckily there are so-called orthogonal tables available (e.g. in reference [139] or on the internet [140]) which allow us to select the best subset. Such a table guarantees that all parameter values of all parameters are used equally frequently enough in the subset, and that the subset is of minimal size.

Let \( f(p_1, p_2, \ldots, p_n) \) be the figure of merit (e.g. etch depth or selectivity) as a function of the individual input parameters \( p_i \) (e.g. ICP power, \( \text{Cl}_2 \) flux). To extract the contribution of an individual parameter \( p_i \) to the figure of merit \( f \), an averaging over all the other parameters \( p_{i\neq j} \) according to equation (3.3) is calculated.

\[
\bar{f}_{p_i}^j(k) = f(\ldots, p_i = k, \ldots),
\]

where \( k \) are the parameter values for the parameter \( p_i \) and \( \bar{f}_{p_i}^j(k) \) denotes the dependence of the figure of merit on the parameter \( p_i \). Performing this averaging for each parameter value \( k \) gives us the relation \( \bar{f}_{p_i}^j(k) \). Repeating this operation for all input parameters \( p_i \), we obtain the impact of each parameter, as shown in Figure 34, Figure 35 and Figure 36.

Using DOE to speed up process development is simple. However, some drawbacks should not be concealed:

- The quality of the results depends on the sampling of the parameter values. A too large difference of the parameter levels may miss a maximum between two

---

16 The number of experiments \( n \) is equal to \( n=p^m \), where \( p \) is the number of discrete parameter levels, and \( m \) the number of parameters.
levels, and a too fine choice may result in an optimum outside of the investigated parameter range. To avoid such a failure of the DOE experiment, general experience of the process should be available for the choice of meaningful input parameter levels.

- The DOE performs only a coarse optimization when the dependence between parameters is weak or insignificant. For fine-tuning of the process the interdependence between the parameters may no longer be ignored, and DOE is not longer applicable.

In our case, the DOE is applied to the optimization of the hole etching process. In the next section, we will present the design of the experiment and the results. After the coarse optimization using DOE, we present the required fine-tuning of the process parameters at the end of the section.

### 3.4.3. Application of the DOE method to photonic crystal etching

#### 3.4.3.1. Introduction

Based on considerations in section 3.4.1, we have decided to use a Cl$_2$/Ar/N$_2$ process for the fabrication of the PhC holes. The DOE method was used for the coarse optimization. For our application, we need to optimize the following input parameters:

- (Relative) Chemical plasma composition (determined by chlorine, argon and nitrogen flux),
- ICP power,
- RF power, and
- Chamber pressure.

The temperature is not considered here, as it was previously investigated (section 3.4.1.1). The most important figures of merit for hole etching process which need to be achieved simultaneously are:

- Maximal hole depth,
- Cylindrical hole shape, and
- Best surface quality, minimal surface roughness.

Additionally, we are also interested (but with lower importance) on the following characteristics:

- Etch rates of InP, InGaAsP and the mask (and their selectivity against each other)
- Sidewall angles of large-area structures
- Surface quality of large-area structures (bottom and sidewall)

The first row of Table 9 defines the chosen parameter levels for the DOE run we use for the coarse optimization. While keeping the Cl$_2$ flux constant$^{17}$, the pressure, the

---

$^{17}$ As only the partial pressures (relative fluxes) of the gas sources in the plasma are relevant for etching, we can keep the flux of one arbitrary source constant during the DOE.
ICP and RF power and the amount and the composition of the additional plasma components were varied. We have chosen to fix the Cl₂ flux and only optimize the relative chemical composition of the plasma by varying the nitrogen and argon flux. The relative chemical composition has a major impact on the etching results. In contrast, the absolute gas flux has an impact on the replacement of etchants in the plasma and on load effects\(^{18}\) and less on the hole shape or surface roughness.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Process parameters ranges and optimum</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cl₂ flux</td>
<td>DOE ranges 10 or 15 sccm</td>
<td>sccm</td>
</tr>
<tr>
<td>Total neutrals flux</td>
<td>around 7.1 sccm</td>
<td></td>
</tr>
<tr>
<td>% of N₂ in the neutrals</td>
<td>0%-100% around 30% around 2.4</td>
<td>% sccm</td>
</tr>
<tr>
<td>Ar flux</td>
<td>7-16 5 sccm</td>
<td></td>
</tr>
<tr>
<td>N₂ flux</td>
<td>7-16 around 2.1 sccm</td>
<td></td>
</tr>
<tr>
<td>He flux</td>
<td>0-15 sccm</td>
<td></td>
</tr>
<tr>
<td>ICP power</td>
<td>1000-2000 600 W</td>
<td>W</td>
</tr>
<tr>
<td>RF power</td>
<td>140-215 160 W</td>
<td>W</td>
</tr>
<tr>
<td>Pressure</td>
<td>3-6 2.2 mTorr</td>
<td></td>
</tr>
<tr>
<td>Stage temperature</td>
<td>200°C</td>
<td></td>
</tr>
</tbody>
</table>

Table 9: Ranges of the chosen process parameters for the DOE runs and the optimized parameters for the subsequent investigations. For the subsequent optimization, also parameter values outside the DOE ranges are considered, if the optimum of the DOE was found to be at one side of the range.

All figures of merit are qualified based on SEM micrographs, which have the advantage of providing a fast characterization technique compared to time-consuming optical characterization by e.g. the internal light source [58] or the endfire [28] techniques. However, they do not deliver loss figures for PhC waveguides but they provide an accurate three-dimensional picture of the exact hole geometry. The link between the extracted figures of merit for holes from SEM images and the loss values has to be verified later by a corresponding set of optical calibration experiments or with theoretical loss models [69, 70].

Obvious figures of merit in process development are InP and InGaAsP etch rates, mask etch rate and large-area sidewall angles. Therefore, we define for this investigation the following additional quantities

\[
\text{Mask selectivity} = \frac{\text{InP etch rate}}{\text{Mask etch rate}} \tag{3.7}
\]

\[
\text{Quaternary material selectivity} = \frac{\text{InGaAsP etch rate}}{\text{InP etch rate}} \tag{3.8}
\]

A high quaternary material selectivity makes it difficult to etch the holes through the core layer (e.g. with methane-containing chemistries [141]), leading to shallow holes.

\(^{18}\) Load effects will only be considered later (section 4.1.1) and not during the DOE run.
• All samples are etched for the same time duration. For less aggressive plasmas, not all mask material is eroded during the experiment and longer etching time and therefore deeper holes are finally possible. The extrapolated maximal etch depth (eMED)

\[
\text{eMED} = \frac{\text{Measured depth} \times \text{Initial mask thickness}}{\text{Etched mask thickness at the facet}}
\]

(3.9)

accounts for a possible longer etching time due to remaining mask material after the etching. Mask faceting (higher mask etch rates at the edge of the masked area, see Figure 33) is the limiting factor for the etching time. The eMED calculation has a limited depth accuracy of ±400nm as the measurement of the remaining mask thickness is difficult due to the mask rounding off at the facet. Mask faceting is most likely caused by strong ion bombardment. It can be reduced by lowering the DC-bias during etching or switching to metal masks [142]. This however causes other difficulties, so these possible improvements were not further pursued.

In addition, the etching rate for holes may slow down with increasing depth due to aspect-ratio dependent etch rates [96], which is also not considered for the eMED.

Surface roughness, hole shape and undercut [48] are quantified by comparing and ranking the SEM micrographs by visual impression, assigning “marks” (numerical quality ranking) to the image. The ranking does not deliver absolute values, only relative comparison between the different processes, which are, however, sufficient for the DOE runs.
3.4.3.2. Etching properties of a Cl2/Ar/N2 plasma for large-areas

We present here the etching results for large areas. They already give an insight into the etching mechanism of InP and its compounds. Large-area etching is required during the PhC devices fabrication for the access waveguide structures (trench waveguides).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>ICP power [W]</th>
<th>RF power [W]</th>
<th>Total neutrals flux [scm]</th>
<th>% of N2 in the neutrals [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sidewall angle</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Surface quality</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sidewall quality</td>
<td>✧</td>
<td>✧</td>
<td>✧</td>
<td>✧</td>
</tr>
<tr>
<td>InP etch rate</td>
<td>-</td>
<td>✧</td>
<td>✧</td>
<td>✧</td>
</tr>
<tr>
<td>Maximal achievable etch depth</td>
<td>-</td>
<td>-</td>
<td>✧</td>
<td>✧</td>
</tr>
<tr>
<td>Selectivity against the mask(^{19})</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 10: Influence of the process parameters on quantities of interest for large-area etching. Up ✧ or down ✧ arrows indicate a larger parameter value to be beneficial or detrimental, respectively. The number of arrows relates to the strength of the trend. For the sidewall angle verticality is optimal. Therefore ✧ ✧ means that higher parameter values lead to a smaller/larger angle between the sidewall and the vertical direction. From the trends, it is obvious that a pure Cl2 process is optimal for large-area etching. A dash (-) indicates that no significant influence is observed.

The impact of the etching parameters on the etch result is summarized in Table 10. The chemical composition of the plasma clearly dominates the result of the etching process. In comparison, the RF power has a weaker influence.

The following observations with respect to figures of merit for large-area etching have been made:

- All measured *etch rates* in this DOE run lie in the interval between 1μm/min and 3μm/min. While higher RF power increases the etch rate, it does not improve the maximum achievable etch depth, as the mask is also etched faster. However, a low fraction of neutrals has a positive effect on both etch rate and maximal achievable etch depth. With fewer neutrals, the etching of the semiconductor is more chemical, which enhances the selectivity.

- The *bottom surface quality* (required to be flat and smooth) is determined only by the nitrogen content in the plasma due to passivation of the surface and the subsequent micro masking or so-called “grass formation”. Other parameters have no significant impact on this figure of merit.

- The *sidewall quality* (compare with Figure 34) is positively influenced by high ICP and RF power and the chemical composition. Again, the chemical composition is more relevant for the surface quality than power.

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\(^{19}\) As lag-effects do not play a role, the selectivity is directly linked to the maximal achievable etch depth.
3.4 Hole etching for photonic crystals in InP/InGaAsP/InP

![Graph](image)

**Figure 34:** Influence of the process parameter on the sidewall quality (numerical quality ranking). The parameter values are set according to Table 9 in the parameter range: ICP power 1000-2000W, RF power 140-215W, neutrals flux 7-15sccm, N₂ percentage 0-100%.

- An important parameter is the **sidewall angle** of large-area structures. Close to vertical (0°) is advantageous. The impact of the different etching parameter on this figure of merit is depicted in Figure 35. The ICP and RF power are irrelevant for the sidewall angle. A high content of neutrals in the plasma moves the etching from the chemical regime towards physical etching, which results in sloped sidewalls. The passivation capability of nitrogen also results in sloped sidewalls.

![Graph](image)

**Figure 35:** Influence of the process parameters on the sidewall angle. Parameter values: ICP power 1000-2000W, RF power 140-215W, neutrals flux 7-15sccm, N₂ percentage 0-100%. The most prominent influence arises from the neutrals content and composition in the plasma. A very chemical process is beneficial for vertical sidewalls.
We found no distinct influence of the process parameter on the \textit{quaternary material selectivity} (equation 3.8). The quaternary material selectivity value lies mostly between 0.8 and 0.9 over the 16 etching experiments DOE run, in contrast to methane-based plasmas for which the selectivity is as low as 0.25.

Pressure has no significant influence on any quantity of interest.

In conclusion, we can state now the optimal conditions for etching large areas is a chemically dominated process (high Cl\textsubscript{2} content, low neutrals content). The use of high powers, both RF and ICP, are also a good choice. However, the final goal is the etching of small holes, which will require a differently tuned etching process. The detailed optimization will be presented in the next section.

3.4.3.3. Hole etching properties of a Cl\textsubscript{2}/Ar/N\textsubscript{2} plasma

A suitable process for the fabrication of large area structures is not necessarily optimal for deep etching of deep, narrow holes for PhCs. The etching condition of high-aspect-ratio structures is different from those of large areas. Issues like ion deflection from electrically charged opposed sidewalls or etchants diffusion in- and reactants diffusion out of the narrow holes need to be addressed. In this section, we discuss the optimization strategy for a PhC hole etching process.

For holes, the figures of merit are \textit{hole shape}, \textit{hole surface roughness} and \textit{hole depth}. In addition, a low quaternary material selectivity is favorable to avoid differential etching of the core and the claddings. Typical hole diameters for wavelengths of $\lambda=1550\text{nm}$ are in the range of about 300nm. Again we use the DOE approach to get insight in the etching process of the holes. The same DOE parameters as in section 3.4.3.2 (Table 9) are used. The qualitative behavior of the etching is assumed to be independent of hole size. Table 11 summarizes the influence of the process parameters on the hole characteristics.

<table>
<thead>
<tr>
<th></th>
<th>ICP power [W]</th>
<th>RF power [W]</th>
<th>Total neutrals flux [sccm]</th>
<th>% of N\textsubscript{2} in the neutrals [%]</th>
<th>Pressure [mTorr]</th>
</tr>
</thead>
<tbody>
<tr>
<td>eMED</td>
<td>(\uparrow)</td>
<td>(\downarrow)</td>
<td>(\downarrow)</td>
<td>(\downarrow)</td>
<td>(-)</td>
</tr>
<tr>
<td>Hole shape</td>
<td>(\uparrow)</td>
<td>(-)</td>
<td>(\downarrow)</td>
<td>(\downarrow)</td>
<td>(\downarrow)</td>
</tr>
<tr>
<td>Conicality</td>
<td>(\downarrow)</td>
<td>(-)</td>
<td>(\downarrow)</td>
<td>(\uparrow)</td>
<td>(\downarrow)</td>
</tr>
<tr>
<td>Undercut</td>
<td>(-)</td>
<td>(-)</td>
<td>(-)</td>
<td>(\uparrow)</td>
<td>(\uparrow)</td>
</tr>
<tr>
<td>Hole surface quality</td>
<td>(-)</td>
<td>(\uparrow)</td>
<td>(-)</td>
<td>(\downarrow)</td>
<td>(-)</td>
</tr>
<tr>
<td>Grass-like vertical stripes on the surface</td>
<td>(-)</td>
<td>(-)</td>
<td>(-)</td>
<td>(\uparrow)</td>
<td>(-)</td>
</tr>
</tbody>
</table>

\textbf{Table 11:} Influence of the process parameters on quantities of interest for PhC hole etching. Up \(\uparrow\) and down \(\downarrow\) arrows indicate a larger parameter value to be beneficial and detrimental, respectively. For holes, the absence of undercut is optimal. The number of arrows relates to the strength of the trend. A dash (-) indicates that no significant influence is observed.

We will in the following discuss the individual figures of merit for hole etching separately.
3.4 Hole etching for photonic crystals in InP/InGaAsP/InP

Maximal hole depth

Figure 36 summarizes the results of the process parameters on the extrapolated maximal etch depth (eMED\textsubscript{Holes}) for holes with 200nm diameter. The trends are similar for holes with 500nm diameter. We included lag effects (see section 4.1.1) [96] into our calculation of the eMED\textsubscript{Holes} (according to equation 3.7) to make the extrapolation more accurate. The calculation is based on the eMED and scales it with the lag factor r measured from SEM images.

\[
\text{eMED}\textsubscript{Holes} = \text{eMED} \cdot \frac{\text{Measured etch depth}_{\text{Holes}}}{\text{Measured etch depth}_{\text{Large Areas}}} \cdot r
\]

(3.10)

The eMED\textsubscript{Holes} range in the individual runs of the DOE is 0.8\(\mu\text{m}-4.4\mu\text{m} and 1.3\mu\text{m}-4.8\mu\text{m} for Ø200nm and Ø500nm hole diameters, respectively.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig36.png}
\caption{Influence of the process parameter on the eMED\textsubscript{Holes} for 200nm hole diameter. Parameter value levels: ICP power 1000-2000W, RF power 140-215W, neutrals flux 7-15sccm, N\textsubscript{2} percentage 0-100%.
}
\end{figure}

From the DOE evaluation in Figure 36, we can draw the following conclusions:

- Whereas nitrogen has a negative impact on the eMED for large-area etching (Table 10) due to micromasking, it is beneficial for hole etching (Table 11 and Figure 36).

These seemingly contradictory results can be explained as follows: due to the enhanced surface passivation with higher nitrogen content, ions are deflected toward the center of the holes. We believe that the enhanced ion bombardment allows more efficient cracking of the passivation layer at the bottom and increases the overall etching rate.
• Comparing Table 10 with Table 11, low RF power has a significant influence on hole depth, but not on large-area etching. This behavior cannot be explained by a selectivity enhancement against the mask due to a lower DC-bias as we do not observe a reduction in etch depth for higher power in the case of large-area etching. At higher power, the plasma density and therefore the amount of active species accelerated towards the sample are increased. This enhances the etch rate of the semiconductor, but also the etch rate of the mask, and therefore no increase in the eMED is observed for large areas.

Now let us consider the situation in the holes. With increasing hole aspect-ratio, it becomes difficult for the neutral etch species to diffuse into or to remove the etch products by diffusion out of the hole, and therefore the semiconductor etching rate slows down when the holes get deeper. This hypothesis is supported by the fact that the hole depth reduction at higher power is more pronounced for small holes as shown in Figure 37. Indeed, for large-area structures, only a slight and insignificant decrease of the eMED (6 ± 5nm/W) with power is observed, which can be caused also by other parameters in the DOE. For holes, we measure a clear decrease of the eMED\textsubscript{Holes} with increasing RF power of 12 ± 3nm/W and 22 ± 3nm/W for 500nm diameter and 200nm diameter holes, respectively.

![Figure 37](image.png)

**Figure 37**: Correlation between the RF power and eMED\textsubscript{Holes} for large-area structures and different holes size (200nm and 500nm diameter).

• The ICP power shows less influence on hole depth than the RF power. While a lower RF power not only reduces the plasma density but also the DC-bias, a lower ICP power reduces the plasma density, but increases the DC-bias, leading to a higher sputter efficiency of the mask. This reduces the selectivity of InP against the mask and the eMED\textsubscript{Holes}.

For the pressure and the neutrals content of the plasma, no distinct trend was observed for the eMED\textsubscript{Holes}.
Hole quality and sidewall passivation

Non-cylindrical holes and/or rough sidewalls contribute to optical losses of a PhC device [69, 70]. Therefore it is mandatory to fabricate cylindrical holes. The previous Table 11 lists the contribution of each processing parameter with respect to the hole quality (generic term for hole shape, hole sidewall roughness, undercut).

All these quantities of interest are only strongly influenced by the nitrogen content in the neutrals flux. High nitrogen content is detrimental for the hole shape and surface roughness for both holes and large areas. This behavior results from the passivation capability of the N-P bonds, as discussed earlier.

So far, there is no justification for the addition nitrogen in the plasma. However, when considering the etching of small (~300nm diameter) holes, we are confronted with the problem of undercut just below the mask (an example is shown in Figure 38a and b). As the undercut is only visible in holes but not at the sidewalls of large-area structures, we believe that it is caused by the deflection of the incoming chlorine ions from the opposite sidewalls, as also observed in reference [143]. As the mode intensity at the top of the holes is relatively strong due to the asymmetric slab waveguide structure and the weak refractive index contrast between core and cladding, the undercut may significantly contribute to optical scattering losses due to its very rough and distorted surface. Furthermore, the undercut destroys the cylindrical hole shape, leading to additional losses. The nitrogen passivation can suppress successfully the undercut as shown in Figure 38c by formation of N-P bonds at the sidewalls [136, 137].

In section 3.4.3.2, we only found that nitrogen has a negative influence on the etching result with respect to hole shape and surface roughness. On the other hand, nitrogen is capable to suppress the detrimental undercut. Because of this contribution, we cannot completely do it without nitrogen. Separate and careful optimization of this critical parameter is required.

Therefore, beside the DOE runs, additional fine-tuning has been performed to tackle the undercut issue. The nitrogen flux has been increased from 1.3sccm to 6sccm. It is visible that the undercut disappears with higher nitrogen flux, but unfortunately a more conical hole shape and increased surface roughness arises (Figure 38).
3. Etching of deep holes in InP for photonic crystals

**Figure 38:** Undercut-suppression with the help of nitrogen addition. The holes etched with the optimized Cl2/Ar/N2/He-process. The nitrogen flow is varied from 1.3, 2.1, 2.9, to 6 sccm for a) to d), respectively. All other process parameters are kept constant. The Cl2 and Ar fluxes are 15sccm and 5sccm, respectively. All related images have the same scale. The undercut is disappearing for higher nitrogen fluxes (left images), but the holes get more conical (right images).

The optimal amount of required passivation by nitrogen is mainly dependent on the chlorine content in the plasma. Figure 39 presents the effect of increasing the chlorine flux while keeping the other parameters constant, in particular the N2 flux. The increased chlorine flux enhances the hole depth. However, the nitrogen flux is not sufficient anymore to passivate the sidewalls, as its relative fraction has been reduced. Therefore the flux must be also adjusted according to the used chlorine flux.

**Figure 39:** Depth of holes etched with Cl2/Ar/N2/He-process vs. Cl2 flux. The N2 and Ar fluxes are 2.1sccm and 5sccm respectively. All other parameters are kept constant. The pressure is 2.2 mTorr except for the highest flux where it had to be increased to 2.5mTorr. Insets: SEM micrographs of the hole’s cross-sections and the undercut. With higher chlorine flux, the nitrogen is not capable anymore to sufficiently protect the sidewalls.
Improved process parameter beyond the DOE run

The DOE has given insight into the basic role the different processing parameters. We used this insight to further optimize the etching process beyond the results which were achieved with the DOE run.

- We have seen that the indiffusion of etchants and outdiffusion of reactants in the narrow holes limits the maximal hole depth that can be achieved. To allow for enough time for the diffusion,
  - ICP and RF power were chosen low enough to slow down the etching (RF power 160W, ICP power 600W). A lower limit for the reduction of the power is the stability of the plasma. The above values are chosen well above this limit.
  - To dilute the plasma and enhance its stability (noble-gas addition may stabilize the plasma [105]), some neutral He (the only available noble gas on the system) was added to the chamber. This resulted in smoother holes. The beneficial effect of He addition has been also reported in [144].
- We observed a weak positive influence from low plasma pressure.
  - We reduced the pressure for the process slightly above the limit of the machine, to still be able to control the pressure with the valve (pressure 2.2mTorr).
- Chemical etching enhances the selectivity and therefore the eMEDHoles.
  - Instead of reducing the Ar flux (the flow meter would have been operated outside the operation range) we increased the flux of the chlorine (Ar flux 5sccm, Cl2 flux 15sccm).
  - At the end of the optimization, the nitrogen flux was adjusted to the lowest possible value where we do not observe an undercut. This nitrogen fine-tuning results in an optimal flux between 2.4-3.9 sccm\(^{20}\).

By this optimization, we improved the process for deep holes to the results presented in Figure 40. We achieved holes depths of 4.2μm, 3.8μm and 2.9μm for hole diameters of 417nm, 310nm and 180nm, respectively. Such depths compare very favorably with literature values (Figure 23).

Such depths are sufficient for the fabrication of bulk-PhC devices, as most of the light mode is penetrated and influenced by the holes.

\(^{20}\) The initial value for optimal nitrogen flux after the DOE was found to be 2.4sccm. However, during this work, the optimal value drifted towards higher fluxes, most likely due to chamber contamination. Regular re-adjustment is necessary to maintain a good hole quality.
In summary, we have developed the fabrication technology to create a dense array of holes into InP/InGaAsP, by systematic optimization of the processing parameters. The dominant role of the nitrogen content in the plasma was discussed in detail. Adding a small amount of nitrogen is mandatory to protect the sidewalls against underetching. However, it has a detrimental effect on the quality of surface and the hole shapes. Therefore a careful balance of the nitrogen in the plasma must be achieved.

3.5. The fabrication flow of a complete PhC device

In the preceding sections, the fabrication of deep holes arranged in a dense array has been presented. In this context, we should not forget the typical dimensions of the structures: PhC devices are barely more than a few tens of micrometers in size. For simple device handling and mechanical stability issues, however, the final chips must be a few millimeters in size. This requires additional access structures – waveguides between the device and the cleaved chip facets – included on the chip, to connect the PhC devices with the outside world. The design of such waveguides will be discussed in Chapter 5. Here we focus on different ways to fabricate these access waveguides.

The requirements for the connecting waveguides are manifold. On the wish list are:

- Single-mode operation
- Mode-matching at the cleaved facet and the interfaces to the PhC
- Low propagation loss (or at least limited and well controlled losses)
- Short processing time and simple processing
- Flexible design from one fabrication run to the next

So far, we are not aware of any technology that simultaneously fulfills these requirements entirely. In the following sub-chapters we present two possible fabrication processes.
3.5 The fabrication flow of a complete PhC device

3.5.1. The endfire process: Single-mode ridge waveguides

If low propagation loss and single-mode operation of the access waveguides are given highest priority, a so-called *endfire process* is the method of choice. It has been already discussed in-depth in [1] and therefore only briefly sketched here. The fabrication sequence allows the combination of the PhC device with shallow-etched single-mode ridge waveguides (1.5\( \mu \)m ridge width). Therefore, at least two masking steps are required for the PhC structures (EBL) and the ridge waveguides (optical lithography). The crux of the matter is the alignment of the two mask layers to each other. We have two contradicting fabrication issues:

- Optical alignment has a precision down to a few hundred nanometers, whereas EBL can achieve a precision which is almost an order of magnitude smaller. Therefore, it would be obviously desirable to align the EBL mask to the optical mask.

- The etching of the PhC starts with a thin PMMA mask layer (210nm). Such thin layers are incapable of covering and protecting the previously etched ridge waveguide structures (height around 300nm). Therefore, the PhC structures must be fabricated first, as it is possible to protect the holes with the thick mask (500nm photoresist and 400nm silicon nitride) for the ridge patterning.

As it is not possible to sufficiently cover the ridge waveguides with the hard-mask for the PhC etching, the PhC structures must be fabricated first. To solve the alignment challenge, the *endfire process* as presented in Figure 42 was developed. A total of 3 masks are required:

1. In a first mask step, gold (Au, 200nm thick) markers are created on the full wafer by optical lithography and lift-off technique. The mask contains small markers for EBL alignment close to the future PhC devices, and large global markers for optical alignment. The subsequent mask steps are aligned onto these markers.

2. The second mask (200nm PMMA, 30nm titanium and 400nm SiN\(_x\)) is EBL written. It defines the PhC device and short trench access waveguides. The individual devices are each aligned to the EBL gold markers to compensate for stage drift during the long (several days) exposure time of all PhC devices. The processing of this mask (hard-mask build-up, patterning and semiconductor etching) was previously described in sections 3.3 and 3.4, respectively.

3. The third mask (500nm photoresist AZ1505 and 400nm SiN\(_x\)) step is again patterned by optical lithography. The mask is aligned to the global gold markers from the first mask. It defines the ridge access waveguides. The subsequent processing (SiN\(_x\) mask etching and semiconductor shallow etching) is presented elsewhere [1].
3. Etching of deep holes in InP for photonic crystals

The process sequence is always performed on a full wafer, and several 100 devices can be fabricated simultaneously\textsuperscript{21}. Alignment precision between the gold markers and the optical ridge waveguide mask / PhC EBL mask is around 400nm / 30nm, respectively, and therefore the alignment precision between the two waveguide sections also between 400nm. Figure 41 presents the image of a final device fabricated with the endfire process.

\textbf{Figure 41}: Microscope image of the final device fabricated by the endfire process.

\textbf{Figure 42}: The process steps of the endfire process: A) Metal-marker-fabrication, B) PhC and photonic wire fabrication (EBL), and C) Ridge waveguide fabrication (optical lithography).

\textsuperscript{21} Optical alignment on a full wafer is much more accurate than on small pieces.
3.5 The fabrication flow of a complete PhC device

3.5.2. The rapid prototyping process: Quick and simple fabrication

If quick and flexible processing is given highest priority, the rapid prototyping process is the method of choice. The process sacrifices single-mode operation of the access ridge waveguides in favor of faster and simpler processing. The rapid prototyping process EBL-writes and etches the PhC device and all accessing waveguides in one single step. This reduces the amount of total processing steps and, therefore, increases the fabrication speed. However, this decision has the following consequences:

- As all structures are etched together in one step, it is not possible to fabricate shallow-etched ridge waveguides, but only deeply etched trench waveguides. Such waveguides require a width smaller than 437nm to be TE single-mode. Single mode operation is, therefore, not possible, as such thin trench waveguides are highly lossy (in the order of several 10dB/cm to 100dB/cm).

- Patterning of access waveguides using EBL implies an increased exposure time due to the large structures. However, short writing times are crucial for the fabrication, as only limited writing capacity is available. We reduced the writing time of the chip by
  
  → writing only narrow trenches (1μm) on both sides of the access waveguides. The width is chosen as small as possible to reduce writing time, but large enough to avoid lateral outcoupling of the waveguide.

  → writing the trenches for the waveguides with a higher exposure current than the complicated structures of the PhC devices. This requires careful calibration of the EBL system to avoid an offset between the structures written with different currents. The offset is below 200nm (Figure 44) and identical for all structures written in the same batch. The offset can further be reduced by splitting the full design into smaller parts and change the current between each part, to avoid the accumulation of the drift during long writing times.

- As shown in section 3.4, the etching of holes and trenches behaves differently. As now all structures are etched together, the process is optimized for the PhC holes and not the trench waveguides. Therefore, the losses in the access waveguides will be higher (around 5-10dB/cm for a 3-5μm wide trench waveguide) than they would be with an optimal fabrication process.

A microscope image of a rapid prototyping chip is shown in Figure 43.
3. Etching of deep holes in InP for photonic crystals

![Image](image1)

**Figure 43**: Microscope image of a chip fabricated with the rapid prototyping process. Several devices are placed on one chip. The light will propagate from left to right along the waveguides through the PhC devices. For the measurement setup and the light shields, we refer to Chapter 5.

![Image](image2)

**Figure 44**: Interface between the trench waveguide written with the 30mm (left) and 10mm aperture (right). The offset between the structures written with different apertures is below 200nm.

### 3.5.3. Comparison of the endfire process and the rapid prototyping process

Neither of the two presented processes for the fabrication of PhC devices (including access waveguides) fulfill all requirements listed at the beginning of section 3.5. Unfortunately, the “perfect” fabrication process is not possible with our available equipment. Table 12 compares the two fabrication processes.
Table 12: Advantages and disadvantages of the different fabrication processes.

For the quick development of devices, rapid prototyping is preferred, in spite of the missing single-mode operation. For a detailed discussion of these multi-mode waveguides, the reader is referred to Chapter 5. Processing cycles of several weeks are undesirable for quick device testing and development. The rapid prototyping is, therefore, used for almost all devices presented in this work, except when stated otherwise.

The rapid prototyping process has proven to be suited for the research on PhC. Despite the large structures, EBL exposure time is short enough to pattern a large number of devices at the same time. Therefore the main limitation of the rapid prototyping process is the propagation loss of the trench waveguides, what inhibits single-mode operation. It is not easy to overcome this limitation, as

(i) either a separate etching process for the trench waveguide is required, what leads us again to the endfire process with its long processing time, or

(ii) an “ideal” process must not only be optimized towards high-quality PhC holes, but also towards low trench waveguide propagation loss. As the focus of this work lies on PhCs, such a traded-off fabrication process is undesirable.
Chapter 4

Hole characterization

“Why should I have to WORK for everything?! It's like saying I don't deserve it!”
Bill Watterson

So far, we have discussed the fabrication of photonic crystal holes in InP/InGaAsP. Using advanced EBL techniques and complex dry-etching processes, vertical holes with a – at least in scanning electron (SEM) images – optimizes surface smoothness have been obtained. As a key parameter for the etching result, the nitrogen concentration in the etching plasma must be carefully adjusted to get optimal results.

So far, we have only characterized holes by using SEM. Although this method allows for quick measurements of the hole depth and hole shape, it does not reveal other interesting properties of the etching process like e.g. surface roughness on the nanometer scale (section 4.2) or carrier lifetime (section 4.3).

In this chapter, we present characterization results of our fabricated holes. The design and characterization of PhC building blocks and complete PhC-based devices will be presented finally in Chapter 6.

4.1. Lag- and load-effects in narrow holes

Feature size dependent etching and plasma loading effects complicate the etching of the holes for a PhC. Depending on the hole diameter, the structural density and the chip size, the etch result from the same process is different. In this section, the optimized process for PhC etching presented in the preceding chapter is characterized in terms of:

- The observation that the etch speed decreases with increasing aspect-ratio of the structures is commonly referred as aspect-ratio dependant etching (ARDE) or RIE lag. A detailed discussion of this effects can be found in references [96,
4. Hole characterization

RIE lag is evident during etching of a wide range of materials (silicon, oxides, metals or III-V-semiconductors) and for different equipment (reactive ion beam etching, reactive ion etching or plasma etching). Lag-effects scale with aspect-ratio rather than the absolute feature size of the etched structure [96]. Different effects are reported to be responsible for lag effect:

- **Knudsen transport of neutrals** [145]: Knudsen transport refers to neutral transport for the case where reactants are reflected diffusively from the sidewalls without a chemical reaction is taking place. The neutrals stick to the surface and leave it under a cosine angular distribution in thermal equilibrium with the surface [96]. The probability that a neutral reaches the bottom of a hole under these conditions is reduced with increasing aspect-ratio of the structure.

- **Ion shadowing** [109]: Due to collisions during acceleration in the sheath, ions may arrive at the wafer surface at non-normal incidence. The angular distribution of the ions and the aspect-ratio of the structure determine the amount of ions reaching the bottom surface and therefore the etching speed. The narrow slits of high-aspect ratio structures shields non-normal incidence ions form the bottom.

- **Neutrals shadowing** [146]: Under reactive-ion etching conditions (pressure < 75mTorr), the mean free path for collisions of neutrals is much longer than the dimensions of the holes. Thus gas-phase collisions can be neglected compared to collisions of the neutrals with the sidewall. Under these conditions, the same shadowing effects occur as for ions.

- **Charging effects** [147, 148]: Surface charges are capable to deflect ions. For high-frequency power supply or conducting masks, total mask charging is irrelevant. Also the electric field (DC-bias) distortion due to the non-planar wafer surface does not contribute to lag-effects, as it would scale with feature size rather than with aspect-ratio [148]. Still, differential charging of the microstructure may distort ion-transportation into high-aspect ratio structures.

- **Material redeposition** [112]: Sputtered semiconductor atoms or reactants may not leave the holes directly, but are redeposited at the sidewall of the holes. Such material must be etched again and thus lower the etch rate. The redeposition is stronger the higher the aspect ratio is. Therefore it contributes to lag effects.

- **Loading effects**. Depending on the amount of etched material, etching species might become depleted during etching. In the case of reactant transport-rate-limited etching, loading effects changes the etching characteristics and slows down the etching speed with increasing wafer size. The relevant parameter for loading effects is the distance \( \Lambda \) over which the reactants are depleted. \( \Lambda \) depends on the relative rates for the transport and reaction, fluid dynamics and
properties of the surfaces in contact with the plasma and reactive gases [96]. One distinguishes \textit{micro-} and \textit{macroloading}. 

- \textit{Microloading} ($\Lambda \approx \text{structure size}$) addresses the topic of local depletion of the etchants due to locally dense structures.

- \textit{Macroloading} ($\Lambda \gg \text{structure size}$) addresses the topic of global depletion of etchants due to the total amount of exposed material in the chamber. As we work with samples starting from pieces as small as 0.36cm$^2$ up to a full 2”-wafer, this effect cannot be ignored.

As photonic crystals are – in terms of exposed area – low-density structures, only macroloading is considered in this work. Loading effects can be reduced either by shifting the regime to surface-rate limited etching, or by adding dummy patterns (“thieving”) on the chip to avoid different surface pattern densities [96].

- \textit{Hole widening} (section 4.1.2, Figure 50). As perfect anisotropic etching cannot be achieved, holes are also slightly etched laterally. This results in enlarged hole size during etching. The hole widening has to be taken into account while drawing the mask. The drawn hole size on the mask is reduced by the expected widening.

These three effects are discussed in the following sections in detail. First, the evaluation method is presented in section 4.1.1, followed by the discussion of the lag effect, load effect and the hole enlargement. As these effects can hardly be avoided during fabrication, it is mandatory to characterize in order to feed them into the optimization cycles of the device design.

\section*{4.1 Lag- and load-effects in narrow holes}

\subsection*{4.1.1. Evaluation method}

Lag-effects were investigated by etching holes of different diameter and measuring their etch depth. The characterization is based on scanning electron microscope (SEM) imaging. The used test pattern consist of a large opening (30x60$\mu$m), where we assume that ARDE effects do not influence the etch rate (we will later verify that this assumption holds), and 4 pads of PhCs of a triangular array of holes of different hole size. All chips are of the same size (6x6mm). The hard-masks for all samples are patterned and etched in the same batch to minimize wafer to wafer variations from the mask fabrication. Samples were fabricated from pure InP wafers and also in our standard InP/InGaAsP/InP slab waveguide structure on InP substrate.

\textit{Hole depth} is directly measured from the SEM images of cleaved facets. As the cleaving precision is very low (at best 10$\mu$m), a full array of holes is patterned and slightly (2°) tilted against the semiconductor crystal orientation. This ensures that at least a few holes are centrally cleaved. The \textit{hole diameter} is extracted from top-view SEM images by automated image-processing to statistically determine the average diameter. The method of the diameter extraction is described in-detail in reference [93].
4. Hole characterization

All results presented below have been obtained from the samples without the InGaAsP core layer for the vertical confinement. It has, however, been verified that there is no measurable influence of the core layer on the obtained results.

4.1.1.2. Lag effects

For the characterization of the lag effects, the etching depth of holes is compared against the etching rate for large areas. Figure 45 presents the results. The depth of the holes have been measured for different etching times and compared with the large-area etch depth.

![Figure 45: Etching depth of InP as a function of time for different hole sizes. The hole radius in the legend refers to the radius of the hole in the hard-mask.](image)

In Figure 45, we compare the etch-depth as a function of time for different hole diameter. The etch rate for large-area structures was found to amount to 2980±82nm/min\(^2\) based on the slope of the linear fit of the etch depth as a function of etching time. As the measurement points could be fitted smoothly with a straight line, we conclude that no lag effects affect the etching. It must be mentioned that the linear fit does not go through the origin of the coordinate system, as it would be theoretically expected. We attribute this observation to the polymer-formation (teflon, Figure 46) during the CHF\(_3\)/O\(_2\) etching of the SiNx hard-mask [92]. Indeed, a hard polymer film

\[\sigma_m = \sqrt{\frac{\sum_{i=1}^{n} (m \cdot x_i + b - y_i)^2 \cdot n}{(n-2) \cdot \left( \frac{n \cdot \sum_{i=1}^{n} x_i^2 - \left( \sum_{i=1}^{n} x_i \right)^2 \right)}} \]

\[\sigma_b = \sqrt{\frac{\sum_{i=1}^{n} (m \cdot x_i + b - y_i)^2 \cdot \sum_{i=1}^{n} x_i^2}{(n-2) \cdot \left( n \cdot \sum_{i=1}^{n} x_i^2 - \left( \sum_{i=1}^{n} x_i \right)^2 \right)}} \]

whereas \(n\) ist the number of points, \(m\) and \(b\) the slope and the intercept of the regression line, respectively, and \((x_i, y_i)\) the measurement points. \(\sigma_m\) and \(\sigma_b\) are the standard deviation for the calculation of the slope and the Y-axis offset, respectively. These equations will also be used in the remainder of this section to calculate the error of regression lines.
is formed on the surface of the InP during the etching of the dielectric hard mask. Therefore the InP is masked during the first few seconds of the etching time. Chlorine plasma is capable of cracking the film. From the linear interpolation of the etch depth, we assume that it takes around 10sec to remove the polymer film.

The lag effect becomes obvious when we compare the etch depth of the holes with the large-area etch depth. For short etching times (<60sec), the difference between the large-area and the hole depth is small. Lag effects start to reduce the etch speed in holes after an aspect-ratio between 6 (for small holes) and 11 (for the largest holes) is achieved. This results in a reduced etching depth compared to the large-area. The depth is reduced by up to 50% for the holes with 61nm diameter after 115sec.

![Image of polymer formation after RIE etching](image1.png)

**Figure 46**: Hard-mask after etching and InP-surface. The polymer formation during over-etching the hard-mask on the InP surface creates bubbles from Teflon. These bubbles are hard to remove and very resistant against the semiconductor etching plasma.

![Graph of etch depth vs. hole diameter](image2.png)

**Figure 47**: Lag-effect simulations of CAIBE-etching of InP, using the model of Berrier et.al. [97] (Reprinted with permission from A. Berrier, M. Mulot, A. Talneau, R. Ferrini, R. Houdré, and S. Anand, Feature size effects in chemically assisted ion beam etching of InP-based photonic crystals, Proc. SPIE Nanoengineering: Fabrication, Properties, Optics, and Devices III, 6327, 2006).
4. Hole characterization

A simple 1D model for CAIBE etching of holes is published in reference [97]. It calculates the time evolution of the bottom of the holes. The following effects are considered: (i) the chlorine coverage at the bottom of the hole, (ii) the removal of the reactants out of the holes and (iii) the reactants re-deposition. They calculated the hole depth for different hole diameters and etching times. Their theoretical results are presented in Figure 47. Although a quantitative comparison between the results (Figure 48) is not possible (they used different processing parameters and particularly a different etching system), the qualitative agreement between the model and our measurements presented in Figure 48 is obvious.

![Figure 48: Measured hole depth of InP as a function of hole radius for different etching time. The lines are to guide the eye, only. The numbers next to the lines indicate the etching time.](image)

4.1.1.3. Mask erosion and maximal etching time

The limiting factor for etching time is the mask etch rate. Due to physical bombardment and chemical etching, the thickness of the mask is reduced continuously. The wear of the mask is stronger close to an edge, resulting in a lateral erosion of the mask at the edge (Figure 33) [106]. We therefore must define two etch rates for the mask, the bulk mask etch rate = 167nm/min and the mask etch rate at the facet = 224nm/min. With 400nm silicon nitride, the mask can withstand a maximal etching time of 107s until the faceting reaches the InP, independently of the etched hole size. A maximum of 4800nm etch depth for large areas can be achieved until the mask is removed down to the semiconductor at the facet (Figure 33 right, b). For holes with a radius of 62nm, 80nm, 109nm and 131nm, etch depths of 2200nm, 2700nm, 3100nm and 3500nm can be achieved, respectively.

The maximal etch time and therefore the maximal hole depth discussed above is only valid for low filling factors (around r/a<0.36). In the experiment, r/a=0.31 is used, which results in a distance between the holes of 0.38a (160nm at a=425nm). This distance is enough for a stable mask fabrication. For PhCs with a TM bandgap [35], for example, higher filling factors up to r/a=0.41 are required. Such a high filling factor gives an interhole-distance=0.18a (77nm at a=425nm). Such narrow distances require thin lamellae of SiNₓ as a hard-mask between the holes. As thin structures are
attacked from all sides, they are much faster etched or eroded than the rest of the mask (Figure 49). This reduces the maximal etching time until the semiconductor is attacked between the holes, and results in reduced hole depth. Therefore the fabrication process presented above is limited to low filling factors (around \( r/a < 0.36 \)).

**Figure 49**: Extended mask erosion between narrow-spaced holes. Such thin lamellae of SiN\(_x\) between the holes are attacked heavily from all sides by the semiconductor etching plasma and are therefore eroded much faster.

### 4.1.2. Hole enlargement

Although the photonic crystal etching process is very anisotropic, holes become larger with increased etching time. Figure 50 presents the hole diameter for different initial mask hole diameters as a function of etching time. The enlargement of the hole radius is linear in time with typically around \( 13 \pm 2 \) nm/min and independent of hole size. No undercut directly under the mask is observed for any etching time for the used optimized process. Therefore the measured hole radius in the semiconductor corresponds to the hole size in the mask. We therefore attribute the hole enlargement in the semiconductor to lateral mask etching. The lateral mask etching is not influenced by hole size.

The lateral mask etching requires calibration of the design hole size used for writing. Holes must be drawn in the design with a smaller hole size than required for the final design (design bias), to account for the hole enlargement. This correction not only accounts for hole enlargement during ICP etching, but also for hole radius change during electron beam writing (EBL) and hard-mask etching. For typical hole radius between 175 nm, this correction predicts a total hole enlargement of around 30 nm during the whole fabrication process. The design uncertainty according to the error values of equation 4.1 is

\[
\Delta r_{\text{design}} = r_{\text{target}} \cdot \Delta m + \Delta b = 5.5 \text{ nm} = 3\% \\
\text{at } r_{\text{target}} = 175 \text{ nm.} 
\] (4.1)

Due to process variations during EBL exposure, hard-mask etching and semiconductor etching, this variation of the hole-size is higher between different runs.
4. Hole characterization

**Figure 50**: A linear increase in hole diameter as a function of time can be observed, with the same slope for all hole diameters. The hole radius enlargement during ICP etching is $13\pm2\text{nm/min}$, $12\pm2\text{nm/min}$, $11\pm2\text{nm/min}$ and $15\pm2\text{nm/min}$ for the smallest to the largest holes, respectively.

4.1.3. **Macroloading**

The loading effects arising from different amounts of exposed semiconductor surface to the plasma. To assess macroloading, samples of different size were etched for the same time. After the experiment, etch depth and hole diameter were extracted from SEM micrographs. We investigated the effect of loading both with InP and hard-mask material (SiN$_x$) exposed to the plasma.

4.1.3.1. **Macroloading caused by the InP surface area size.**

Macroloading arising from InP surface area size is measured by etching a quarter, a half or a full wafer of blank InP together with the test sample. This additional wafer consumes etch species and therefore introduces load effects. The sample itself was placed in the middle of the chamber, whereas the additional material (blank InP wafer) is arranged around the sample.

The resulting etch depth after a fixed etching time (100sec) is presented in Figure 51. The etch rate drops significantly with increasing amount of InP that has to be etched. The effect is strong for large areas, whereas for holes the effect is less pronounced due to additional limitations, e.g. lag effects. The mask etch rate is not influenced by the amount of InP in the chamber. Therefore, the load effects cannot be compensated by longer etching times, as the overall selectivity decreases.
4.1 Lag- and load-effects in narrow holes

Figure 51: InP load effects of the etching process after 100sec etching. With an increasing InP surface area in the chamber, the etch rate drops. The radius refers to the radius of the hole in the hard mask prior to ICP etching. The mask etch rate is independent of load effects.

Also the hole radius after etching is influenced by macroloading. Figure 52 presents the measured hole diameter for different amounts of exposed wafer surface. Clearly, the hole diameter drops. However, the strength of the effect is weak, so that it can be almost neglected during fabrication. The measured decrease in the hole radius due to lag effect is in the order of -8nm to -10nm between a small piece and a full wafer.

Figure 52: Hole diameter as a function of the etched surface. A decrease in the hole diameter as a function of etched surface can be observed, with the same slope for all hole diameters. A linear fit through the point predicts a decrease of the hole radius of -8±3nm, -8±4nm, -10±4nm and -10±5nm per full InP wafer load.

4.1.3.2. Macroloading with SiNx

We also investigated the impact of loading the process with a wafer covered with SiNx (masked wafer). We found that the loading with a full wafer covered by silicon nitride has only a weak impact on the hole depth:
4. Hole characterization

- The hole and large-area-etch depth is only reduced by around 5% and 10%, respectively by adding the wafer covered by SiNₓ.
- The loading with SiNₓ has almost no impact on the hole diameter (<3%).

Therefore we can conclude that the amount of masked material has only a minor influence on the etching result, compared especially to the influence by the amount of unmasked InP.

4.1.4. Conclusion on lag and load effects

In conclusion, macroloading leads to a lower selectivity and therefore a lower maximal hole depth. To achieve the best results with respect to quality and reproducibility, we derive the following guidelines

(i) The sample size should be the same for the optimization of the process and the final device, and

(ii) The amount of InP exposed to the plasma should be minimized.

4.2. Hole surface roughness measurement by AFM*

A key figure of merit for PhC devices is the propagation loss. Apart from intrinsic effects, losses originate from (i) insufficient hole depth, (ii) a non-cylindrical vertical hole shape or (iii) surface roughness [70, 74].

Scanning electron microscope (SEM) micrographs are the method of choice to characterize fabricated PhC holes. They have the advantage of a fast characterization compared to a time-consuming optical characterization by the internal light source [58] or the endfire techniques. Vertical hole shape and hole depth can easily be extracted from SEM micrographs [99], whereas sidewall roughness can only be qualitatively estimated due to the 2D nature of SEM images. This qualitative information is insufficient to relate the surface roughness to other PhC properties like propagation loss [74] or carrier lifetime [149]. Therefore, other characterization methods for sidewall roughness are required. Several tools and methods were proposed in the literature:

- Electron-probe-surface-roughness-analyzers use a SEM with four secondary electron detectors at different locations with respect to the sample to extract the surface profile [150]. This method allows a fast and simple measurement of the roughness. However, it is not reported to be applied to hole surfaces. Furthermore, the equipment is not widely available.

- Transmission electron microscopy (TEM) [151]. In consequence of the measurement method, only 1-dimensional roughness profiles (cross-section through the rough surface) can be obtained. A full 2D mapping of the roughness is not possible.

- Atomic force microscopy (AFM, [152]) using a special mask pattern (staircase pattern of etched semiconductor fins [153]).
• AFM using a modified scanning process with a lateral instead of vertical feedback loop and with a boot-shaped tip [154] to extract surface roughness.

However, all these methods were so far applied only to flat surfaces and not inside of cylindrical holes, or require special techniques or equipment which is not widely accessible. As shown before, the etching results differ between large area openings and high aspect-ratio holes. Therefore it is important to directly investigate the etched holes themselves. To the best of our knowledge, only Rong et al. [155] have used AFM-scanning so far inside etched holes to report a rms surface roughness of 0.8nm. They, however, scanned only a very small (17x15nm) window to avoid the influence of the hole curvature but miss long-range roughness caused by a non-circular hole shape. We now present the extension of this method to much larger scanning windows by subtracting the three-dimensional conical vertical hole shape from the scanned surface. We are therefore able to quantify surface roughness and the deviation from the ideal desired hole shape. For the measurement of the sidewall roughness with the presented method, only conventional AFM scanning technique is required.

### 4.2.1. AFM scanning method

To assess the hole surface roughness, we fabricated holes with a radius of ~170nm, arranged on a triangular lattice. As it will become obvious later, it is important to mention that the holes are exposed as octagons to gain patterning speed during EBL writing. The PhC arrays are tilted by ~1° with respect to the semiconductor crystal orientation, in order to intersect holes with different cross-section depth in a cleaving plane (crystal plane). The total size of the PhC is sufficiently large (~15μm x 80μm) to yield several holes with suitable (see Figure 55) cross-section depth at the cleaved surface and to have enough spatial tolerance when cleaving through the hole array.

![Figure 53](image.png)

*Figure 53:* Schematic of the cleaved surface of a PhC array and the scanning window. The scanning window covers several holes with different shallow cross-section depths (right-hand side of the sample). The white box marks holes suitable for scanning and fitting.

For AFM scanning, the samples are mounted on a carrier plate in such a way that the cleaved facet faces towards the scanning tip of the AFM. Figure 53 presents a schematic of the scan procedure. The cleaved facet is scanned by the AFM, whereby the fast scan direction (x) is perpendicular to the holes, and the holes are scanned from
4. Hole characterization

bottom to the top. The scan is performed on an Asylum Research AFM in tapping mode with conventional MicroMash NSC35 tips. The radius of the apex is smaller than 10nm and the tip is pyramid-shaped with a full tip cone angle of 30° and a height of ~22μm, according to the manufacturer (Figure 54). The tip-surface distance is reduced by lowering the setpoint (compared to the standard settings of our AFM) until the tip resolves the hole profile. The measurement is aborted as soon as the tip leaves the cleaved surface to avoid damage of the tip.

![Figure 54](image)

**Figure 54:** SEM images of the AFM tip at different magnifications. The image with the highest resolution allows estimating the tip-radius smaller than 12nm. The effective radius is most likely smaller but cannot be resolved by the SEM.

Due to the pyramid-shaped AFM tips, the measurement must be restricted to holes with a shallow cross-section depth. Only the apex of the tip should be in contact with the sample. To estimate the maximum measurable hole cross-section depth without touching the sample with the side of the tip, we use the 2D model presented in reference [156]. Within this model, the scanning tip is approximated by a sphere mounted on a pyramid shaped support. Only a 2D cross-section is considered. The scanning process is modeled by touching the surface with the tip in one point. On flat surfaces, this is the apex sphere of the tip, but while scanning high aspect-ratio structures, the pyramid shaped support may come into contact with the structures and strongly distort the obtained image. This defines the maximum measurable cross-section depth. The limit is reached when the tangent to the hole arc at the top of the hole cross-section is parallel to the sidewalls of the tip support (point $x$ in Figure 55). For holes with radius $r=170$nm and assuming the dimensions of the tip given by the manufacturer, the maximum cross-section depth is $r[1-\sin(15°)]=126$nm This corresponds to an opening angle of the hole arc of 150°.

This value is an upper limit. We even limit ourselves to hole cross-section depths below 90nm (corresponding to an opening angle of the hole arc of 124°) to be on the safe side. This ensures that the top contact point is always located on the sphere of the apex and the pyramid-shaped tip sidewalls do not interfere with the sample. Extreme tip-surface orientations are avoided.
We now discuss the measurement procedure. The curved hole arc is discretized at equidistant locations along the scanning direction. This results in an uneven sampling along the curve of the hole, notably in a reduction of the number of scanned points per unit arc towards the edges of the holes. With our choice of dimensions, the resolution per unit arc is doubled in the middle of the hole arc as compared to the edges. As long as the roughness is homogeneous over the entire hole sidewall, this will not affect the quality of the presented results.

Although AFM is able to provide nanometer resolution (1nm, [152]) in the vertical direction (along with the tip axis), the lateral resolution (perpendicular to the tip axis) is worse. It is limited by the tip shape and the hard- and software of the scanning equipment. As lateral resolution, we define the minimal distance between two obstacles on a flat surface for which they are identified as separate objects.

- The discretization of the sample surface is limited by the hardware and software of the AFM equipment (analog to digital converter). For our Asylum Research AFM, memory constraints of the software and the size of the required scanning window for a full hole cross-section limit the resolution to 1 to 2 sampling points per nm². This limit can be pushed down by reducing the scanning area, but then the full hole does not fit into one scan.
- The relation between the dimensions of the roughness and the tip-shape determines the lateral resolution of the AFM. Deep and narrow grooves do not allow the same resolution as shallow features. Values down to 3nm are reported in reference [152] for a simple case. However, to the best of our knowledge, no detailed report that discusses the aspect of lateral resolution of AFM is published.

Coming back to our simple model [156] for AFM scanning, we estimate the lateral resolution of our scanning procedure. We use a topography for the roughness depicted in Figure 56A. The groove of depth h and width d is scanned. We make the following
assumptions: (i) the distance $d$ is smaller than $2\cdot R$, as we are interested in fine roughness on the surface (ii) the groove is too deep for the tip to touch the bottom. Under these assumptions, we calculate the measured depth $h'$ (Figure 56a) of the groove to be

$$h' = R - \sqrt{R^2 - \left(\frac{d}{2}\right)^2} \iff d = 2\cdot\sqrt{2\cdot R \cdot h' - h'^2}.$$  \hspace{1cm} (4.2)

The measured depth $h'$ must be of course larger than the vertical resolution $\delta_{\text{vert}}$ of the AFM to recognize the structure, $h' > \delta_{\text{vert}}$. Using this equation with $R=10\text{nm}$ (value from the tip manufacturer) and $\delta_{\text{vert}}=1\text{nm}$ (value from the reference [152]), the lateral resolution is >9nm. This limit is caused by the overestimate of the actual width of an object on the surface (Figure 56B). The excess width $w$ per side is $w=4.5\text{nm}$.

Figure 56: Definitions of the variables used for the estimate of lateral resolution. A) for a groove and B) for a hill.

Although these calculations use a very simple 2D model, we state that the lateral resolution is in the order of 10nm due to the rounded tip-shape. From the equations, it is obvious that the resolution can only be improved if the radius of the tip apex is reduced, e.g. with carbon-nanotube tips [157]. The found lateral resolution is insufficient to resolve every detail of the hole surface (e.g. the openings in the hole sidewall, as shown in Figure 38). Therefore the roughness of the holes is underestimated.

The direct extraction of the RMS roughness from the AFM micrographs is only possible for flat surfaces. For non-flat surfaces, the roughness must be separated from the topography of the scan. To obtain a value for the hole sidewall roughness without being limited to very small scanning windows, the overall hole profile must be subtracted from the measured data. The subtraction was carried out for each fast line scan (x-coordinate in Figure 53) to ensure insensitivity to AFM drift and the conical vertical hole shape. Figure 57 illustrates the fitting procedure. The required data processing steps are:

1. The raw data from the AFM is first leveled by subtraction of a possible tilt of the sample. The scanning window compasses not only the hole arc, but also a part of the adjacent flat cleaved facets on both sides. A linear fit through the scan-points in these flat regions is subtracted from the whole scan line. Figure 58a shows a typical subset of an AFM scan after this processing step.
2. The scan area is automatically separated into hole area and the cleaved facet area by intersecting the scan with a threshold plane (Figure 57) lower than the cleaving plane. The offset between the surface and threshold level is chosen to be larger than the tip radius of curvature (10nm) to suppress the complex convolution of the tip apex with the edge of the hole cross-section.

3. Each scan line is fitted to a circle. The three variables circle centre \((x_0, y_0)\) and its radius \(R\) are free parameters for the fit. The norm

\[
\sum_i \left( (x_i - x_0)^2 + (y_i - y_0)^2 - R^2 \right)
\]

is minimized for the fitting procedure, whereby \(x_i\) and \(y_i\) are the measured data points on the arc representing the hole sidewall. Although octagons are patterned with EBL, a circle is a reasonable first order analytical approximation for the rounded hole shape at nanometer scales\(^{23}\). We will subsequently quantitatively analyze the error of this assumption. Furthermore, the fitting algorithm for octagons is considerably more complex than for circles. To the first order, the fitted circle radius \(R\) represents the fabricated hole radius reduced by the radius of the tip apex.

4. To quantify the RMS roughness, we use the value \(R - r_i\), where \(R\) is the fitted hole radius and \(r_i = \sqrt{(x_i - x_0)^2 + (y_i - y_0)^2}\). \(R - r_i\) represents the deviation of the fabricated hole from a perfect circle for each scanned point. The whole hole segment below the threshold plane is used for the RMS calculation. The RMS is calculated according to

\[
\text{RMS} = \sqrt{\frac{1}{n} \sum (R - r_i)^2}
\]

The processed AFM scan after circle subtraction is shown in Figure 58b. The developed data processing routine allows calculating a quantitative value for the surface roughness inside the holes. As hole radius and tip influence the measurement, the results only allow for a comparison of different results under the same scanning conditions. Absolute values are hard to achieve with AFM, as the de-convolution of the tip-shape from the measurement is difficult.

This data processing method will now be applied to the investigation of the effect of nitrogen passivation on the surface roughness.

\[^{23}\text{Fitting a perfect octagon would not improve the quality of the results, because of proximity effects and limited resist contrast, the hole shape lies in-between a true circle and an octagon.}\]
4. Hole characterization

**Figure 57:** Schematic of the data processing geometry. The measured data after leveling (thick line) is thresholded by the dashed line to determine the arc for fitting. The deviation from the perfect circular shape (dotted line) is then calculated as $R-r_i$. The inset presents the SEM top-view of a hole after ICP-RIE etching. The octagonal shape is barely visible because it is smoothed by proximity effects and limited resist contrast.

**Figure 58:** (a) Raw data of a part of the hole after flattening and drift-compensation. Note the different scales on the horizontal and vertical axes, respectively. (b) Surface roughness plot after subtracting the circular fit from image (a). Although lateral drift of the AFM does not alter the RMS roughness extraction, it is compensated for in the viewgraphs of Figure 58 by aligning the hole centers.
4.2.2. The influence of nitrogen in the etching plasma on sidewall roughness

The N$_2$ concentration in the plasma has a dominant influence on the vertical hole shape and the surface roughness. From SEM images, the balance between over- and under-passivation is qualitatively obvious (Insets of Figure 59). We apply the above-mentioned scanning and data processing technique to quantify this dependence.

Three different etching experiments were performed, whereby all processing parameters were kept constant except for the N$_2$ flux, which was set to 1.9sccm, 2.9sccm and 6sccm, respectively. The sample with 2.9sccm nitrogen flux shows the best surface quality in SEM micrographs. Seven to eleven holes with a radius of ~170nm on several samples are scanned for each process condition with the same kind of tip. The RMS roughness is determined for each hole scan individually and subsequently averaged over all scanned holes fabricated with the same process. The results are presented in Figure 59. A RMS roughness of 3.5nm, 2.5nm and 5.25nm is measured for the samples with 1.9sccm, 2.9sccm and 6sccm nitrogen flux, respectively. The measured values agree well with the qualitative impression from the SEM images. For a 2.9sccm N$_2$ flux, an optimum is achieved for which the SEM images and the measurements show minimal RMS roughness.

![Figure 59](image)

**Figure 59:** Measured RMS roughness as a function of N$_2$ flux in the etching plasma. The error bars represent the standard deviation over the scans of different holes fabricated with the same process. The insets show the corresponding SEM images. The dashed line indicates the estimated lithography-induced (see section 4.2.3) deviation from the perfect circle due to the smoothed octagonal shape.

Very small and high-aspect-ratio dint-like structures of the sample fabricated with a nitrogen flux of 1.9sccm (left inset in Figure 59) are visible. They are caused by strong isotropic chemical etching of chlorine at the top of the holes. Due to their high aspect-ratio, they are only partially resolved by our conventional AFM tips. This leads to an underestimation of the RMS roughness of the sample with 1.9sccm nitrogen flux.
4. Hole characterization

As a reference, for a flat cleaved surface we measured a RMS roughness of 0.3nm. In the best case, the roughness is still higher than an atomically flat surface. Apart from the rough surface, the octagonal patterned hole shape will have a small impact on the roughness value, as we will discuss in the next section.

4.2.3. The influence of the octagonal hole shape

To enhance patterning speed, holes are e-beam written as octagons. Due to proximity effects and limited resist contrast, the octagonal hole shape is smoothed during the processing, resulting in an intermediate contour between a circle and an octagon. This smoothed octagon shape introduces a lithography-induced deviation from the assumed perfect circle, which cannot be separated in a simple way from etching-induced roughness by our measurement and evaluation method. This results in an overestimation of the etching-induced roughness.

In this section, we provide an estimate for the contribution of this lithography-induced deviation from the perfect circle to the measured RMS roughness value. We generated with Matlab data sets of scans of hole shapes ranging from perfect circles to perfect octagons, without roughness. Intermediate data sets (smoothed octagons) are created by (weighted) averaging the data from circles and octagon data sets created with the same parameters. These data sets represent ideal scans of perfect round or octagonal holes (no surface roughness) scanned with the perfect tip (apex radius=0). The data sets were created with different hole cross-section depths with a nominal diameter of 170nm. Our data post-processing method is then applied to these sets to quantify the lithography-induced deviation.

![Figure 60: Deviation from a circular shape caused by a non-circular hole shape. The curves are obtained by applying the rms calculation procedure to numerically generated hole structures ranging from perfect circles to perfect octagons for holes with a diameter of 170nm.](image)

The results are presented in Figure 60 for a nominal diameter of 170nm. Other diameters show very similar results. The upper-most line corresponds to an octagonal hole
shape, whereas the perfectly circular hole shape obviously leads to no lithography-induced deviation from the perfect circle for all cross-sections depths. From top-view SEM micrographs, we see that the real shape of the hole is close to a circle. However, the octagonal hole shape from patterning can still be vaguely discerned. Therefore we believe that the thicker lines indicates the shapes matching best the fabricated hole shapes.

For hole cross-section depths scanned in the experiment (<90nm), we found a perfect octagonal hole shape to result in a lithography-induced deviation from the perfect circle of up to 4nm. These values drastically increases for larger cross-section depths (>110nm). The lithography-induced deviation from the perfect circle for smoothed octagonal hole shapes lies below at around 1nm and 2nm.

Therefore, the RMS measurement can partly be attributed to the lithography-induced deviation from the perfect circle due to the non-circular hole shape. This value varies strongly with the hole cross-section depth for small values (< 60nm), as seen in Figure 60. For larger values (60nm – 120nm), it is constant. The lithography-induced deviation from the perfect circle varies again strongly above 120nm, but no scans with such high hole cross-section depths are used.

4.2.4. Conclusion on surface roughness measurement

In this section, we have developed a method to quantitatively measure sidewall roughness inside PhC holes. The method only requires a standard AFM and does not rely on equipment that is not widespread in laboratories. Applying that method, we quantified the surface roughness and confirmed the qualitative observation of the roughness in SEM images. An increased accuracy of the method could be achieved by using ultrasharp and high-aspect-ratio tips, which can further relieve the restriction to shallow holes and better resolve the fine structure of the roughness.

Only limited models are available to relate the surface roughness to the effective propagation losses. Bogaerts et al. [74] extended the \( \varepsilon^\prime\)-model [69] for the losses caused by surface roughness. However, due to its simplicity, it is not capable to translate the rms-value (which is an aggregated figure for roughness without the fine details about the surface topography) into a loss figure. Therefore the relative impact of roughness to the propagation losses remains unclear from the modeling side. The most promising strategy would be a set of calibration experiments of samples with different roughness but otherwise identical holes (which is not simple to achieve), measuring from a set of samples the rms roughness and the propagation losses. As for our process, hole shape, hole depth and hole surface roughness cannot be controlled independently, such a calibration experiment would demand further process development effort. A possible strategy is the development of a wet chemistry to “smooth” the hole surface afterwards by removing the rough layer of the hole surface.

4.3. Carrier lifetime inside a photonic crystal

For active photonic crystal (PhC) based devices like lasers and semiconductor optical amplifiers, the lifetime of free carriers inside the gain region is a key parameter, as the lasing threshold is inversely proportional to the carrier lifetime and influences the cur-
rent efficiency for amplification. Unfortunately, the presence of the dry-etched periodic hole array penetrating the active core layer drastically reduces the carrier lifetime inside the PhC ($\tau_{\text{PhC}}$), as shown already in reference [158]. Carriers can then recombine non-radiatively via surface states on the hole sidewalls and therefore do not contribute to light amplification. On surfaces of the semiconductor, many recombination centers are present, due to (i) the abrupt termination of the semiconductor crystal and therewith many electrically active states, and (ii) due to impurities from the etching process. In this work, we assessed the impact of the holes on the carrier lifetime, as the process will be used later for the fabrication of active PhCs. The impact of the design and the processing is quantified.

4.3.1. Measurement setup

Carrier lifetimes were obtained from pump-probe measurements in transmission. For that, the typically used InGaAsP quaternary core layer ($\lambda_{\text{PL}}=1200\text{nm}$) was replaced by the In$_{0.60}$Ga$_{0.40}$As$_{0.88}$P$_{0.12}$ ($\lambda_{\text{PL}}=1540\text{nm}$) material that absorbs light at $\lambda=1550\text{nm}$. The pump beam then excites the charge carriers in this layer and pumps it to transparency. The attenuation of the probe beam while passing through the pumped area of the quaternary layer is inverse proportional to the excited carrier density, as they absorb the light by electron-hole recombination.

150µm×150µm large triangular PhC hole arrays with the different lattice constants $a$ and hole radii $r$ were fabricated to assess the influence of the PhC design on $\tau_{\text{PhC}}$. The effective hole diameter after processing was extracted after fabrication by top view SEM micrographs and the sidewall density (SD) was calculated [158] according to

$$\text{SD} = \frac{\text{sidewall length per unit cell}}{\text{area of a unit cell}} = \frac{2\pi \cdot r}{\sqrt{3} \cdot a^2} = \frac{2\pi}{\sqrt{3} \cdot a} \cdot \text{ff}.$$  (4.4)

Note that the SD is not scalable, as it depends not only on the filling factor ff, but also on the absolute lattice constant $a$. As mentioned in Chapter 3, the nitrogen content of the semiconductor etching plasma has a dominant influence on the hole shape and hole sidewall roughness. To explore its influence on $\tau_{\text{PhC}}$, 5 different chips were fabricated by varying the nitrogen content in the etching plasma, with flow rates varied from 2.7sccm, 3.3sccm, 3.6sccm, 3.9sccm to 5.1sccm. Each chip contained PhC arrays with several sidewall densities ranging from 0.0041nm$^{-1}$ to 0.0074nm$^{-1}$.

The carrier dynamics within the active layer region of the PhC was investigated employing the pump-probe technique in transmission. The setup is sketched in Figure 61. The output from an optical parametric amplifier producing 150fs optical pulses at a repetition rate of 82MHz with a central wavelength of 1550nm, was split into a pump beam and a probe beam and focused onto the PhC at 45° and 0° angle of incidence, respectively. Care was taken to ensure that the injected optical carrier density ($\sim 1.8 \cdot 10^{18}\text{cm}^{-3}$) was constant for all of the measured samples to avoid saturation effects. To suppress the influence of carrier excitation due to the probe beam, only the pump beam was chopped with 3.1kHz and the signal was measured with a lock-in amplifier. The temporal change of the carrier density was sampled by monitoring the background-free transmitted average probe signal as a function of the relative pump
4.3 Carrier lifetime inside a photonic crystal

probe delay time. The set-up reproducibility is verified by a variance of the carrier lifetime between the measurements below 5%. $\tau_{\text{PhC}}$ was extracted by fitting a single time-constant exponential decay to the measurement. The fitting error is less than 5% for all measurements.

![Diagram of pump-probe setup](image)

**Figure 61**: The pump-probe-setup in transmission. The setup is described in-depth in the text.

### 4.3.2. Measured carrier lifetime as a function of fabrication and design

The unpatterned InP/InGaAsP/InP wafer was found to have a bulk carrier lifetime of $\tau_b > 10\text{ns}$ (due to the long carrier lifetime, the exact value cannot be determined). The samples with the etched PhC pattern, however, show a drastically reduced carrier lifetime $\tau_{\text{PhC}}$ compared to $\tau_b$ as a consequence of the high carrier recombination velocity at the hole sidewalls [158]. Figure 62 presents $\tau_{\text{PhC}}$ as a function of the nitrogen flux in the etching plasma for different SDs. A maximum of $\tau_{\text{PhC}}$ within the investigated range has been found at a nitrogen flux of 3.9 sccm for all different designs. The investigation showed that the maximum $\tau_{\text{PhC}}$ as expected coincides with high surface quality. At low nitrogen flux ($<3.9\text{sccm}$), $\tau_{\text{PhC}}$ is reduced. We believe that this reduction is caused by the presence of the undercut due to the lack of sidewall passivation and the very rough surface at the top of the holes (compare Figure 38). This effects increase the effective hole surface and therefore the number of surface recombination centers. Also for a high nitrogen content in the semiconductor etching plasma ($>3.9\text{sccm}$), the reduced $\tau_{\text{PhC}}$ is assigned to the increased surface roughness caused by too much physical etching. The maximal observed variation of $\tau_{\text{PhC}}$ as a function of nitrogen content within a PhC design is achieved for the lowest sidewall density and does not exceed a factor of 2 (from $\tau_{\text{PhC}} = 505\text{ps}$ to $\tau_{\text{PhC}} = 910\text{ps}$). For higher sidewall densities, the $\tau_{\text{PhC}}$ behavior is less pronounced.
4. Hole characterization

Figure 62: Active layer carrier lifetime $\tau_{\text{PhC}}$ as a function of the nitrogen flux and the sidewall density. A maximum $\tau_{\text{PhC}}$ is measured for the etching process where SEM micrographs show the smoothest holes. The variation of $\tau_{\text{PhC}}$ with the nitrogen flux is more pronounced for PhC arrays with low sidewall density. The structures with high SD and low N$_2$ content (missing white diamonds) were outside the fabrication tolerance and could not be measured. The measurement error is estimated to be 5%, mainly due to the spatial precision of the delay stage. The inset shows a representative SEM micrograph for the holes with the smoothest surface (N$_2$ flux of 3.9sccm), the dashed lines indicating the location of the absorbing core region. The hard mask is still visible on top.

On the other hand, the sidewall density has a more pronounced influence on $\tau_{\text{PhC}}$. For the optimal nitrogen flux N$_2$=3.9sccm, $\tau_{\text{PhC}}$ varies by a factor of 4.6 (from $\tau_{\text{PhC}}$ =194ps to $\tau_{\text{PhC}}$ =910ps) between the smallest and highest sidewall densities. Therefore, to achieve a high $\tau_{\text{PhC}}$ in an active PhC device, a PhC design with low SD should be chosen. This implies the use of a low PhC filling factor $f_f$. However the narrowing of the photonic bandgap of triangular, hole-type PhCs[5] at small $f_f$ sets a lower limit on this $\tau_{\text{PhC}}$ optimization scheme.

4.3.3. Conclusion on carrier lifetime measurement

By measuring $\tau_{\text{PhC}}$ for different fabrication processes and PhC designs, we quantified the impact of the holes for the suitability of future active PhC devices. A maximal $\tau_{\text{PhC}}$ =910ps was found for the sample etched with optimum nitrogen flux where the smoothest surface is obtained simultaneously, which is still an order of magnitude shorter than in the unperturbed material. The maximal variation of $\tau_{\text{PhC}}$ with the semiconductor etching processes does not exceed a factor of 2. In contrast, the dependence of $\tau_{\text{PhC}}$ on the PhC SD is stronger with up to a factor 4 enhancement of $\tau_{\text{PhC}}$ for low filling factors $f_f$. From this results we conclude that an improvement of $\tau_{\text{PhC}}$ by fabrication shows only limited applicability, as other constraints like optical loss or hole shape have to be considered. On the other hand, PhC designs with low filling factors are promising to achieve high $\tau_{\text{PhC}}$. 
4.4. Summary and outlook

In Chapter 3, we have presented the fabrication technology for photonic crystal holes. This discussion ended with the presentation of the best achievable holes. In this chapter, we have characterized these holes:

- Lag effects and load effects have a significant impact on the holes. Unfortunately, they cannot be avoided at all. Therefore the exact knowledge of the behavior of the etching result under such effects is mandatory to control the reproducibility of the fabrication and the device characteristics. Especially the limited hole depth of small holes, which are required e.g. for the central hole in the directional coupler, section 6.3, influences the device properties and performance.

- SEM images give a fast but only qualitative impression of the material surface inside a hole. The quantification of the roughness from SEM micrographs fails due to the 2D nature of the images. Attempts in literature to measure roughness from etching either require special mask patterns or special equipment, and conventional AFM fails due to the corrugated surface inside a hole. We therefore developed a method to separate the corrugated surface from the roughness using conventional cross-section scans of holes, and were able to quantify the roughness inside the holes. To relate the rms value to propagation losses, a set of calibration experiments is required.

- In passive devices, carrier lifetime (CL) is not an important issue. However, with the ongoing work to extend the technology towards active photonic crystal devices, the CL inside the active layer becomes an issue, as it directly influences the pump current required for the light amplification. The PhC design and the fabrication technology greatly influences the carrier lifetime. Even in the best case (low density of sidewalls, optimized process), the CL is still reduced by an order of magnitude compared to the unperturbed semiconductor material.

Holes alone cannot provide a useful PhC device. Connections of light sources and detectors with the PhC device are required. The embedding of PhC devices in such an access structure is discussed in the next chapter.
Chapter 5

Integration of photonic crystal devices for port-to-port measurements

“There's never enough time to do all the nothing you want.”
Bill Watterson

Not only the fabrication, but also the measurement of a photonic crystal (PhC) device is a challenging task. Measurement equipment and chip size (typically 3mm wide and 3-8mm long) are orders of magnitude larger than the actual PhC device. These tiny PhC structures – seldom more than a few tens of micrometers in size – need, therefore, an optical connection to the outside world. Hence, special measurement equipment and auxiliary structures on the chip must be developed and used to obtain measurement data from the PhC devices. In this chapter, we present all relevant results with respect to these auxiliary structures on the chip for PhC device measurement, and the optical measurement setup.

5.1. Introduction

From literature, three different approaches for optical passive device characterization are commonly used. They are briefly presented below. A comparison between the different methods can also be found in Table 13 at the end of this section.

A. The internal light source technique (ILS, Figure 63A) [58] is a relatively simple approach to characterize PhC devices. Quantum wells (QW) or quantum dots (QD) are embedded into the vertically guiding core layer and excited by
an external light source from top. The generated light propagates through the PhC device to the cleaved facet. The device must be placed close (~40 μm) to a cleaved chip faced to reduce re-absorption by the non-excited QWs/QDs. Due to the short propagation distance of the light in the chip, no auxiliary lateral guiding structures are required. After leaving the chip, the light is collected by a microscope objective and projected onto the detector. By normalizing the measured transmission signal after the PhC device against the signal from a non-patterned part of the chip, the transmission spectrum of the device is obtained. As ILS measurements require no additional auxiliary structures next to the PhC device, the measurement is relatively straight-forward and fast. On the other hand, the method is limited to rather simple PhC devices, as complex access guiding structures are not part of the design.

Figure 63: Different measurement principles (sketch in lateral cross-section): A) Internal light source measurement, B) scanning near-field microscope measurement, C) endfire measurement.

B. Recently, PhC devices have also been characterized by scanning near field optical microscopy (SNOM, Figure 63B) [77, 159-161]. SNOM is a powerful tool to obtain sub-wavelength spatial information about the light distribution in a device by probing the evanescent light field. The optical power is usually delivered by external sources (laser or broadband light source) and coupled
laterally into the device. Additional auxiliary waveguides for light guiding between the cleaved facet and the PhC device must be included on the chip. The evanescent tail of the vertical light mode profile is collected from top by a tapered fiber. By scanning with the tip over the surface and linking the tip’s position with the measured collected light intensity, the evanescent field intensity distribution can be mapped. The scanning window covers either the full or a part of the PhC device.

Even time-resolved field information (real-space pulse tracking) can be obtained by interfering the collected light with a reference beam [161]. The dispersion relation in a PhC waveguide can be probed by using a so-called “standing-wave-meter” [77], realized by a reflecting terminated waveguide which gives rise to a standing wave.

SNOM measurements are slow and time-consuming, and do not deliver transmission- but rather scattering information.

C. Port-to-port measurements [28] (also referred to as endfire measurements (EF), Figure 63C) allow transmission spectrum characterization for a broad diversity of devices [162, 163]. Light is externally generated (laser or broad-band light source) and coupled into the chip from the side through a cleaved facet. Auxiliary access waveguides are required between the PhC device and the cleaved facets on both sides, as light must be guided over long (>1mm) distances. After passing the chip (auxiliary waveguides and PhC device), the transmitted light is collected and analyzed externally (optical power-meter or optical spectrometer). The transmission characteristics of the auxiliary access waveguides are superimposed to the transmission characteristic of the PhC device. Careful de-embedding of the different spectra is necessary with the help of additional reference structures. EF measurements allow us to obtain the transmission spectra from complex devices.

<table>
<thead>
<tr>
<th>Light source</th>
<th>ILS</th>
<th>SNOM</th>
<th>EF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measurement time per device</td>
<td>Short</td>
<td>Long</td>
<td>Short</td>
</tr>
<tr>
<td>Obtained data</td>
<td>Transmission</td>
<td>Field distribution</td>
<td>Transmission</td>
</tr>
<tr>
<td>Auxiliary structures</td>
<td>None</td>
<td>Incoupling waveguides</td>
<td>In- and outcoupling waveguides</td>
</tr>
<tr>
<td>Advantages</td>
<td>• Simple, no auxiliary structures required</td>
<td>• Field distribution visible</td>
<td>• Allows the measurement of complex devices</td>
</tr>
<tr>
<td>Disadvantages</td>
<td>• Light re-absorption at the quantum wells/dots • Limited to simple PhC structures</td>
<td>• Long measurement time • Very limited transmission results • Complicated measurement procedure (long learning time)</td>
<td>• Complicated de-embedding of the measurement • Access waveguide structure adds complexity to the fabrication</td>
</tr>
</tbody>
</table>

Table 13: Comparison of the different characterization methods.
Our characterization work focuses on the endfire measurement. This method is best suited to obtain the transmission spectra of our basic and more complex devices. ILS would not provide sufficient flexibility, and SNOM delivers the “wrong” information for input-output relations.

In the following sections, we will first present our measurement setup, before we discuss the design (dimensions) and transmission properties of the auxiliary waveguides. The auxiliary trench waveguides (width 3-5\(\mu\)m, section 5.3.2) between the PhC device and the cleaved facets are fabricated by etching narrow trenches (trench width 1\(\mu\)m, trench depth \(\sim\)4\(\mu\)m) on both sides of the waveguide into the semiconductor. Their fabrication was already discussed in section 3.5 and is not repeated here. The light collected by the power detector of the EF setup is attenuated by orders of magnitude compared to the source light intensity. In section 5.4, we will therefore discuss the different sources of optical power loss, before we draw the conclusions of this chapter.

5.2. The endfire measurement setup

Endfire measurements are in principle rather simple. In brief, we shine light onto the cleaved facet on one side of the chip, and measure the transmission through the chip from the other side. Figure 64 illustrates the endfire setup used in this work. The following sections will now describe the individual parts of the setup.

**Figure 64**: Schematics of the endfire setup used in this work. The light is provided by two tunable laser sources and combined in a 2:2 fiber coupler. One output of the coupler is recorded by a reference power meter, the other output is used to couple light into the chip by a lensed fiber (focus spotsize 3\(\mu\)m, working distance [WD] 14\(\mu\)m). After the chip (DUT), the light is collected by a microscope objective (magnification [Mag] x40, numerical aperture [NA] 0.65). The degrees of freedom for the alignment of the chip are indicated in the sketch.
5.2 The endfire measurement setup

5.2.1. Light source

Two basic types of light sources are suited for endfire measurements. (i) A tunable laser source in combination with a power meter, or (ii) a broadband white-light source in combination with an optical spectrometer as a detector. This work is based on tunable laser sources. The requirements for such a light source are the following:

- **High power.** The photonic crystals are lossy structures; therefore a bright optical power source is advantageous. For our application, 20mW maximal optical output power has proven to be sufficient.

- **High bandwidth.** A photonic bandgap is a structure with a large bandwidth. Typical bandwidth of the bandgap for our structures are $\Delta \nu=0.10$ around a central reduced frequency of $\nu=0.28$. This translates directly into a bandwidth from 1330nm to 1870nm with a central wavelength of 1550nm. No tunable laser source was available to cover such a broad bandwidth, and lithographic tuning [58] of the PhC devices is unavoidable. Still, a broad bandwidth of the source helps to reduce the number of tuning steps and, thus, the measurement time.

- **Stability and precision.** The optical power level and the emission wavelength of the tunable laser source must be stable and precise during the measurement.

- **Flat spectrum:** Thanks to the reference power meter at the input, a flat spectrum is not inherently necessary for our measurement setup.

![Laser source characteristics](image)

**Figure 65:** Laser source characteristics. The 13dBm level is reached from 1510nm to 1620nm, but a wider wavelength range can be used thanks to our calibration branch. The spectra overlap each other, as no laser sources with better frequency matching (less overlap) have been available.

To obtain a broad bandwidth, we combined two tunable laser sources (source 1: Agilent 81980A, $\lambda=1465$nm-1575nm and source 2: Agilent 81940A, $\lambda=1520$nm-1630nm). A total bandwidth of 160nm (instead of 100nm for a single source) is provided around the center wavelength of $\lambda=1550$nm. Figure 65 depicts the maximal output power spectrum of both sources. For the major part of the bandwidth, a power
level above 20mW (13dBm) is provided. The output signal from the sources is polarized. Agilent provides the following specs for the sources: (i) Absolute wavelength accuracy: $\pm 20\text{pm}$, (ii) Power stability at $\pm 1\degree C$ environment condition (constant temperature): $\pm 0.01\text{dB/h}$, (iii) power repeatability: $\pm 0.01\text{dB}$.

5.2.2. Fiber optics and reference beam

The output of the lasers is delivered to the samples with single-mode fiber optics. Polarization maintaining (PM) fibers are used. The two beams from the fibers are combined by a broadband 2:2 PM coupler. 50% of the light is coupled to each output branch of the coupler. The (small) deviation from this ideal splitting ratio is compensated by data calibration. One output branch is used as a reference beam and recorded by the reference power meter. The other branch is the signal beam and is coupled into the sample. Due to the reference branch, 50% of the light is lost for the signal beam. To best of our knowledge, a commercial PM coupler (-combination) with a different splitting ratio 2:x is not available.

To assure a good beam quality at the incoupling facet of the chip, the following characteristics were verified: (i) a low noise and (ii) negligible interference fringes from parasitic cavities in the fibers. We measured the spectrum of the signal beam after the lensed fiber, where the light is normally injected into the chip. It shows a noise level of only 0.02dB and the fringes due to reflections at interfaces have an amplitude of 0.02dB (Figure 66). Frequency features of the PhC devices which we want to measure are much stronger. As an example, the even mode gap of a W1 waveguide in section 6.1 introduces a dip of several dB even for the shortest measured waveguide. Therefore, the beam quality is sufficient for our measurements, and these small disturbances are not detrimental for the measurement.

![Figure 66: Power spectrum of the signal beam that is outcoupled from the lensed fiber and measured directly (without chip) by the power meter. The data is normalized against a linear fit through the data (offset removal).](image-url)
5.2.3. Light incoupling into the chip

As our light sources are not on-chip, the problem of efficient incoupling of the externally generated light into the semiconductor chip (into the auxiliary trench waveguides) must be solved.

5.2.3.1. Standard technologies for light incoupling

Standard techniques are input couplers with a lens, butt-coupling, grating couplers and prism couplers (Figure 67) [56].

- **Input couplers with a lens.** The light is directly focused on the facet of the chip (Figure 67A). Efficient incoupling can be achieved, but the alignment is difficult, as the chip cannot be pre-aligned by visual inspection. A special case of the incoupling by a lens is the use of a lensed fiber, which will be discussed in the next subsection.

- **Butt-coupling.** The light source – usually a semiconductor diode – is mounted directly on the cleaved facet of the chip (Figure 67B).

- **Prism and grating couplers.** The light can be coupled from top into a slab waveguide, either by a grating (Figure 67C) or by a prism (Figure 67D). The condition for an efficient coupling is that the k-vectors in the propagation direction must match according to equation (5.1) and (5.2) for grating and prism couplers, respectively. The coupling condition imposes a limit for the bandwidth of the incoupling.

\[
\begin{align*}
    k_{WG} &= k_{\text{free space}} \cdot \cos(\theta) + \frac{2\pi \cdot q}{\Lambda} \quad \text{for the grating} \\
    k_{WG} &= k_{\text{free space}} \cdot n_{\text{Prism}} \cdot \cos(\theta) \quad \text{for the prism}
\end{align*}
\]

*Figure 67: Different incoupling schemes: A) Lateral incoupling by a lens, B) butt-coupling, C) grating coupler, D) prism coupler.*
5.2.3.2. Incoupling with a fiber

Due to its simplicity, we have chosen to couple the light into the chip by using a lensed fiber. Because InP is brittle, it provides perfectly flat surfaces on vertical cleaved facets, which can be used to couple light into the semiconductor waveguide.

The lens of the fiber has a focal length (working distance) of 18μm and a minimal circular spot-size of 3μm (minimal spot size in the focus, 1/e² intensity decay) according to the manufacturer. The core has a diameter of 8μm. Proper spatial mode-matching between the lensed fiber mode and the waveguide mode is required for best incoupling efficiency. Due to restrictions by the fabrication and design, perfect mode matching cannot be achieved. For a detailed discussion of the optimal incoupling, the reader is referred to section 5.3.3. Here, we only briefly summarize the most relevant facts.

- **Vertical direction.** The upper cladding of the slab waveguide is thin (300nm) to ensure a good overlap of the vertical optical mode with the etched PhC holes. The vertical mode profile dimension is 487nm and 694nm for TE and TM polarization, respectively (Full width at half maximum (FWHM) for the intensity distribution, \(\lambda=1550\text{nm}\), calculated with [86]). Therefore, the vertical overlap between the slab waveguide mode and the mode from the lensed fiber (spot size 3μm) is small.

  To enhance the mode overlap between the vertical slab waveguide mode and the mode of the lensed fiber, it would be required to make the upper cladding thicker and/or to reduce the core refractive index. These measures would enlarge the extension of the vertical slab waveguide mode. However, this is not possible without losing the overlap of the light mode with the upper part of the PhC holes. Therefore, there is no degree of freedom left to optimize the mode overlap with the excitation beam in the vertical direction. In this work, we therefore accept the bad vertical mode matching and the resulting low coupling efficiency of the incoupling interface, as a good overlap of the slab waveguide mode with the PhC holes is more important to obtain meaningful measurements of a PhC device, than a perfectly matched incoupling.

- **Horizontal direction.** Horizontal light guiding (in the access structures apart from the PhC device) is achieved by laterally hard-confined trench waveguides. The only degree of freedom to achieve good lateral mode matching between the trench waveguide mode and the lensed fiber mode is the width of the waveguide at the cleaved facet. The optimal width of the trench waveguide is discussed in section 5.3.3. From that discussion, a 5μm wide waveguide yields to the best coupling efficiency (for values see section 5.4).

The 5μm wide trench waveguide at the cleaved facet with our vertical layer structure supports 15 TE(-like) modes, not all perfectly TE polarized due to the vertical slab asymmetry [41]. The properties of the modes are presented in Table 14. The Eₓ-component of the first 4 modes is shown in Figure 68. For the total incoupling efficiency, the overlap integral of all modes (with the same alignment) with the excitation beam is relevant. We here only consider the first and second order mode, as the other
modes all have a vanishing overlap integral. The total overlap integral increases only by 0.9% to maximal 55.9% including the second order mode, compared to only the fundamental mode. The maxima is, however, quite broad. We obtain an overlap integral of 55.8%-55.9% from 400-700nm horizontal offset from the center of the waveguide). In this region, between 6% and 17% of the light is coupled into the 2nd TE mode.

<table>
<thead>
<tr>
<th>Mode</th>
<th>Group index</th>
<th>Horizontal Symmetry</th>
<th>2D-Overlap integral of the mode with a Gaussian Beam of waist radius of 1.5(\mu m) (optimized position).</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fundamental TE mode</td>
<td>3.255</td>
<td>Even</td>
<td>55%</td>
</tr>
<tr>
<td>2(^{nd}) TE mode</td>
<td>3.244</td>
<td>Odd</td>
<td>20% (off-center excitation by 1.48(\mu m))</td>
</tr>
<tr>
<td>3(^{rd}) TE mode</td>
<td>3.226</td>
<td>Even</td>
<td>1%</td>
</tr>
<tr>
<td>4(^{th}) TE mode</td>
<td>3.200</td>
<td>Odd</td>
<td>0%</td>
</tr>
<tr>
<td>5(^{th}) TE mode</td>
<td>3.166</td>
<td>Even</td>
<td>0%</td>
</tr>
<tr>
<td>6(^{th}) TE mode</td>
<td>3.125</td>
<td>Odd</td>
<td>1%</td>
</tr>
<tr>
<td>Higher-order TE(^{24}) modes (7(^{th}) to 15(^{th}) modes)</td>
<td>3.166-2.3104</td>
<td>Even and odd</td>
<td>Vanishing (&lt;1%)</td>
</tr>
<tr>
<td>Optimal position considering the ground TE and the 2(^{nd}) TE mode(^{25})</td>
<td></td>
<td></td>
<td>~55.9% (off-center excitation between 0.4(\mu m) and 0.7(\mu m)).</td>
</tr>
</tbody>
</table>

Table 14: The TE-modes of a 5\(\mu m\) wide trench waveguide. Only the ground mode has a high overlap with a Gaussian beam with a waist radius of 3\(\mu m\). The odd modes have a vanishing overlap integral with the Gaussian beam for a centered excitation. The 2D overlap integral is a good approximation to the real situation, as the lensed fiber core is only 8\(\mu m\) in diameter, and therefore its beam close to a parallel beam.

![Mode-profiles (E\(_x\)-field) of the first 4 modes of the 5\(\mu m\) wide trench waveguide. Between each tick on the axis is a distance of 1\(\mu m\). The cross-hairs in the first two modes indicate the optimal position of the excitation with the lensed fiber. As for the 3\(^{rd}\) and the higher modes, the overlap integral almost vanishes, no optimal position is indicated.](image)

Figure 68: Mode-profiles (E\(_x\)-field) of the first 4 modes of the 5\(\mu m\) wide trench waveguide. Between each tick on the axis is a distance of 1\(\mu m\). The cross-hairs in the first two modes indicate the optimal position of the excitation with the lensed fiber. As for the 3\(^{rd}\) and the higher modes, the overlap integral almost vanishes, no optimal position is indicated.

---

\(^{24}\) These modes are not completely TE polarized, as the vertical slab waveguide is asymmetric. They are only TE-like.

\(^{25}\) Higher-order-modes have in any case an overlap integral close to 0, and will therefore not contribute to the total incoupling efficiency.
• Reflections. Due to the refractive index contrast between air and InP, reflections at the interface are unavoidable. The reflections can be estimated by

\[ R = \left( \frac{n-1}{n+1} \right)^2 = 28\% \text{ for } n = 3.26, \]  

using the effective refractive index of the vertical slab waveguide. Anti-reflection coatings (ARC) introduced at the facets may reduce the reflections and enhance the incoupling. However, ARC were not available for this work.

From the maximal overlap integral and the reflection coefficient, we estimate the power loss from the light incoupling into the chip to be in minimum 56% - 72% = 40% = 4dB (only the fundamental mode and second order mode overlap-integral and the surface reflection is considered). This value is lower than the measured incoupling loss in section 5.4 of around 7-8dB. However, for our calculations, we assume ideal conditions and that the waist of the focused beam is on the cleaved faced of the chip. If this condition is not fulfilled precisely, higher interface loss result, because the beam from the lensed fiber has a larger spotsize on the cleaved facet. Therefore the calculated interface loss represents a lower limit for the best achievable power transmission into the chip.

5.2.3.3. Required alignment precision

For the reproducibility of the measurements, the alignment between the waveguides on the chip and the lensed fiber is crucial. The degrees of freedom for the alignment are indicated in Figure 64.

• For the movement from device to device on the chip and the orientation of the chip along this movement direction, the sample holder can be translated along the x-direction and rotated around the z-axis manually.

• Both the input lensed fiber and also the output microscope objective (section 5.2.4) were placed on an xyz-stage, for which only x and z are motorized by a step-motor with a resolution of 50nm. The motorized x and z-axes are used for alignment, whereas the y-axis is used to control the focus of the lensed fiber/microscope objective with respect to the sample.

This configuration of the degrees of freedom allows to perform the alignment of the lensed fiber/microscope objective automatically. The proper alignment is assumed when most of the light passes through the device. The sensitivity of the alignment towards the transmitted power is displayed in Figure 69. Accepting a reduced transmission of 1dB compared to the optimum, the alignment between fiber and chip must be better than 1μm in the z-direction. The latitude for the x-axis is over 2μm. Such a precision in alignment is achievable with our step motors of a stepsize of 50nm.
5.2 The endfire measurement setup

Figure 69: Measured transmitted power as a function of the lateral (x-axis) and vertical (z-axis) displacement between the trench access waveguide on the chip and the fiber (input). The width of the trench at the facet is 5μm. Accepting 1dB variation (which is much less than typical PhC features) of the transmitted power leads to a required alignment tolerance of 2.2μm and below 1μm for the x-axis and z-axis, respectively.

For comparison with the measurement values in Figure 69, the overlap integral of the trench waveguide modes (fundamental and second order) with the excitation beam from the lensed fiber is shown in Figure 70. Also numerically, the alignment latitude for a tolerated 1dB reduced power transmission is in the order of 1μm and thus well within the capability of our endfire setup axis step motors. We can therefore expect that the alignment of the fiber to the chip is well optimized and reproducible.

Figure 70: The overlap integral of the ground mode and the second-order mode with the Gaussian beam from the lensed fiber (simulated with a 2D mode solver Lumerical [90]). The red curves are calculated for the ground mode (line: x-axis, dashed line, z-axis), the blue curves for the second-order mode (line: x-axis, dashed line, z-axis). The black lines indicate the 1dB reduced overlap integral, compared to the maximal overlap integral value at zero displacement, for each mode.

5.2.4. Outcoupling from the chip and light detection

After the chip, the light is collected by a microscope objective (magnification x40, numerical aperture 0.65) from the cleaved facet and projected through an iris (to suppress stray light) onto the InGaAs detector. The chip and the detector are fixed, whereas the microscope objective is placed on a motorized xyz-stage for precise alignment. The modal shape at the output of the chip is not relevant for the measure-
5. Integration of photonic crystal devices for port-to-port measurements

5.2.4.1. Straylight reduction

Complete material removal apart from the waveguide or wider trenches on both sides of the waveguides along the full length are not possible, because of the very long EBL writing time that would be required to expose such a large area. Therefore there is also a vertical guiding layer outside the waveguides. Several trench waveguides (typically 20-40 waveguides) are lined up in parallel. The situation is sketched in Figure 71. Two parallel waveguides form a low-loss parasitic trench waveguide in-between, which can guide straylight generated at the incoupling or on the chip. Therefore, straylight form these parasitic waveguides and the substrate (Figure 71) must be suppressed for reliable EF measurements. We mastered the reduction of the straylight by a combination of an iris with on-chip so-called “light shields”, as explained subsequently.

![Figure 71: Microscope image of the coupling region on one side of a rapid prototyping chip prior to cleaving. Both sides of the chip (incoupling and outcoupling) are identical.](image)

Figure 72A depicts the image of a cleaved facet without light shields and the iris. Next to the guided light in the trench waveguide (bright spot in the middle of the image), straylight is guided all over the chip along the slab waveguide. The (narrow) trenches on both sides of the waveguide, which do not guide light, cannot be seen in the image. The resolution of the camera is not sufficient. It is obvious that it is necessary to suppress the straylight guided by the parasitic waveguides. For that, we implemented the following measures:

- At the cleaved facet, the trenches on both sides are broadened from 1µm to up to 10µm width, to enlarge the gap between the parasitic and the trench waveguides. As there is only air in these gaps, no (stray) light can be guided there. These so-called “light shields” protect the detector from the straylight in the vicinity of the guided signal beam (Figure 72B). The width of these light shields is limited by the writing time on the EBL system.
• An iris is placed after the microscope objective. It shields the straylight that is far away from the guided signal beam (Figure 72C) which is not suppressed by the light shields. However, it cannot shield the straylight in the very vicinity of the guided mode, as the iris cannot be closed enough.

**Figure 72:** Collected signal with the IR camera (schematics): A) No measures against straylight, B) with on-chip light shields, C) with the iris, D) both measures combined. The dashed red areas indicate the regions that are suppressed by the iris and/or light shields.

Both measures together allow the total protection of the detector from straylight, as shown in Figure 72D. Note that no straylight is seen above or below the slab waveguide in the infrared camera.

### 5.2.4.2. Alignment of the microscope objective to the chip

**Figure 73:** Measured transmitted power as a function of the lateral (x-axis) and vertical (z-axis) displacement between the trench access waveguide on the chip and the microscope objective (output). The width of the trench at the facet is 5μm. Alignment tolerances of up to 12μm are measured, within no change in the transmitted power is observed.

Compared to the required precision for the alignment between the lensed fiber and the chip (see section 5.2.3.3), the alignment requirement for the microscope objective is much more relaxed. Figure 73 shows the measured transmitted power as a function of the placement of the microscope objective. Thanks to the large detector size (several
millimeters in diameter) and the use of free-space optics, we do not observe a significant change of the transmitted power over a displacement of the microscope objective of up to 6μm in each direction. As our step motors have a stepsize of 50nm, well-controlled alignment of the output detector can be achieved.

5.2.5. Light detector and measurement
The signal and the reference light beams are recorded by two InGaAs-detectors from Agilent. The detector covers the full range of both tunable laser sources. The reference beam must be attenuated (-6dB), because the unattenuated power would be almost outside the allowed power range specification for the detector (-90dBm to 10dBm). According to the manufacturer, the power meter has an accuracy of ±3.5% and a noise level of <5pW. With closed measurement setup cover, a background power level maximal -68dBm is measured. However, straylight in the chip raises the noise level to around -35dBm. The straylight there comes from multiple scattering of the light from the laser source inside the cover (not necessarily passing through the chip).

<table>
<thead>
<tr>
<th>Cover</th>
<th>Room light</th>
<th>Setup under direct illumination</th>
<th>Noise</th>
</tr>
</thead>
<tbody>
<tr>
<td>Laser off</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Closed</td>
<td>On</td>
<td>Off</td>
<td>Below threshold</td>
</tr>
<tr>
<td>Laser on</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Closed</td>
<td>On</td>
<td>Off</td>
<td>-68dBm</td>
</tr>
<tr>
<td>Open</td>
<td>On</td>
<td>Off</td>
<td>-55dBm</td>
</tr>
<tr>
<td>Open</td>
<td>Off</td>
<td>Off</td>
<td>-65dBm</td>
</tr>
<tr>
<td>Open</td>
<td>On</td>
<td>On</td>
<td>-45dBm</td>
</tr>
</tbody>
</table>

*Table 15: Measured background noise of the measurement setup for different conditions of the light in the room and open or closed setup cover (without the chip).*

Fabry-Perot-fringes in the measurement are unavoidable due to the reflections at the cleaved facets, except for very lossy devices. They can be used for the measurement of waveguide losses using the fringe-contrast method. The fringes (typical fringe spacing ~0.1nm) are recorded with high resolution (typically δλ=0.001nm) over a very narrow frequency range (Δλ~1nm). Such a measurement takes up to one hour.

For the broadband transmission measurement of PhC devices, the resolution must be reduced to typically δλ=0.5nm too keep a reasonable measurement time (~20min per device). Hence, the fringes are now not sufficiently resolved to remove them by Fourier analysis. They are removed by smoothing the measurement data over several fringe periods, although this reduces the frequency resolution of the measurement.

5.3. Access waveguide structures
In this section, we discuss the influence of the lateral dimensions of the waveguide (section 5.3.2) and the incoupling section (section 5.3.3) on the optical power transmission through the chip.
5.3 Access waveguide structures

5.3.1. Single-mode ridges vs. multi-mode trench waveguides

Single-mode waveguide operation allows for a good control of the light coupling and propagation. The beam power propagates in the same mode. As soon as several modes are involved, a precise control of the propagation behavior and a calculation of the reflection and transmission coefficients from a waveguide interface become difficult. It is not a priori clear in which mode(s) the light propagates, and all modes may have different k-vectors and, therefore, different dispersion characteristics. Furthermore, imperfections of the fabrication unpredictably scatter the light between the modes.

5.3.1.1. Trench waveguide modes

For our measurement, mostly 5μm wide trench waveguides fabricated with the rapid prototyping process (section 3.5.2) are used. Figure 74 presents the number of modes and their mode refractive index as a function of the waveguide width. Single-mode waveguiding is only achieved for a waveguide width below 437nm and 288nm for TE and TM polarized light, respectively, for our material system. Due to the slab waveguide asymmetry, not all modes are perfectly polarized [41]. As it will be shown in section 5.3.2, such narrow trench access waveguides suffer from huge losses due to surface roughness. They are therefore not suited for guiding light through the whole chip (1-3mm), and wider waveguides with far lower losses must be used.

Figure 74: TE and TM modes of a trench waveguide with the vertical layer structure used in this work, as a function of waveguide width. Only the perfect polarizations are shown (not the TE- and TM-like, except for the ground TE mode [white triangles]). The waveguide is single-mode for a width below 437nm and 288nm for TE and TM polarized light, respectively. For comparison, the single-mode width for a ridge waveguide (300nm etch-depth) in our material system is at 1.75μm. All values calculated for λ=1550nm.

5.3.1.2. Mode-conversion in the multi-mode trench waveguide

The requirement for single-mode waveguide operation can be fulfilled by the endfire process (section 3.5.1). The required spatial dimensions are well within the fabrication
tolerances of the process. It is favorable for processing to etch the ridge down to the core layer (300nm etch depth) due to its etch-stop capabilities. For this depth, the width of the ridge waveguide for single-mode operation is 1.75μm and 1.46μm for TE and TM polarized light, respectively. Such ridges widths can be easily patterned by photolithography, and exhibit only low losses.

However, the endfire process is unpractical for device development. The long processing time (several weeks per run) impedes the rapid development cycles for novel device designs. Therefore, the rapid prototyping process is used (section 3.5.2) despite its unfavorable multi-mode trench access waveguides.

These multi-mode trench waveguides may suffer from mode-conversion between the TE-modes in the waveguide. Such a conversion is difficult to control or simulate, and may further depend strongly on the exact incoupling at the beginning of the waveguide. At the end of the waveguide, before the incoupling into a single-mode (PhC) device, the unknown distribution of the energy between the modes makes a controllable incoupling difficult.

To exclude that our measurement – and especially the comparison between the measurements of different devices on the same chip – are spoiled by mode conversion and the resulting “arbitrary” incoupling efficiency into the single-mode part of the (PhC) device, we verified that the multi-mode waveguides are not a limiting factor for our measurement. For that, we measured a multi-mode ridge waveguide of 5μm width, including in the middle a short single-mode trench waveguide (width 400nm) section including interface tapers to the wide trench waveguides. The transmission spectrum was measured several times, re-aligning the setup between the measurements. We only observe a standard deviation 0.4dB between the measurements, over the full spectrum. Therefore we can conclude that reliable measurements are possible with our setup and the chosen auxiliary trench waveguides, despite the risk of mode-conversion in the waveguides.

5.3.1.3. Conclusions

Although multi-mode behavior is not favorable, it must be tolerated and controlled to achieve low propagation losses in trench waveguides. The reproducibility of the alignment procedure and the down-conversion from the multi-mode trench waveguide to a single-mode trench waveguide for incoupling into the PhC waveguide was verified by aligning and measuring the same access trench waveguide – including a short single-mode section – several times. The standard deviation from measurement to measurement is only 0.4dB, and therefore sufficiently low compared to the frequency features we observe in PhC devices (compare with Chapter 6).

5.3.2. Trench waveguide propagation losses

In contrast to shallow-etched (~300nm) ridge waveguides, the etched sidewalls of the used trench waveguides with their substantial roughness and imperfections strongly scatter the guided light. We have measured the optical propagation losses for different trench waveguide widths. The fringe-contrast method was used (appendix B, reference [71]), which makes the measurement independent of the incoupling efficiency.
The results for different trench waveguide widths are presented in Figure 75. The losses increase with decreasing trench waveguide width. For the use of the trench waveguides as access waveguides, single-mode operation (below a width of ~437nm) is out of reach due to the high losses that are expected for these thin waveguides. For trench waveguides wider than 3μm, however, the loss reduction is only marginal and not much is gained by making them wider. Therefore we conclude that the best width for our trench waveguides is between 3μm to 5μm, with a propagation loss of around 8-9dB/cm. Wider trench waveguides suffer from incoupling difficulties and a worse incoupling efficiency (see section 5.3.3), and are therefore less suited as access waveguides.

**Figure 75**: The propagation losses in a trench access waveguide as a function of its width. Because of its very high loss value, single-mode propagation losses values could not be measured quantitatively. All the measured trench waveguides do not include tapes at the cleaved facets, to avoid effects from tapering.

### 5.3.3. Incoupling taper design

In the previous section, we determined the optimal trench waveguide width to be higher than 3μm, with respect to acceptable propagation loss. In this section, we will discuss the incoupling into the waveguide in more detail. As a result we will show that we should not use waveguides wider than 5μm.

A good spatial mode-matching of the light spot from the lensed fiber and the trench waveguide mode is crucial. Therefore, we investigate the dependence of the incoupling efficiency (mode overlap) as a function of the beam (from the lensed fiber) properties and the trench waveguide width. Figure 76 presents the overlap integral for
three different circular spot sizes/waist\textsuperscript{26} diameters of the exciting beam. The relative position of the modes is optimized with respect to maximal power transmission. The values presented in Table 14 and Figure 76 do not include reflections from the index contrast between the air and the semiconductor slab waveguide at the cleaved facet. They are added separately to the loss balance (section 5.4).

- For the used fibers (waist diameter 3\,\mu m, working distance 14\,\mu m according to the specification of the manufacturer) with the waist of the beam exactly on the cleaved faced (ideal case), we see that the overlap integral only marginally changes between 3\,\mu m and 8\,\mu m waveguide width (Figure 76, blue line). The maximal overlap integral is only 55\% for the fundamental mode. This low value is caused by the low vertical mode overlap due to the small vertical extension of the waveguide mode. Horizontally, the matching can be optimized by the trench waveguide width.

- Better overlap integral values can be achieved with a smaller waist radius of the Gaussian input beam (Figure 76, red line, waist diameter 2\,\mu m). As the spot-size is smaller, the vertical mode matching is better, and the horizontal mode matching can again be optimized by using a narrower waveguide. The smaller spot size therefore results also in a shift of the maximum overlap integral towards lower trench waveguide width and results in a better maximal overlap integral (75\%, Figure 76). However, fibers with such small spot sizes are not available for this work.

- For beams with larger waist diameters, or when the illumination is out-of-focus (resulting in a larger spot size), we observe the opposite trend (Figure 76, green line, waist diameter/spot size 5\,\mu m). Due to the worsened vertical mode matching, the maximal value is decreased to 38\%, and the maximum is shifted towards higher trench waveguide widths.

From the calculation of the overlap integrals, we see that a small spot size is beneficial for a high incoupling efficiency, as long as we adjust the width of the trench waveguide at the facet to the smaller beam waist radius. As 3\,\mu m is the smallest available spot size for a lensed fiber, a trench waveguide width of 3-5\,\mu m is the optimal size with respect to incoupling. Larger waveguide widths have lower incoupling efficiency, but only marginally lower (<1\,dB/cm) propagation losses. Therefore there is no gain for larger waveguide widths. 3-5\,\mu m waveguide width represents an optimum with respect to incoupling efficiency and propagation losses.

\textsuperscript{26} Waist diameter denotes the smallest diameter of the Gaussian Beam (1/e\textsuperscript{2}-decay in the lateral intensity profile), whereas spot size refers to the diameter for the illuminated spot on the cleaved faced. If the Gaussian Beam is focused on the cleaved facet, both figures yield the same value. For all other cases, waist diameter < spot size.
5.3 Access waveguide structures

Figure 76: Overlap-integral between the fundamental TE mode of the trench waveguide of different widths and the beam from the lensed fiber, for different Gaussian beam waist radii. The relative position between the modes was optimized with respect to maximize the overlap.

5.3.4. Design guidelines for the access waveguides

Summarizing the results from the preceding sections, we recommend the use of a very simple design for the access trench waveguides:

- **Waveguide width between 3-5μm.** Narrower waveguides lead to higher losses, and wider waveguides support more modes without reducing the propagation losses substantially, but lower the incoupling efficiency. Only shortly before the PhC-device, the trench access waveguides must be tapered down to the PhC waveguide width.

- **Avoid any tapers at the input and output of the fibers.** There is no benefit from different waveguide widths at the input cleaved facet and the rest of the waveguide, with respect to our propagation loss measurements and also with respect to the simulated overlap integral between the beam and the waveguide mode (Figure 76). Both factors yield the same optimum. On the other hand, tapers may lead to mode conversion, which is hard to control and introducing additional hassles for reproducible measurements.

- **De-embedding:** For every measurement, the contribution of the transmission spectra from the access waveguides must be de-embedded to obtain the device properties. The procedure for the de-embedding depends on the device characteristic that needs to be measured. The following methods are used:
  - **Cutback-method:** Comparison of the transmission spectra of devices (e.g. a waveguide) of different length. The slope of a linear fit to the measurements, plotted in the power vs. device-length diagram, provides the propagation losses of the device (used e.g. for the W1 propagation losses, section 6.1).
5. Integration of photonic crystal devices for port-to-port measurements

- **Reference-device**: Comparison against a reference device of the same structure, but without the feature in which we are interested in (used e.g. for the losses introduced by a PhC bend, section 6.2).

- **Normalization**: If light is split into two (or more) branches, the different intensities in the branches can be used to normalize the output signal (used e.g. for the directional couplers, section 6.3).

The exact de-embedding procedure is discussed in the corresponding sections.

- **Incoupling from the 5μm wide trench waveguide into a PhC device**. The performance and the efficiency of the incoupling into a PhC device strongly depends on the device itself. Therefore it is not possible to give general guidelines designing such an interface, without specifying the exact device, its filling factor and its operation wavelength. For example, it is well known that the incoupling into slow light requires a careful optimized interface [34] for an relatively efficient incoupling. On the other hand, incoupling into a PhC waveguide outside the slow-light region is relatively simple by butt-coupling, as shown by the measurements of a W1 waveguide in section 6.1.

### 5.4. Power budget of the endfire setup

Several sources of losses are present in the optical path of our endfire setup. In this section, we try to estimate the contribution of each source to identify the dominant factor of loss and the possibilities for improvement. We discuss the loss budget for the example of a simple trench waveguide of 5μm width, measured with the maximal available laser power at λ=1550nm. Such a waveguide is considered as the reference structure for standard PhC devices measurements. The power budget for such a measurement can be estimated as follows (compare with Figure 64):

The tunable laser source delivers a maximal power of +13.5dBm at λ=1550nm, which is perfectly coupled into the glass fibers of the endfire setup.

- The polarization-maintaining fibers are lossless (in good approximation compared to other sources of losses), but the 2:2 power combiner/splitter introduces 3dB loss of optical power.

  \[ +13.5\text{dBm} \]

  \[ -3\text{dB} \]

  Losses at air-fiber interfaces in the connectors and at the end of the lensed fiber are low (4% each) and therefore not relevant for this coarse power budget.

- The incoupling from the lensed fiber into the chip introduces additional losses of optical power, due to mode-mismatch and reflections. These effects are discussed in section 5.2.3. A lower limit for the losses of -4dB, composed by 56% transmission because of the mode overlap and additional 28% loss due to the refractive index contrast into a 5μm wide ridge is calculated. However, the real losses are

  \[ > -4\text{dB} \]
higher, as the model in section 5.2.3 describes an idealized situation. We will later give an estimate for the total loss of this interface.

- The propagation through the trench waveguide (5μm width) introduces loss of optical power. The total length of the trench waveguide is 3mm. We measured loss of -8dB/cm.

Due to the high losses in the trench access waveguide and the small (28%) reflection coefficient at the interface, multiple roundtrips of the light between the facets are not taken into account.

- The reflection at the output facet is 28% and the transmission therefore 72%, as already mentioned earlier. We neglect multiple-roundtrip light propagation.

- Loss in the free-space optics is very small. Neither the microscope objective nor the iris do block the optical power substantially.
  
  - **Microscope objective / Outcoupling**: the NA of the objective is 0.65, acceptance angle is 40°. Figure 77 shows the far field of the ground mode. Most of the light can be collected by the microscope objective (red circle) and projected onto the detector. The loss is estimated therefore below 1dB.
  
  - **Iris**: Thanks to the on-chip light shields (section 5.2.3.3), it is not required to close the iris completely. All light from the signal beam can pass the iris.
  
  - **Reflections on the detector surface**: none (-60dB, according to the manufacturer). No light is lost for measurement.

Total loss of all loss channels

As a result of all losses, an absolute power level of -1.1dBm is measured by the detector.
It was not possible to ab-initio determine the incoupling losses correctly by calculating the overlap integral and reflection, as the exact spot size of the incoming beam on the cleaved facet is unknown. Only a lower limit for the loss is obtained by considering ideal conditions for the overlap integral and the reflections. However, the real value for the incoupling can be calculated from the other known values by completing the power balance above. We estimate the incoupling loss in this case to be -6.7dB to -7.7dB, being therefore the largest contribution to the optical power loss.

The setup as in its present configuration has been proven to transmit sufficient optical power for our measurements. However, should it become necessary to improve the overall power flow through the sample in the future, the following measures would most effectively:

- -3dB is lost by combining the signal of the two tunable laser sources in the polarization maintaining splitters. So far, it is not possible to improve this value. It is no polarization-maintaining coupler available, which can combine the laser beams without the 3dB loss. To eliminate this loss source, the coupler must be removed and the setup must be operated with only one laser source.

- -2.4dB optical power is lost by propagation losses in the 3mm long trench access waveguide. This value can be reduced by choosing shallow etched ridge waveguide instead of a trench waveguide (→ endfire process, section 3.5.1), or by improving the etching process with respect to trench propagation losses (at the expense of hole quality and depth).

- -6.7dB to -7.7dB is lost at the incoupling interface, due to reflections and mode-mismatch. With the current incoupling scheme, the room for improvement is exhausted as the main limitation is the vertical waveguide structure. Different coupling schemes like polymer auxiliary taper or grating couplers [164] may enhance the coupling. The use of ARC offers only limited improvement, as reflections are only responsible for -1.4dB (28%) loss per interface. Both other incoupling concepts and the use of ARC introduce additional fabrication steps.
5.5 Summary and outlook

To characterize our devices, we have chosen the *endfire method* for its flexibility and the possibility to measure complex devices. All measurement results of PhC devices presented in the next chapter are obtained from the setup described above. But endfire measurements have the disadvantage of a complex measurement setup and the requirement for additional integrated structures (waveguides and tapers) on the chip. These demand careful de-embedding of the measured transmission spectra.

In this chapter, we first provided a description and characterization of our endfire setup. Some of the most important conclusions are:

- The losses in a waveguide depend strongly on the trench access waveguide width. Narrow trench waveguides are very lossy. Single-mode operation in the accessing waveguide cannot be achieved, as such waveguides loose too much optical power.

- The losses in the trench access waveguides and the incoupling from the lensed fiber into the chip are believed to be the main source of optical power loss of light.

- The use of multi-mode trench waveguide may disturb the reliability of the measurement. However, we have shown that for our structures, we can reproducibility measure a single-mode device (waveguide) embedded in the middle of the multi-mode access waveguide structure. Despite of the risk of mode-conversion in the multi-mode waveguides, our setup and our trench access waveguides work reliably.

The setup – as it is described here – is suited to measure PhC devices. The dynamic range of the frequency features of a PhC device is higher than the oscillations of the Fabry-Perot-fringes arising from reflections at the interfaces, and the noise of the light source. However, if finer structures must be measured, the problem of these fringes must be tackled.
Chapter 6

Photonic crystal devices

“In reality continues to ruin my life.”
Bill Watterson

In the preceding chapters, we have discussed the fabrication and characterization of photonic crystals in InP/InGaAsP. This chapter focuses on the use of the developed PhC technology to fabricate basic building blocks for optical signal processing. Starting from simple PhC waveguides presented in section 6.1, we present the PhC waveguide bend in section 6.2. Whereas bends and waveguides are elementary devices for integrated optics, we report on a more complex and advanced device in section 6.3: a PhC based power splitter. This device is a good example to demonstrate that with the help of PhC it is possible to realize optical functionalities on a smaller footprint compared to conventional power splitters.

6.1. Photonic crystal waveguides

6.1.1. Introduction

Classical waveguides in integrated optics rely in the ray optics picture on the total internal reflection between two materials of different refractive indices. Most waveguides can be classified into two types: (i) Weak index-contrast guiding (e.g. shallow-etched ridge waveguides, $\Delta n \approx 0.02$) and low light confinement and (ii) High index-contrast guiding ($\Delta n \approx 2$) and strong light confinement (e.g. photonic wires [165] or deep trench waveguides [166]). PhCs, however, rely on guiding by a photonic bandgap (PBG). By locally disturbing (“doping”) the periodic pattern, we can create light states within the bandgap. In practice we just need to connect single defects to a transmission line. The light propagates along these defects. Such a defect waveguide, based on defects in the lattice, relies not on total internal reflections, but on constructive and destructive interference caused by the periodic modulation of the refractive
The most interesting difference of such waveguides in comparison with conventional waveguides is the nonlinear dispersion relation of the guided modes. For certain frequencies, the group velocity becomes very low (slow-light regime) and the light can even be slowed down at least conceptionally to a zero group velocity.

These special PhC waveguiding properties are the most important for integrated optics. All devices presented later in this chapter are based on PhC waveguides. Its aim for finally implementing complex functionalities such as add/drop filters, all-optical switches, it is, therefore, necessary to study first a straight PhC waveguide.

6.1.2. Waveguide designs in triangular lattice photonic crystals

Many combinations of defects behave as a waveguide, as long the defects are close enough for efficient coupling. Therefore, there is a considerable variability of possible designs for PhC waveguides (Figure 78). In the following, the most common designs for a triangular lattice are presented and discussed.

- A coupled cavity waveguide (CCW) is presented in Figure 78 A and B. Such a waveguide is build from a line of defects, closely spaced but not directly connected to each other. The light can then couple from one defect state to the next and thus propagate along the row of defects. Such waveguides have interesting properties, e.g. they can exhibit strong slow-light effects [63] when the guided mode dispersion becomes flat.

- If we directly connect the defect states without separating holes in-between (as shown in Figure 78 C), waveguiding is achieved along this defect row.

- As a special case of a defect row waveguide, completely removing one or more rows of holes at last leads us to the most-used waveguide types, the Wx waveguides (x stands for the number of omitted holes), as shown in Figure 78 D (W1) and Figure 78 E (W3).

Figure 78: Different types of waveguides inside a PhC: (A) Coupled cavity waveguide by modifying the hole diameter, (B) coupled cavity waveguide by omitting holes, (C) wave guiding along a continuous line of hole of modified radius, (D) W1 waveguide and (E) W3 waveguide. The dashed circles indicate omitted holes.

27 Modifying the hole shape is theoretically also possible, but not very practical with respect to manufacturability.
Not surprisingly, these Wx waveguides therefore became the work-horse for PhC devices. The W1 waveguide is mostly used due to its relatively simple requirements on fabrication tolerances (not critical to lag effects due to different hole radius nor is a shift of holes necessary) and due to its unique optical properties - the large single-mode bandwidth or the pronounced slow-light regime. The often required transverse single-mode frequency operation range\textsuperscript{28} appears only in the W1\textsuperscript{[1]}. Therefore, the remainder of this chapter deals exclusively with W1 waveguides.

### 6.1.3. Dispersion relation of a W1 PhC waveguide

![Dispersion Diagram](image)

**Figure 79:** Schematic of the dispersion diagram $\omega(k)$ of the TE polarized modes of a W1 waveguide with $r/a=0.34$ and $n_{\text{eff}}=3.258$. The dark regions indicate PhC modes where no guiding by the PBG-properties can be achieved (unguided modes). Distinct features of the modes are indicated in the diagram. The insets show representative filed plots of the modes (MPB-calculation).

As mentioned above, the dispersion relation $\omega(k)$ of PhC waveguides modes is very different compared to conventional waveguides. Figure 79 presents a typical dispersion diagram of a W1 waveguide with $r/a=0.34$ and $n_{\text{eff}}=3.258$. The dispersion diagrams of PhCs with different filling factors $r/a$ are very similar. For bulk-type photonic crystals, the whole bandgap lies above the light line of the substrate\textsuperscript{[5]}.

The modes can be categorized according to their lateral symmetry into even and odd modes. The order of a mode refers to the number of nodes in of the lateral field (the order is equal to the number of nodes + 1).

\textsuperscript{28} Single-mode operation must often be required for controlling the coupling properties at interfaces.
Odd mode:

- The **second-order odd mode** in the middle of the PBG separates the even fundamental **single-mode region** into two parts. For \( r/a > 0.33 \), a higher-order odd mode appears in the PBG and sets an upper limit to the single-mode region.

- The **second-order odd mode** has for any \( k \) along the propagation direction a low group velocity \( v_g = \partial \omega / \partial k \).

Even mode:

- The **first-order even mode** spans almost the whole PBG, ending slightly above the lower bandedge (even mode-cutoff). Below the even mode-cutoff, no modes at all are supported and transmission through the PhC waveguide is not possible.

- The even mode supports a **large region of linear dispersion** in the upper half of the PBG.

- An **even mode-gap**\(^{29} \) (eMG) close to the upper bandedge (the next higher even mode lies outside the PBG) is present. The even mode-gap might lie outside the PBG for filling factors \( r < 0.34a \).

- The even mode possesses a **slow-light regime** close to the even mode-cutoff, where the group velocity \( v_g = \partial \omega / \partial k \) becomes low. This makes the W1 interesting for functionalities requiring slow-light modes. However, efficient incoupling within this frequency range is a very challenging task [34]. On the potential down-side of this effect, very high propagation losses are observed for a waveguide in slow light operation [22].

The frequency-dependence of the transmission features can be used to determine the filling factor of the fabricated sample [94], as an alternative to the measurement by SEM images. Mostly suited is the eMG of the W1 waveguide, as the position of the even mode-cutoff is very distinct in the measurement.

### 6.1.4. Propagation loss measurements

This section presents a transmission measurement through a W1 waveguide to demonstrate the performance of our PhC fabrication process. The measured transmission spectrum was acquired with the endfire setup presented in section 5.2. Cutback measurements were used to evaluate the propagation losses. Waveguides with at least three different lengths (expressed in lattice periods, 60a, 120a and 180a) have to be measured. The propagation loss is obtained by a linear fit onto the measured power transmission through the waveguides as a function of the waveguide length. The full frequency spectrum was covered by applying lithographic tuning (see section 2.1.3.2, or reference [58]). The samples were fabricated using the so-called **endfire process** (sec-

\(^{29}\) A frequency range where no (even) mode is present.
tion 3.5.1). The lossy trench waveguides are only used in the vicinity (at maximum the last few tens of micrometers) of the PhC device.

![Figure 80](image-url): Transmission-measurement through a W1 waveguide. The device was 60 (blue), 120 (magenta) and 180 (yellow) lattice constants long. The filling factor of the structure is \( r = 0.335a \), determined by the position of the eMG. The location of the different frequency features are indicated in the diagram. The single-mode regions are shaded in orange, the region outside the bandgap in gray. The thin lines show the direct measurement including the Fabry-Perot fringes caused by the reflections at the interfaces; the thick line is smoothed. The schematic dispersion relation can be found in Figure 12.

![Figure 81](image-url): Total incoupling losses (blue) and transmission losses (red) of the W1 waveguide, obtained by applying the cutback method to the measurements presented in Figure 81. The location of the different frequency features are indicated in the diagram. The single-mode regions are shaded in orange, the region outside the bandgap in gray. In the region of high incoupling loss (0.20u-0.24u), the propagation loss measurements are unreliable, as the total losses are dominated by the incoupling.

Figure 80 and Figure 81 present the result of a transmission measurement through a W1 PhC waveguide. The position of the eMG – which depends on the filling factor – was used to determine the filling factor to be \( r = 0.335a \). The even mode-cutoff is not
clearly visible in the measurement and is therefore not considered for the determination of the filling factor, as the high (incoupling and propagation) losses of the slow-light mode above the cut-off prevents a precise determination of the spectral position.

The measurement shows that the light is guided in both single-mode (SM) regions above and below the odd mode. There is no obvious difference in loss between the single- and the multi-mode (MM) region. We believe that only the even mode is excited to transmit light, because the excitation is even and the transversal symmetry is not broken. This assumption is supported by the measured dip in transmission at the frequency where the even mode-gap is located. Light guiding by the odd modes would transmit also light at frequencies in the eMG (as it is only a gap for the even mode), and the eMG would be covered by the transmission in the odd mode. Also outside the PBG (grey shaded region in Figure 80), good waveguiding properties are observed. Transmission losses between -1500dB/cm and -400dB/cm are obtained, depending on the frequency (Figure 81). For comparison, literature values listed in Table 3. Our loss values are state-of-the art for the InP bulk material system. Such high loss value forbids the use of PhCs for millimeter-distance wave guiding. The values are, however, still acceptable low for typical PhC device sizes. The directional coupler, e.g., presented at the end of this chapter has only a length of a few microns. A PhC W1 waveguide of the same length shows losses in the order of 1dB, which is acceptable.

The relative incoupling loss is depicted in Figure 81. The losses have been determined from the Y-axis intersection of the linear fit. They comprise all other loss sources apart from the W1. We observe a relative constant incoupling losses over the whole bandwidth of the W1, except for the slow light region [34]. Below the even mode cut-off the incoupling losses are huge (up to -20dB stronger), since no propagating mode exist for these frequencies and all light is reflected.

Summarizing, we were able to demonstrate successful operation of a PhC W1 waveguide. This is a prerequisite for all further devices presented in this chapter.

6.2. The optimized W1 bend*

The next step towards integrated optics is the waveguide bend. Seldom is a straight waveguide sufficient when we integrate several functionalities on one single chip. Such a bend requires low bending losses and low reflections to improve the overall light transmission on the chip.

6.2.1. Introduction

A waveguide bend is an indispensable building block for device interconnection for integrated optics. For the realization of a bend, the classical integrated optics based on low refractive-index contrast waveguides using the InP material system provides two different types of waveguide bends:

- *Weakly-guided single-mode ridge waveguides.* Low bending losses are only obtainable for sufficiently large bending radii (e.g. up to a few millimeters) in order to maintain total internal reflection. This is not compatible with dense integrated optics and boosts the cost per device.
6.2 The optimized W1 bend

- Smaller bending radii (sub-micrometer) have been achieved with lateral high-refractive index contrast, tightly-confined photonic-wire (PW) [167] or trench waveguides. Bending radii down to a few micrometer without notable loss are reported for Si PW [168]. By introducing a waveguide mirror, the radius of the bend can even be pushed down to below 1μm [169]. However, single-mode photonic wires or trench waveguides are very narrow. Such thin lamellae of only a few 100nm width are very lossy (section 5.3) because of the increased light intensity at the (rough) sidewall.

Alternatively, as light guiding in PhC waveguides relies on the PBG[5] and not on total internal reflection, waveguide bending within one lattice constant (less than 1μm) is feasible. For our triangular lattice, the bending angle of 60° is given by the lattice symmetry. Such simple bends are however subject to high light reflection due to mode conversion and modal mismatch in the bending region. To enhance the transmission of the bends, several improvements on the canonical design have been proposed (sketched also in Figure 82, a-d):

a. Adding smaller holes into the waveguide close to the bend [170]. Such an approach suffers from lag effects in the etching process due to inhomogeneous hole radius of the design.

b. Replacing the hole at the outer edge of the bend by a more complex design [23, 24]. Such an approach requires a more complicated lithography and etching process.

c. A resonant cavity in the bend with uniform hole radius is more favorable for fabrication, as e.g. demonstrated for W3 (three missing rows of holes) bends [171]. However, a W3 waveguide does not meet the requirement for transverse single-mode operation.

d. Bends of any bending angle are also obtained by stretching the lattice around the corner [172], but such an approach is, however, not easy to combine with the integration of other devices on the same lattice.

To circumvent all these drawbacks, we present here a single-mode W1 waveguide bend optimized for high bandwidth, which relies only on the local displacement of individual, uniform holes.
6. Photonic crystal devices

6.2.2. Optimization procedure

The optimization of the bend is performed in 2D, as the large size of the structure and the correspondingly large computation time makes 3D optimization virtually impossible. Our 2D computations include a frequency dependent effective refractive-index \( n_{\text{eff}}(\lambda) \) of the vertical waveguide structure. We therefore lose the scalability (section 2.1.3.2) of the PhCs and it is necessary to specify the actual lattice constant \( a=425\,\text{nm} \) of the device in the 2D simulations in order to calculate \( n_{\text{eff}}(\lambda) \). The hole radius \( r \) is chosen as \( r=0.33a \), which provides a large PBG while keeping an acceptable inter-hole distance larger than \( \sim 80\,\text{nm} \) [93] for the smallest lattice constant used for lithographic tuning [58]. Dispersion diagrams and transmission spectra are calculated with the plane-wave expansion method (using MPB [61]) and the finite element (FE) (COMSOL [85]), respectively. The 2D COMSOL simulation used for the optimization does not include loss. As radiation leakage is very low, all input power is either transmitted or reflected.

Figure 83 presents the dispersion diagram of a W1 waveguide for \( r=0.33a \). The PBG extends from \( u=0.229-0.318 \) while the odd and even W1 waveguide modes span the reduced frequency range \( u=0.234-0.318 \) within the PBG. Single-mode operation of the bend is only possible outside the frequency range covered by the odd modes. Only between \( u=0.234-0.258 \) (single-mode window B) and \( u=0.270-0.309 \) (single-mode window A), the waveguide is (even) single-mode. In the multi-mode frequency region, mode conversion between the odd and even modes will occur at the bend due to the symmetry breaking of the waveguide geometry [167]. Region A has a larger bandwidth than region B, which suffers additionally from difficult light incoupling from a trench access waveguide mode into the W1 waveguide due to the large group-velocity mismatch in the slow-light regime [34].
6.2 The optimized W1 bend

Figure 83: Schematic of the diagram of a W1 waveguide with r/a=0.33 calculated in 2D with the plane wave expansion method [61] with a frequency-dependent $n_{\text{eff}}(\lambda)$. The PBG extends from $u=0.229$ to $u=0.318$. For single-mode operation, the frequency range above the odd mode (A, $u=0.270-0.309$) has a larger bandwidth than the frequency range below (B, $u=0.234-0.258$). The insets show representative filed plots of the modes (MPB-calculation).

The power transmission spectrum of the canonical unoptimized 60° bend is presented in Figure 84. It has been simulated with the area integration method presented in section 2.3.3. Accurate results are only obtained within the two single-mode windows with this technique. This is no restriction, as we are only interested in these regions.

Figure 84: Power transmission for the unoptimized bend computed by the 2D FE method. The yellow regions in the transmission spectrum indicate the single-mode frequency range below (B) and above (A) the odd mode. High transmission in B can be achieved at the expense of a narrow 3dB bandwidth which spans from $u=0.239-0.255$ (18% of the bandgap width, arrow).
The unoptimized bend shows a narrow-band spectral response of the power transmission peaking at 99% close to in the middle of frequency range B around $u=0.245$. However, the 3dB bandwidth is small and spans only the reduced frequency range of $u=0.239-0.255$ ($\lambda=1470\text{nm}-1570\text{nm}$, $\Delta\lambda=100\text{nm}$ for $a=375\text{nm}$). This corresponds to only 18% of PBG. As a further drawback, the operation region of the bend lies in the slow-light region of the W1 waveguide, where we additional suffer from incoupling difficulties [34] due to the high group velocity mismatch.

In the upper single-mode window A, the transmission is very low. Most of the light is reflected at the bend.

Before we can discuss the optimization, we must understand technological constraints. In order to keep a good process latitude, we impose the following conditions on the optimization:

(i) The shape and diameter of the holes shall remain unchanged. This avoids difficulties with lag effects.

(ii) Holes may not overlap and must maintain a minimum distance of 80nm to avoid mask breakdown due to faceting.

(iii) Except for the vicinity of the bend, the holes are not allowed to be shifted away from their lattice position.

(iv) The bend must be symmetric in order to preserve reciprocity with respect to power transmission, meaning that the bending loss due to out-of-plane scattering should be independent of the propagation direction. The solution of the Maxwell equations is indeed only reciprocal when we consider all channels (transmission, reflection, scattering) for light propagation. As in the case of an asymmetric bend, the scattering channels are different depending on the direction of the operation direction, and therefore the behavior of the bend is different.

![Figure 85: Labeling of the holes in the bending region. Only the locations of the two black holes at the apex of the bend are parameterized within the optimizer. The arrows indicate the definition of the positive directions for the displacement values in Figure 86. The dashed circles indicate the position of holes 1 and 2 after the optimization. The background shows the field plot ($H_y$) of the optimized bend at $u=0.294$. The energy density integration areas for the simulations are indicated by the rectangles.](image)
The coupling of the even and odd modes in the multi-mode region (u=0.258-0.270) cannot be prevented. A bend always breaks the transversal symmetry of the waveguide. Therefore we must limit our operation range to the single-mode regions A or B (Figure 83) to avoid the coupling. Since the single-mode frequency range A is larger than B, it is more suitable for broadband power transmission. To broaden the bandwidth, the optimization goal is to move the operation window into this frequency range.

As shown by means of a sensitivity analysis performed in reference [28], the holes with the strongest influence the transmission are the two holes of the apex of the bend (hole 1 and 2 in Figure 85). We therefore restrict ourselves to a rigorous optimization of these two hole positions to limit computational cost. The requirement for symmetry and the restriction to only the two holes closest to the apex of the bend leaves two optimization degrees of freedom: moving the holes 1 and 2 along the symmetry axis of the bend (black line in Figure 85).

The bend is optimized by a complete parameter sweep of the location of the two degrees of freedom. For each design, the maximal power transmission, and the 1.5dB and 3dB bandwidth in the upper single-mode window A are determined. The simulation domain comprises the bend and a 16 lattice constant long input- and 13 lattice constant long output W1 waveguide (Figure 85). The energy density integration method (section 2.3.3) was used to determine the power transmission through the bend. The step size for the optimization of $\Delta x_1$ and $\Delta x_2$ was chosen to be 0.04a, corresponding to a hole position variation step of 17nm for a=425nm lattice constant. This value is a good trade-off between accuracy and simulation time (in the order of 1h per design). The maximal 3dB and 1.5dB bandwidths and the maximal power transmission in the upper single-mode window were used as optimization goals. As will be subsequently shown, all three goals can be fulfilled simultaneously.

Figure 86(a) shows the results of the 3dB bandwidth optimization. A high transmission bandwidth ($\Delta u>0.036$, corresponding to 40% of the bandgap) is achieved over a large range of hole displacements (white region in Figure 86(a)) between $\Delta x_1=0a-0.18a$, and $\Delta x_2=0.66a-0.90a$ for holes 1 and 2, respectively. The fact that the area of maximized bandwidth lies along the diagonal in the $\Delta x_1-\Delta x_2$ plot suggests that the dominant dimension for the optimization is not the position of the individual holes alone, but the distance between the two holes. The limits for the optimization are typically as follows:

- **Hole 1 ($\Delta x_1$):**
  
  **Upper limit:** The position of hole 1 for which maximal transmission is achieved extends to up to $\Delta x_1=0.18a$, solely limited by the capability to manufacture closely-spaced holes. For higher $\Delta x_1$-values, the high transmission and broad bandwidth are still maintained, but the design is outside the fabrication tolerances.

  **Lower limit:** For small negative displacement values $\Delta x_1$, the transmission at low frequencies inside the single-mode region A drops and the bandwidth therefore shrinks. The full bandwidth of this window cannot be used anymore.
• Hole 2 ($\Delta x_2$):

Both directions: Moving the position ($\Delta x_2$) of hole 2 away from the optimal position introduces sharp dips in the frequency spectra. These drop divides the usable bandwidth of single-mode region A into two parts and thus lowers the maximal bandwidth.

![Figure 86](image)

**Figure 86:** (a) 3dB bandwidth as a function of the holes shifts $\Delta x_1$ and $\Delta x_2$. A large range of shifts (bright region) allows for maximal power transmission and large bandwidth ($\Delta u>0.036$, corresponding to 40% of the bandgap). The plot for the 1.5dB bandwidth looks very similar. (b) Maximal transmitted power within the upper single-mode window A as a function of the hole shift $\Delta x_1$ and $\Delta x_2$. The circles indicate the optimized position ($\Delta x_1=0.15a$ and $\Delta x_2=0.80a$).

The 1.5dB bandwidth and the maximal power transmission are also considered for the optimization. The 1.5dB bandwidth shows similar behavior as the 3dB bandwidth in Figure 86(a), but with a slightly better performance for higher $\Delta x_1$.

Figure 86(b) shows the results for the transmission optimization. The maximal lossless (i.e., $\varepsilon''=0$) transmitted power lies above 98% for the overall region where we simultaneously achieve high transmission bandwidth.

Around $\Delta x_1=0.15a$ and $\Delta x_2=0.80a$ a maximal broad 3dB and 1.5dB bandwidth (40% and 37% of the bandgap, respectively) is achieved (Figure 87), while the distance between hole 1 and its nearest neighbor is still 0.19a (corresponds to 80nm at $a=425nm$) and offers therefore sufficient process latitude for the hole fabrication. A maximum simulated peak transmission of 99.4% is obtained (lossless case). These displacement values were therefore chosen for the optimized bend. We attribute the improved performance of the optimized bend to the smoother bend apex.
6.2 The optimized W1 bend

*Reduced frequency \[ u = a / \lambda \]*

**Figure 87:** Power transmission of the optimized bend computed with the 2D FE method. Hole 1 is displaced by \( \Delta x_1 = 0.15a \) and hole 2 by \( \Delta x_2 = 0.80a \) along the symmetry axis of the bend. The frequency range for high transmission is shifted above the odd mode, and the 3dB bandwidth has increased from 18% to 40% of the PBG.

To estimate the influence of inaccuracies induced by the process technology on the transmission characteristic of the optimized design, the region around \( \Delta x_1 = 0.15a \) and \( \Delta x_2 = 0.80a \) was simulated with a finer resolution of 0.01a (=0.43nm). For deviations from the optimized design smaller than 0.02a (=0.85nm) in \( \Delta x_1 \) and \( \Delta x_2 \), the change in the 3dB and 1.5dB bandwidths is smaller than ~5%. Such a deviation corresponds to a position variation of only 9nm at 425nm lattice constant. This precision can be achieved using electron-beam lithography. This validates the robustness of the optimized design on small variations due to the process inaccuracies.

**Figure 88:** The simulated transmission through an optimized bend with different filling factors \((r/a=0.31-0.33)\). The lines indicate the single-mode transmission window A for the corresponding filling factor. The shaded area corresponds to the frequency range for which the bend is designed (single-mode transmission window for \( r/a = 0.33 \)). The investigated \( r/a \)-range spans 0.06a, corresponding to a radius variation of 26nm at the typical lattice constant of \( a = 425nm \). Losses are not considered for these simulations.
The results presented above were obtained for \( r/a = 0.33 \). However, even a careful calibration of the design hole radius may lead to inaccurate hole radius, as the hole diameter is very sensitive to changes in the fabrication process. To judge the stability of the determined optimal bend design, we have simulated it for different filling factors (\( r/a = 0.31 \)-0.36). The outcome of these simulations is depicted in Figure 88. The plots show that the bends 1.5dB or 3dB bandwidth are only weakly affected by the hole radius variation, or are even enlarged (due to the larger bandgap for higher filling factors). Still a high transmission can be expected in the upper region of single-mode transmission window A.

However, due to the changed hole radius, the bandgap and the therefore upper single-mode window A and the high transmission range of the bend shifts in frequency. Table 16, left part, shows this observation. The lattice constant is determined by the operation point (center wavelength) \( u_0 \) of the device and the wavelength \( \lambda \) of the light source according to \( a = u_0 \cdot \lambda \). This lattice constant can be achieved with high (2\( \sigma(dx) \leq 5.4 \text{nm} \), [1]) precision. The lattice constant is chosen so that the tuning range (1470nm-1630nm) of the laser source used in our endfire setup overlaps with the bend bandwidth, for the PhC filling factor \( r/a = 0.33 \). When we obtain a different filling factor after fabrication, the bandwidth of the fabricated bend is shifted against the bandwidth of the designed bend. Therefore, we only consider the overlap of the fabricated bend bandwidth with the designed bend bandwidth with \( r/a = 0.33 \) as usable. The frequencies outside the overlap are not covered by the frequency range of the source. For our bend, a reduction of the bandwidth up to a third or 15% is observed when we miss the target hole radius by 0.02\( a \) (8.5nm at \( a = 425 \text{nm} \)) or 0.01\( a \) (4.3nm at \( a = 425 \text{nm} \)), respectively. Achieving such a precision in hole radius is a difficult task and requires careful calibration of the whole fabrication process.

<table>
<thead>
<tr>
<th>( r/a )</th>
<th>Absolute</th>
<th>Overlap with the -3dB SM range of the bend with ( r/a = 0.33 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-3dB SM range [( u )]</td>
<td>Bandwidth [( u )]</td>
</tr>
<tr>
<td>0.31</td>
<td>0.267</td>
<td>0.296</td>
</tr>
<tr>
<td>0.32</td>
<td>0.270</td>
<td>0.303</td>
</tr>
<tr>
<td>0.33</td>
<td>0.273</td>
<td>0.308</td>
</tr>
<tr>
<td>0.34</td>
<td>0.277</td>
<td>0.315</td>
</tr>
<tr>
<td>0.35</td>
<td>0.281</td>
<td>0.320</td>
</tr>
<tr>
<td>0.36</td>
<td>0.290</td>
<td>0.325</td>
</tr>
</tbody>
</table>

| Table 16: The -3dB-bandwidth of the optimized bend (optimized for \( r/a = 0.33 \)). Left part: Absolute -3dB bandwidth, right part: Overlap of the -3dB-bandwidth with the nominal -3dB-bandwidth of the bend with \( r/a = 0.33 \). The percentage value sets the bandwidth in relation to the nominal -3dB-bandwidth of the bend with \( r/a = 0.33 \). |

### 6.2.3. Bend fabrication and characterization

Optimized and unoptimized bend designs, as well as reference W1 waveguides, were fabricated using the standard endfire fabrication process presented in Chapter 3, to verify the predicted transmission enhancement gained by the optimization. The filling
factor of the fabricated device was validated using top SEM micrographs and found to be higher (r/a=0.36) than designed (section 6.2.2), due to fluctuations of the fabrication process.

Measurements were performed using the endfire setup presented in section 5.2. We apply lithographic tuning [58] to enhance the measured bandwidth. Scaled devices with lattice constants ranging from \(a=375\text{nm}\) to \(a=500\text{nm}\) in 25nm steps were fabricated. This procedure covers the whole PBG. To avoid a non-perpendicular (to the cleaved facet) out-coupling of the light at the opposite cleaved facet, the bended part of the trench waveguide turns the light propagation direction back to the perpendicular orientation.

Figure 89: Access structures to measure the bend.

Figure 90 presents the transmitted power for the fabricated structures. The upper single-mode transmission band for the fabricated filling factor \(r=0.36a\) spans from \(u=0.281\) to \(u=0.325\) (yellow region). Taking a W1 waveguide of the same unfolded length as a reference, the optimized bend shows a decrease of 3dB in transmission within the relevant single-mode window. In comparison with the unoptimized bend, however it improves the transmission by about 5dB.

To understand the measurement results, we simulated the fabricated structure by 2D FE including losses (applying the \(\varepsilon''\)-model [68, 69]). We applied again the energy density integration method to calculate the transmission. However, this method becomes inaccurate, as the energy conservation \(P_{\text{source}}=P_{\text{reflection}}+P_{\text{transmission}}\) is only fulfilled approximately (See appendix A). This inaccuracy only allows qualitative comparisons with the measurements. For all simulated devices, the distinct frequency features become smoothed with higher \(\varepsilon''\). This smoothing of the power transmission spectrum is also present in the measurement, as no distinct frequency features are visible.

In the measurement, the optimized bend shows a lower transmission than the W1 waveguide of the same length (22 lattice constants). This contradicts the (lossless) results of the optimization, where we found almost 100% transmission. Including
losses in the simulation ($\varepsilon''>0$), we qualitatively confirm that the W1 waveguide has a higher power transmission than the optimized bend, but only by around 1dB (for $\varepsilon''=0.4$). As the attenuation increases with increasing $\varepsilon''$-value, we believe that the bend shows lower transmission than the W1 because the mode penetrates deeper into the holes at the apex of the bend than into the holes along the W1 waveguide.

![Graph showing transmission through optimized and unoptimized bends](image)

**Figure 90**: Measured transmitted power through optimized and unoptimized bends in comparison with a reference W1 waveguide of the same length (total 22a). The shaded region indicates the single-mode frequency range above the odd mode ($u=0.281-0.325$). An increase of about 5dB has been achieved by the optimization. The optimized bend has a device loss of 3dB.

### 6.2.4. Conclusion on the 60° bend

We demonstrated the full optimization cycle of a 60° waveguide bend, restricting the optimization to local hole displacements for improved process control. By shifting the holes along the symmetry axis of the bend, a design was found resulting in an improvement of the 3dB bandwidth from 18% to 40% of the PBG width, with a maximum power transmission for the lossless 2D model of 99.4%. The measurement of the fabricated optimized bend showed an increase in the transmission of 5dB compared to the unoptimized bend, leading to a bending loss of 3dB.

### 6.3. Parallel PhC waveguide directional couplers as power splitters

Power splitting is another basic building block for integrated optics. The splitting of a light signal into several branches is required to feed a signal into separate paths, e.g., for a Mach-Zehnder-interferometer, or to create a monitor branch of the output power. For the latter, normally another splitting ratio than 1:1 is required. The most compact form of a power splitter is the conventional Y-branch splitter [28, 174]. Unfortunately, the simplest implementation of the splitter implemented in a W1 waveguide (Figure 91a) suffers from high reflections between 40-100% [28]. It was demonstrated that by adding a small resonant hole in the middle of the Y-junction (Figure 91b), the
reflections can be reduced close to the theoretical limit of 11% [28]. Indeed, for a symmetrical power splitter, the upper limit for transmission is 4/9 for each branch, 1/9 of the light being unavoidably reflected [28, 175]. A simple mathematical proof can be found in reference [28] on page 79. Furthermore, the influence of the position of the central hole on the power balance between both arms is large. Even a misplacement of 0.05a (21nm at a=425nm) of the central hole contributes significantly to an imbalance between the two output branches [113]. This sensitivity challenges the accuracy of the electron beam lithography tool.

Although simple, the Y-power splitter is technologically hard to control and suffers from reflections.

Thus, the objectives for an optimal implementation of the splitter are:

- No reflections to maximize power transmission and avoid parasitic reflections into the precedent device.
- Small device size to increase integration density and yield.
- Flexibility (any ratio between 1:1 and 1:0) in the splitting ratio between the branches.
- Broad bandwidth and constant coupling length (strength) for all frequencies within the bandwidth.

A promising approach for power splitters are parallel coupled waveguides (Figure 91c). Directional PhC couplers (DC) have already been widely investigated, both theoretically [176-180] and experimentally [27, 176, 181-183]. For the InP low-refractive index contrast system, to our knowledge, only Qiu et al. [27] present an asymmetric bidirectional coupler. They designed the splitter for wavelength-selective operation in an optical filter.

### 6.3.1. Introduction and theory

Conventional PhC DCs consist of two parallel W1 waveguides separated by one or several rows of holes (Figure 91c), depending on the desired degree of coupling [28]. The close proximity allows the modes to couple and transfer optical power back and forth.
Figure 92: Dispersion diagram of a W1 waveguide (blue dashed lines) and a DC (red lines) with a reduced central hole radius \( r_c = 0.25a \), restricted to the upper half of the PBG, where broadband single-mode operation is possible. The shaded area represents the area of bulk photonic bands. The quasi-single-mode region is limited by higher-order modes, and the odd mode in the middle of the PBG.

Figure 92 shows a photonic band diagram with the dispersion relation of a single W1 (blue, dashed) and two coupled W1 waveguides (red). The diagram shows that the W1 waveguide mode splits into two modes with different propagation constants \( k \). As we will show in the next paragraph, this splitting into two modes is the base for the operation principle of the DC. For the rest of this section, we focus only on the even (with respect to the center of a single W1 waveguide) W1 waveguide mode, as only this mode guarantees single-mode operation. In addition, only the quasi-single-mode region is of interest, where exactly two DC modes are supported by the parallel waveguides.

The dispersion curve of the odd W1 waveguide mode is centered in the middle of the PBG and splits it up into two halves. Two quasi-single-mode regions lie above or below the odd W1 mode. The odd/even mode splitting \( \Delta k(u) \) below the odd W1 waveguide mode depends strongly on the reduced frequency\(^{30} \) [176]. Above the odd W1 waveguide mode, \( \Delta k \) is relatively constant. Therefore the upper region of the PBG is more suited for broad-band power splitters with a frequency-independent \( L_C \).

\(^{30} \) A strong variation of the \( L_C \) as a function of frequency might raise the idea to use of the DC as a wavelength demultiplexer. Although the variation is too strong for a broad-band power splitter, it is still far to weak to design an efficient \( \lambda \)-demultiplexer with sufficient large suppression or narrow channel spacing.
6.3 Parallel PhC waveguide directional couplers as power splitters*

**Figure 93**: Modes in (A) an undisturbed waveguide, (B) in coupled waveguides and (C) at the input interface of the directional coupler.

Mathematically, the coupling of the light can be described as follows:

Only considering undisturbed (uncoupled) waveguides, each W1 waveguide supports one lateral optical even mode (single-mode operation), their electromagnetic field being denoted as $|W_{1\text{upper}}\rangle$ and $|W_{1\text{lower}}\rangle$\(^{31}\) (Figure 93A). In the DC, two different coupler modes with odd and even symmetry with respect to the middle of the two waveguides co-exist, denoted as $|\text{odd}\rangle$ and $|\text{even}\rangle$. These modes have – as visible in Figure 92 – different propagation constants $k_{\text{odd}}$ and $k_{\text{even}}$ due to their different lateral field distribution. The total resulting field at position $z$ along the DC is indicated as $|\text{DC}(z)\rangle$. Here, the origin for the $z$-direction is at the interface between the W1 and the DC. Knowing the mode properties, the DC properties can be calculated. We assume the following:

\(^{31}\) The symbol represents the whole mode of the form

$$|\psi\rangle = \hat{a}(x,y) \cdot e^{i\psi} \cdot e^{i(k_z \cdot z - \omega t)} ,$$

describing the real field distribution, its phase and the spatial and temporal evolution.
1. The DC modes can be approximated by a superposition of the undisturbed W1 waveguide modes according to

$$|\text{odd}\rangle \approx \frac{|W_{\text{upper}}\rangle - |W_{\text{lower}}\rangle}{\sqrt{2}}, \quad |\text{even}\rangle \approx \frac{|W_{\text{upper}}\rangle + |W_{\text{lower}}\rangle}{\sqrt{2}}.$$  \hspace{1cm} (6.1)

2. At the interface between the incoming W1 waveguide and the DC (Figure 93C), the spatial field distribution must match ($|\text{DC}\rangle = |W_{\text{upper}}\rangle$). Best matching is achieved by

$$|W_{\text{upper}}\rangle \approx \frac{|\text{even}\rangle + |\text{odd}\rangle}{\sqrt{2}}, \quad |\text{DC}(0)\rangle.$$  \hspace{1cm} (6.2)

Both DC modes are therefore equally excited by the $|W_{\text{upper}}\rangle$ mode at z=0. The phase of the $|\text{odd}\rangle$ and $|\text{even}\rangle$ mode is identical. A similar relationship can be found for the $|W_{\text{lower}}\rangle$ mode.

3. Both DC modes propagate along the DC with their own propagation constant $k_{|\text{odd}\rangle}$ and $k_{|\text{even}\rangle}$. At any time, the resulting field distribution in the DC is the superposition of both coupler modes:

$$|\text{DC}(z)\rangle = \frac{|\text{even}\rangle}{\sqrt{2}} e^{-i k_{|\text{even}\rangle} z} + \frac{|\text{odd}\rangle}{\sqrt{2}} e^{-i k_{|\text{odd}\rangle} z}$$

$$\approx \frac{|W_{\text{upper}}\rangle + |W_{\text{lower}}\rangle}{\sqrt{2}} e^{-i k_{|\text{even}\rangle} z} + \frac{|W_{\text{upper}}\rangle - |W_{\text{lower}}\rangle}{\sqrt{2}} \frac{e^{-i k_{|\text{odd}\rangle} z}}{2} \left( (e^{i \Delta k z} + 1) |W_{\text{upper}}\rangle - (e^{i \Delta k z} - 1) |W_{\text{lower}}\rangle \right)$$ \hspace{1cm} (6.3)

For the calculation, we use equations 6.1 and 6.2, and the relation $k_{|\text{odd}\rangle} = k_{|\text{even}\rangle} + \Delta k$. The result describes the interference between two coupler modes.

In the transmission experiment, we do not measure the electric field but the transmitted power. The transmitted power as function of the distance z can be expressed as follows:
6.3 Parallel PhC waveguide directional couplers as power splitters

\[
\|DC(z)\|^2 = \left| \frac{\text{even}}{\sqrt{2}} e^{-i k_{\text{even}} z} + \frac{\text{odd}}{\sqrt{2}} e^{-i k_{\text{odd}} z} \right|^2 \\
\approx \frac{1}{4} \left| e^{-ik_{\text{even}} z} e^{-ik_{\text{odd}} z} \right|^2 \left| (e^{-i\Delta k z} + 1) W_{\text{upper}} - (e^{-i\Delta k z} - 1) W_{\text{lower}} \right|^2 = \\
\frac{1}{4} \left( 1 + e^{-i\Delta k z} + e^{i\Delta k z} + 1 \right) \left| W_{\text{upper}} \right|^2 \\
+ \frac{1}{4} \left( e^{-i\Delta k z} - e^{i\Delta k z} \right) \left| W_{\text{upper}} \right|^2 \\
+ \frac{1}{4} \left( 2 - 2 \cos(\Delta k z) \right) \left| W_{\text{upper}} \right|^2 \\
\approx \frac{1}{4} \left( 2 + 2 \cos(\Delta k z) \right) \left| W_{\text{upper}} \right|^2 \\
+ \frac{1}{4} \left( 2 - 2 \cos(\Delta k z) \right) \left| W_{\text{lower}} \right|^2
\]

For the transformation, we used the relation

\[
\left| W_{\text{upper}} \right|^2 \left| W_{\text{lower}} \right|^2 = \left| W_{\text{upper}} \right|^2 \left| W_{\text{lower}} \right|^2.
\]  \hspace{1cm} (6.5)

This relation holds only if the two modes are in phase (this is ensured by equation 6.2). Therefore the mixed-mode terms cancels themselves out. The result above can be rewritten using a trigonometry identity to

\[
\|DC(z)\|^2 = \cos^2 \left( \frac{\Delta k \cdot z}{2} \right) \left| W_{\text{upper}} \right|^2 + \sin^2 \left( \frac{\Delta k \cdot z}{2} \right) \left| W_{\text{lower}} \right|^2
\]  \hspace{1cm} (6.6)

Equation 6.6 describes the power flow from the upper to the lower waveguide, and back. The power in a waveguide as a function of the position varies with \( \cos^2 \) or \( \sin^2 \) in the upper and lower waveguide, respectively. Figure 94 presents typical field patterns of such a power transmission between the waveguides. By ending the power splitter at the right distance \( L \) after the input, any splitting ratio of the optical power in the two branches can be obtained.

**Figure 94:** FE simulations of the \( H_z \) field of a DC.

We define the coupling length\(^{32}\) (\( L_C \)) of the DC as

\[^{32}\text{The reader should not confuse the coupling length } L_C \text{ with the length of a realization of a coupler } L.\]
\[ L_C = \frac{2 \cdot \pi}{\Delta k} \quad \text{with} \quad \Delta k = |k_{\text{even}} - k_{\text{odd}}| \]  

(6.7)

This definition is according to reference [176]. \( L_C \) is the distance required for the light to couple once to the second waveguide and back. This choice for \( L_C \) is somewhat arbitrary, and some literature may use other definitions, e.g. for coupling only once into the other waveguide like in reference [184]. \( L_C \) is related to the classical coupling constant \( \kappa \) as \( \kappa = \frac{\Delta k}{L_C} \). With \( L_C \), we rewrite equation 6.7 the following form, which is usually found in literature [176]:

\[
\| \text{DC}(z) \|^2 = \cos^2\left( \frac{\pi \cdot Z}{L_C} \| W_{1,\text{upper}} \| \right)^2 + \sin^2\left( \frac{\pi \cdot Z}{L_C} \| W_{1,\text{lower}} \| \right)^2
\]

(6.8)

### 6.3.2. Modeling

As shown in the preceding section, \( L_C(u) \) depends on the difference \( \Delta k(u) \) of the propagation constants \( k_{\text{odd}} \) and \( k_{\text{even}} \). In a basic DC design (Figure 95a), this splitting is weak and therefore the \( L_C \) is large. The goal of the optimization is to reduce the \( L_C \) by design changes while keeping a broad bandwidth and a weak change in the \( L_C \) with frequency.

To enhance the coupling between the waveguides, several modifications to the canonical design (Figure 95a, design A) can be envisaged: the separating row may have a reduced hole radius (Figure 95a, design B) [180, 183], or the holes at the outside of the coupled W1 waveguides may have a larger hole radius (Figure 95a, design C). The useful bandwidth \( \Delta u \) of the DC is the frequency range where

(i) the splitting \( \Delta k(u) \) of the modes is large and almost constant.

(ii) only two coupler modes are present, as the beating gets hard to control in the presence of three or more modes. This corresponds to the quasi-single-mode region depicted in Figure 92).

Due to the large relative size of the DC, full-wave 3D simulations are not feasible. The DCs are therefore investigated by means of 2D simulations. The hole radius for the bulk PhC is fixed at \( r=0.31a \), proving good balance between PBG width and fabrication tolerances.

Both the finite element (FE) and the plane-wave expansion (PWE) tool are used to simulate the DC. The comparison of the results between the different methods confirms the reliability of the simulation.

- For the FE simulations, \( L_C \) is obtained by fitting the function \( A \cdot \cos^2(\pi x/L_C) \) onto a line profile of the longitudinal optical power distribution in the middle of upper coupler waveguide. \( A \) and \( L_C \) are fitting parameters.

- For the PWE simulations the \( L_C \) is extracted from the \( k \)-vector splitting \( \Delta k(u) \) of the DC modes in the quasi-single-mode region.

- The bandwidth of the DC is always determined from the PWE computations.
6.3.3. Simulation results

Figure 96 represents the bandwidth $\Delta u$ and the minimal achievable $L_C$ within the bandwidth for all investigated design concepts presented in Figure 95 (standard coupler, coupler with a smaller center hole radius $r_c$, and coupler with additionally enlarged edge hole radius $r_e$). The effects of the different hole configurations are discussed in the subsequent sections. Several goals must be simultaneously met by the optimization with respect to the central and edge hole radii $r_c$ and $r_e$, respectively:

- For high yield and cheap fabrication, the final device length should be low. This requires a short coupling length $L_C$ (strong coupling).
- The benefit of using the upper part of the PBG to design a power splitter is the broad bandwidth of the devices. Although a reduction of $L_C$ must be unavoidably paid by a reduction of the bandwidth (see section ), a sufficient bandwidth for a practical application must be obtained.

Figure 95: Schematic hole configuration of the three investigated coupler designs. The red holes are different from the bulk hole radius $r_b$.

Figure 96: PWE simulations of the bandwidth $\Delta u$ (length of the lines) and minimal coupling length (the frequency dependence of the $L_C$ is shown in the following Figure 98). The red segments represent the DCs with edge hole radius $r_e=0.31a$ for different central hole radii. The blue segments correspond to designs with edge hole radius to $r_e=0.33a$, $r_e=0.35a$ and $r_e=0.37a$ for the upper, middle and lower segment of each group, respectively.
• For broadband power splitters, a weak dependence of $\Delta k(u)$ on the reduced frequency $u$ is obviously required to avoid a varying splitting ratio over the bandwidth.

It is difficult to fulfill all goals simultaneously. Therefore trade-offs have to be made. The choice of the best design must be found with respect to the specific demands of the practical application (especially the required bandwidth).

6.3.3.1. The effect of the center hole radius

The radius $r_c$ of the hole separating the two coupled waveguides has a dominant influence on $L_C$. The basic design A (Figure 95) has a $L_C$ of over 1000a. By reducing the central hole radius from $r_c=0.31a$ to $r_c=0.13a$ (Figure 96, red lines), the coupling strength is strongly enhanced and the minimal $L_C$ is reduced by orders of magnitude down to 34a. However, this reduction is achieved at the expense of the bandwidth $\Delta u$, which is decreased by a factor of 3. The decrease of $L_C$ is visualized in the field plots of the different coupler designs (Figure 97). The minimal central hole radius is technologically limited by the minimal hole radius $r_c$ that can be etched in the semiconductor, and by the required DC bandwidth.

![Figure 97: FE simulations and the coupling length $L_C$ of the $H_z$ field for coupler designs A and B (Figure 95), for different central hole radii $r_c$.](image)

6.3.3.2. The effect of the edge hole radius

Next, we discuss the impact of increasing the hole radius at the edge of the waveguides (Figure 95, Design C). As an example, the design with the central hole radius $r_c=0.19a$ provides $L_C$ as short as 52a and a bandwidth of 16% of the total PBG width. We used this central hole radius $r_c$ as fixed for the discussion of the impact of the edge hole radius $r_e$. The qualitative results are representative also for designs with different central hole radius $r_c$. We increased the edge hole radius from $r_e=0.31a$ to $r_e=0.269a$.
6.3 Parallel PhC waveguide directional couplers as power splitters*

$r_e=0.37a$. The maximal hole radius is technologically limited by the capability to fabricated closely-spaced holes. Figure 98 presents the simulated $L_C(u)$ for different edge hole radius $r_e$. Both simulation methods, FE and PWE, yield very similar results with a discrepancy below 4%.

- Increasing of the edge hole radius to $r_e=0.37a$ decreases $L_C$ by ~16%. The impact of the edge hole radius is, however, much weaker than the impact of the central hole radius (arrow in Figure 98).

- The total bandwidth of the DC is almost not affected by the increase of the edge hole radius, but it is shifted towards higher frequencies. This may lead only to a reduction of the bandwidth if it is shifted into the PhC airband (e.g. for $r_c=0.25a$ and $r_e=0.37a$ in Figure 96).

- The variation of the $L_C$ within the bandwidth is less than 10% for all DCs with fixed $r_c=0.19a$. This makes this DCs useful as broad-band power splitters at any given splitting ratio.

In contrast to the central hole radius $r_c$ which influences $L_C$ and the bandwidth, we found that the edge hole radius $r_e$ mainly influences $L_C$.

![Figure 98: $L_C$ vs. reduced frequency $u$ simulated with the FE (empty blue diamonds) and PWE (filled red squares) techniques for the different DCs. The couplers have a fixed central hole radius $r_c=0.19a$ and different edge hole radii from $r_e=0.31a$ to $r_e=0.37a$. The change of the $L_C$ within the bandwidth is below 10%.](image)

6.3.3.3. Practical coupler application

PhC devices are more complex in fabrication and simulation than conventional optical devices due to the dense spatial variation between semiconductor material and air. A fine grid is required in simulation to sufficiently resolve the strong spatial modulation of the refractive index. Furthermore, the fabrication of high-aspect-ratio holes for PhCs is challenging. Therefore PhC devices are only useful if they provide a benefit over conventional devices. In this section, the length of a 3dB PhC power splitter is estimated and compared it to a “conventional” coupled-waveguide power splitter. The PhC-based DC with $r_c=0.19a$ and $r_e=0.37a$ is considered for this comparison, as it
provides short coupling length and still feasible central hole radii (diameter ~160nm) for fabrication. The minimal $L_C$ for this design is found to be 53 periods.

The power in the different branches is given by equation 6.9:

$$P_{\text{bar}} = P_0 \cdot \cos^2 \left( \frac{\pi \cdot Z}{L_C} \right)$$

$$P_{\text{cross}} = P_0 \cdot \sin^2 \left( \frac{\pi \cdot Z}{L_C} \right)$$  \hspace{1cm} (6.9)

A 3dB coupler based on the above-mentioned design has therefore a length of $L_{3\text{dB}}=14a$. This corresponds at a device length of only $\approx 6\mu\text{m}$. Such a DC has a bandwidth of $\approx 60\text{nm}$ at $a=435\text{nm}$ (for $\lambda=1550\text{nm}$) with a coupling ratio between 47% and 55%.

![Figure 99: Simulated (2D, FEM) 3dB coupler length for a conventional, trench-waveguide based coupler. Only couplers based on very thin waveguides and/or very short separation distance between the waveguides can compete with the PhC DC. However, the fabrication of such structures imposes similar difficulties to the fabrication as the PhC DC. For comparison, the coupling length of the PhC DC is indicated by the red horizontal line.](image)

The length of the PhC DC should be compared to “conventional” directional couplers based on coupled trench waveguides with similar feature sizes in the same material system. We used the same software and simulation method to simulate trench-waveguide based directional couplers. Figure 99 presents the simulated 3dB coupler length $L_{3\text{dB}}$ for different trench waveguide widths and separation distances between the waveguide. Only for very thin and therefore lossy waveguides and for a very narrow separation distance between the waveguides, the conventional DC shows comparable coupling length as the PhC DC, for the same fabrication requirements with respect to feature size and accuracy.
6.3.3.4. Incoupling into the directional coupler

For every optical device, the reflections at the input and output port, as well as at inhomogenities within the device, are crucial for its performance. For almost all devices, such as the PhC DC or for an SOA in particular, reflections are detrimental and lower the overall power transmission. Reflections might occur at the interfaces at the entrance and the exit of the DC. A feeding and continuation of the DC with W1 waveguides is assumed. The relevant interfaces are:

- At the input of the DC, reflections can occur at the interface between the feeding W1 waveguide and the DC. This interface is discussed in this section.

- At the end of the device, the two branches of the DC need to be separated from each other. The separation is achieved in this work by coupling the output into two trench waveguides. However, when the DC is integrated into a PhC circuit, the light must be coupled into a W1 waveguide at the exit of the device. To separate the two waveguides from each other, at minimum one waveguide must contain a bend. The issue of the bend reflection has been addressed in detail in section 6.2 and will not be discussed here again. Both the DC and the bend bandwidth (see Figure 87) are optimized for an operation range above the odd waveguide mode and are therefore compatible with respect to the integration in the same PhC lattice.

We will now have a closer look to the reflections at the DC input. Reflections at an interface might occur due to mode mismatch or group velocity mismatch (Figure 100). We investigate here the impact of adding tapers to the interface between the feeding W1 waveguides and the DC to allow an adiabatic transmission [185] between the feeding waveguide and the DC.

They are realized by a linear change of the hole radius. There are obviously two different positions for a tapers:

- For the separating row of holes, if \( r_c \neq r_b \) (blue in Figure 100).
At the beginning of the cross-waveguide (green in Figure 100).

Three different taper concepts (as shown in the insets of Figure 101, a taper for the cross waveguide and/or a taper for the separating hole of row) and taper length (2, 4 and 9 intermediate hole radii steps) have been investigated for $r_c=0.31a$, 0.25a, 0.19a and 0.13a. $r_e$ was kept equal to $r_b$ for all simulations. As the results are all similar, we restrict our discussion here to the DC with the central hole radius $r_c=0.13a$, which requires the strongest taper for the central hole radius.

As the power reflections are the figure of interest, we make use of the energy density area integration method (section 2.3.3). For our investigation, the modes in the W1 and the DC are different, in contrast to the requirement for identical modes for the area integration method. As a consequence, absolute transmission values through the interface cannot be obtained. The simulation allows only quantitative comparison of different tapers and the butt-coupled interface and therefore a relative comparison between the performance of different incoupling schemes.

We investigated three different concepts of tapers to couple into the DC. (i) Tapering of the cross waveguide and the separating row of holes, (ii) tapering of the cross waveguide and (iii) tapering of the separating row of holes. These are depicted in the inset of Figure 101.

Figure 101 presents the transmission curves of the tapered designs, for $r_c=0.13a$ and $r_e=0.31a$. The simulated transmission is normalized against the untapered interface. None of the presented tapers is capable to significantly enhance the transmission over the full bandwidth. On the contrary, they may show strong dips in the transmission spectra. For the dip frequencies, the transmission through the taper is significantly lowered. No relation between the structure and the location of the dips was found.

An analysis of the $H_z$-field- and energy-density-plots of the interface at the dip frequencies (A representative sample is shown in Figure 102) shows that an intense spot of optical energy exists within the taper in the waveguides. The behavior of the transmission spectra and the field plot let us conclude that a cavity is created by the arrangement of holes of different sizes of the tapers that matches a frequency inside the single-mode window. This cavity disturbs the power flow through the taper and gives therefore rise to reflections.

In conclusion, the untapered interface is the most suited design for the W1 - DC interface. Tapers of any type do not enhance the power transmission, but accidentally create cavities within the taper give rise to reflections. Thanks to the small group velocity difference between the W1 and DC modes (see Figure 92, the dispersion curves are almost parallel) and the good spatial field matching, a taper seems not to be necessary.
Figure 101: The transmission through the W1 waveguide - DC interface with the central hole radius of $r_c=0.13a$ and $r_e=0.31a$, for different taper concepts and taper lengths. The transmission is normalized against the butt-coupled interface. The investigated area is limited to the single-mode window of the DC. The insets show the corresponding taper concept. The tapered holes are filled black. The frequency resolution is $\Delta u=0.0001$. 
6. Photonic crystal devices

6.3.4. Fabrication and measurements

The structures with central hole radius $r_c=0.19a$ were fabricated for experimental verification. A lattice constant of $a=435\text{nm}$ is used, which results in a bandwidth within the tunable range of our laser sources. Apart from the DC, the following auxiliary structures are included on the chip:

- A 10a long W1 waveguide is placed before the DC to allow the mode to settle.
- A short taper of two holes in the upper waveguide was placed in the design, as the results of the simulations presented in the section 6.3.3.4 were not known at the time of fabrication. As shown later, this taper has however no impact on the measured $L_C$.
- The waveguides are separated immediately after the DC by means of multimode trench waveguides. The width and distance of these trench waveguides are matched to the W1 waveguides. No bend is integrated into the PhC to simplify the interpretation of the results. By means of FE simulations and measurements, we have verified that the additional coupling loss by the two trench waveguides can be neglected.

Figure 103 shows as an example a scanning electron micrograph of a DC with reduced central hole radius, the W1 access waveguide including the taper and the access trench waveguides.
6.3 Parallel PhC waveguide directional couplers as power splitters

Figure 103: SEM micrograph of a typical fabricated coupler. A W1 waveguide is preceding the input of the DC. In addition, a short taper in the cross waveguide suppresses reflections between the W1 and the DC.

The device characterization is performed by the endfire technique. The reduced-frequency range of \( u = 0.267 \) to 0.296 (a=435nm) is probed. For each coupler design, couplers of 5 different lengths (10a, 20a, 30a, 40a and 50a) were fabricated. The transmission through the bar and cross states was recorded sequentially without moving the input fiber. A spectral resolution of \( \lambda = 0.5 \)nm was chosen for the tunable sources, and the raw measurements were averaged over a sliding window of 5nm to eliminate the Fabry-Perot (FP) fringes from parasitic FP cavities. The measured transmitted power \( p(u)_{\text{bar/cross}} \) was normalized for each measurement and frequency according to

\[
p(u)_{\text{bar/cross, norm}} = \frac{p(u)_{\text{bar/cross}}}{p(u)_{\text{bar}} + p(u)_{\text{cross}}} \tag{6.10}
\]

This normalization makes the measurement independent of the incoupling efficiency and the waveguides loss. For a particular frequency \( u \), \( L_C \) was extracted by fitting the normalized power \( p(u)_{\text{bar/cross, norm}} \) vs. device length curves with

\[
A \cdot \cos^2\left(\frac{\pi}{L_C(u)} \cdot x\right) \quad \text{and} \quad A \cdot \sin^2\left(\frac{\pi}{L_C(u)} \cdot x\right) \tag{6.11}
\]

for the bar and the cross state, respectively. \( A \) and \( L_C \) are the fitting parameters. As norm for the fitting procedure, the mean least square distance (RMS) over all 10 measurement points was minimized. The fitting uncertainty is on the average around 5%. Due to the normalization, the pre-factor \( A \) is not necessary. Indeed, it is found to be very close to 1. A typical fit result is shown in Figure 104 for \( r_c = 0.19a, r_e = 0.31a \) and \( u = 0.271 \). Other frequencies and designs look similar.

The measured \( L_C \) for all fabricated DCs and frequencies within the single-mode window are presented in Figure 105 together with the PWE simulations. The measured \( L_C \) amounts to 60a to 70a and is between 8a and 12a higher than the corresponding PWE simulations. The reason for this deviation will be discussed in the next section.
6. Photonic crystal devices

**Figure 104**: Fitting of the measured normalized transmitted power for the bar (red filled squares) and cross (empty blue diamonds) states vs. device length. \( r_c=0.19a \), \( r_e=0.31a \) and \( u=0.271 \). The other designs or frequencies show similar fit quality.

![Graph showing normalized transmission vs. fabricated coupler length](image)

**Figure 105**: Comparison of the PWE simulation (dashed blue line) and measurements (red line) of the \( L_C \) for the DCs with \( r_c=0.19a \). Note that the ordinate starts at 50a.

![Graph comparing PWE simulation and measurement](image)

### 6.3.4.1. Sensitivity analysis

We will discuss in this section the stability of the device under variations of the hole diameter. To estimate the impact of hole radius deviations on the \( L_C \), we performed a sensitivity analysis using PWE simulations for each hole type (hole radius of the surrounding crystal \( r_b \), central hole radius \( r_c \), edge hole radius \( r_e \)) separately. The analysis was performed by varying the hole diameter around the nominal design value. The change of \( L_C \) depending on the hole diameter change is extracted (\( \Delta L_C/\Delta \% \), change in coupling length per relative change in hole diameter, first order). The results are presented in Table 17, first column.

- The sensitivity contribution of the central hole radius \( r_c \) is the most significant with \( \Delta L_C/\Delta \%=1.6a/\% \) (Change of the \( L_C \) relative to the percental hole radius variation), as these holes are most strongly interacting to the light mode. A hole radius deviation of only 1\% (e.g. 2nm for holes of 200nm diameter) results in 3\% error in the \( L_C \). This demands a highly precise fabrication technology.
The edge hole radius \( r_e \) has the opposite influence than the central hole radius. For each percent deviation from the target radius, a decrease in coupling length of \( \Delta L_C/\Delta \% = -0.4a/\% \) must be expected.

The hole radius of the surrounding crystal \( r_b \), however, has only a minor impact of about \( \Delta L_C/\Delta \% = 0.2a/\% \) (Change of the \( L_C \) relative to the percental hole radius variation). The mode is mostly shielded from these holes by the edge holes.

Finally we discuss the deviation between the simulations and measurements results for our fabricated DCs. We used a scanning electron microscope (SEM) to record micrographs of the holes from top. These images were used to determine the hole radius after fabrication. The measured hole radius deviations are presented in Table 17, second column. The hole radius of the crystal was measured to be larger than designed, the central and edge hole radius to be smaller. This deviation is used to estimate a deviation of \( L_C \) (third column of Table 17). The strongest impact results from the central hole diameter deviation, which is responsible for an almost 15\% longer \( L_C \), whereas the impact of the other hole types is much weaker. This value is even higher than the observed value of 8\% to 12\% (Figure 105). It should however be considered that real holes are in general not perfectly cylindrical but of conical shape. The hole diameter is however measured from top, where it has the highest value. The averaged hole diameter which the light mode experiences is therefore a bit smaller. This mitigates the change in \( L_C \).

<table>
<thead>
<tr>
<th>Holes</th>
<th>Simulated coupling length variation for 1% hole-radius deviation</th>
<th>Measured deviation from nominal hole radius (SEM)</th>
<th>Expected change in ( L_C ) from the hole-radius deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Central hole radius</td>
<td>1.6a/%</td>
<td>+9%</td>
<td>14.4a</td>
</tr>
<tr>
<td>Edge hole radius</td>
<td>-0.4a/%</td>
<td>-7%</td>
<td>2.8a</td>
</tr>
<tr>
<td>Hole radius of the surrounding crystal</td>
<td>0.2a/%</td>
<td>-4%</td>
<td>-0.8a</td>
</tr>
</tbody>
</table>

Table 17: Comparison between target and fabricated hole radius and impact on the \( L_C \) by means of PWE simulations.

Table 17 allows us to estimate the requirement towards the precision of the hole radius. We consider the coupler with \( r_c=0.19a \) and \( r_e=0.31a \), showing a minimal \( L_C=53a \), and use it as a 3dB splitter. As we will see, this is the most sensitive design. Let’s assume that we accept \( \pm 5\% \) deviation from the ideal 1:1 splitting ratio. We calculate the required precision by taking the derivative of equation 6.9:

\[
\frac{\partial p}{\partial L_C} = -2 \cdot \cos \left( \frac{\pi}{L_C} \cdot L \right) \cdot \sin \left( \frac{\pi}{L_C} \cdot L \right) \cdot \frac{\pi}{L_C^2} \cdot L \leq 1 \quad \forall L \leq \frac{\pi}{L_C} \cdot L
\]

(6.12)

The product \( 2 \cdot \sin \cdot \cos \) is in maximum 1, achieved for the length of the 3dB coupler configuration \( L=1/4 \cdot L_C \).
With \( L_c = 53a \), \( L = 1/4 \cdot L_c \) and \( \Delta p = 0.05 \), we obtain \( \Delta L = 3.4a \). This means that we must have a hole radius/diameter precision for the central hole (which is the most sensitive one) of less than 2\% (according to Table 17, first row). Such a value is hard to achieve by one single fabrication shot. Equation 6.13 also implies that the device becomes more sensitive with increased device length. Therefore, it is important to design the 3dB coupler with \( L = 1/4 \cdot L_c \) and not \( L = 3/4 \cdot L_c \).

### 6.4. Summary

The design and fabrication of the PhC devices is much more challenging than for conventional optical devices. The PhC devices require precise simulation methods with a fine grid, and a well-controlled fabrication technology to achieve the desired function. Hole placement (better than 9\,nm are required, section 6.2.2) and hole diameter (better than 2\% is required, section 6.3.4.1) accuracy are crucial parameters for the devices and need to be controlled during fabrication. The placement accuracy of the used EBL system is sufficient enough for the PhC device fabrication, but the requirement for the precise hole diameter is at the limit of the technology. Dedicated fabrication equipment would be definitely required for commercial devices. Basic functions (waveguiding, bending, power splitting) using our developed fabrication technology have been demonstrated in this chapter. They are the cornerstones to build integrated optical circuits.

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33 For scientific research, several devices with slightly different filling factors can be produced, and the structures with the correct filling factor can be identified and measured after the fabrication. However, such an tuning approach is undesirable for commercial fabrication.
Chapter 7

Summary, conclusions and outlook

“Sometimes I think the surest sign that intelligent life exists elsewhere in the universe is that none of it has tried to contact us.”
Bill Watterson

Over the many pages of this work, a lot was said about photonic crystals, their fabrication and their measurement. Towards the end of this thesis, we would like to summarize the most important aspects, and give an outlook about the future of photonic crystals.

7.1. Summary and conclusions

The following key issues in fabrication, characterization and application of photonic crystal (PhC) devices were addressed and successfully solved:

- *Establishment of a semiconductor processing technology for the fabrication of PhC and trench waveguides*. A complete PhC fabrication process was developed. We achieved holes depths of 4.2μm, 3.8μm and 2.9μm for diameters of 417nm, 310nm and 180nm, respectively. Such depths are comparable with literature values, as presented in section 3.1.2. Not only was a process developed. Also the mechanism of etching and passivation were investigated and understood by systematically exploring the parameter space of the semiconductor etching machine. Especially the strong impact of the nitrogen content in the etching plasma was pointed out. The addition of nitrogen to the plasma is responsible for roughness and conical hole shapes, but beneficial for the sidewall passivation to avoid mask undercut.
• **Detailed characterization of the fabrication process.** The PhC holes were characterized by different methods to quantify the results of the etching process:

  o *Lag effects* become important when we use different hole sizes in the same device. The different hole size may impact the performance of the device. As we cannot avoid lag effects, at least their impact on hole depth should be known.

  o *Load effects* arise from different chip sizes. Reduced etching depth in large substrates has been observed.

  o *Sidewall roughness* inside the PhC holes gives rise to optical propagation losses. We developed a new analysis method to extract roughness values from AFM scans of a curved surface. With this method, we quantified the roughness of PhC holes and also confirmed quantitatively the qualitative impression for SEM images. A balanced nitrogen content in the etching plasma leads to the lowest sidewall roughness.

  o *Carrier lifetime* inside an active layer becomes important for the efficiency of an active device. The carrier lifetime was investigated for different etching processes and different PhC designs. Low sidewall density of the PhC design has proven to be advantageous for high carrier lifetime. Again, a balanced nitrogen content in the etching plasma performs best with respect to long carrier lifetime.

• **Endfire setup.** The micrometer size of PhC devices requires a complex measurement setup to access these structures. We built an endfire setup to measure transmission spectra of PhC devices. The setup consists of external optical parts (laser source, light injection, light collection and power measurement) and on-chip auxiliary structures to guide the light from the cleaved facets to the PhC device. All parts were carefully characterized to understand their impact on the transmission of the light from the source to the detector.

• **Photonic crystal devices.** The practical use of the etching process and the measurement setup were demonstrated on basic building blocks for integrated optics based on PhCs. In particular, the following structures were measured:

  o A *W1 waveguide* as the cornerstone of all PhC devices which require single-mode operation.

  o A *waveguide bend* was optimized by 2D simulations to enhance the bandwidth and the transmission around the corner. The enhancement found by simulations has been confirmed by the measurement.

  o A *directional coupler* used as a broadband power splitter of any desired branching ratio has been demonstrated. Based on hole-size variations around the two coupled waveguides, the required length of the device has been shortened drastically.
All these developments were required to establish a basic technology for passive PhC devices. Successful fabrication and measurement of passive PhC devices were demonstrated in this dissertation.

7.2. Outlook

The work presented in this thesis is only an intermediate step towards practical devices using PhCs. The ultimate goal will be active PhC devices. In this section, we will give an outlook about further steps and tasks towards this goal.

7.2.1. Going active

The developed technology can be incorporated directly for the fabrication of active devices (lasers or semiconductor optical amplifiers based on PhC waveguides). The semiconductor etching process has proven to be unselective towards quaternary material. Therefore the incorporation of quantum well or quantum dots, based on InP-related materials, is straightforward. However, several challenges must be mastered before an electrically pumped active PhC device will be presented:

- **Electrical contacts and alignment**: Photonic crystal waveguides are small compared to conventional ridge waveguides (a few 100nm width). The precise alignment of the metal contact stripe, for electrical current injection into the semiconductor, on top of the waveguide becomes important. Electron beam lithography is required. Furthermore, the resistivity of such a thin contact stripe above a PhC must be addressed.

- **Larger hole depth**: The presented hole depth of over 2μm is by far sufficient for passive devices as the upper cladding is chosen thin. The mode in such a slab waveguide configuration is located close to the air above the upper cladding. Introducing an electrical contact on top of the PhC enhances the losses due to light absorption in the metal. As a consequence, the mode and with it the core layer must be buried deeper below the cladding. In order that holes still penetrate the full light mode, deeper holes are required.

- **Electrical interconnects**: The contact stripes must be connected to the electrical power sources. The electrical interconnects of processors are normally embedded in a passivation layer (e.g. BCB or SiNₓ). A passivation layer may however influence the optical modes. Therefore either careful investigation of the influence of the passivation layer on the PhC properties must be investigated, or an airbridge-technology to connect the contact stripes with power sources must be developed to get rid of the passivation layer.

- **Active and passive integration**: Not the full wafer will be at the end active. Passive sections are required. On large scale, these passive sections must be of different semiconductor material than the active parts to avoid re-absorption of the light on the unpumped active layers. This demands for the development of selective-area re-growth or quantum-well intermixing.
7. Summary, conclusions and outlook

7.2.2. Membrane integration

Membrane-based PhCs, either free-standing or supported by a low-refractive index material have much lower losses (compare section 2.2.3, Table 3) than bulk-type devices. For the latter, values of 500dB/cm for a W1 waveguide still count as state-of-the-art. For single, short devices, such losses can be accepted, as losses per functionality are relevant. However, for large-scale integration, these losses must be reduced.

Using membrane-based PhC device as a solution to avoid high losses complicates the fabrication. The demand to the ICP hole etching process is indeed lowered, as holes need to be less deep. However, depending on the realization of membranes, several pitfalls during processing and measurement must be mastered.

- **Low-reflection, high efficiency membrane/bulk interfaces for local membranes.** An interface between bulk-type PhCs and membrane-type PhCs is not explored in literature. The selective underetching of only a part of the chip becomes difficult, as lateral etch-stops are hardly possible. Furthermore, such an abrupt interface gives rise to very detrimental light reflections.

- **Incoupling from fibers into membranes.** We have discussed in section 5.2.3 the problem of incoupling into a well-confined waveguide mode. This difficulty is further tightened by the even vertically more confined waveguide modes. Incoupling into a membrane becomes less efficient.

- **Wafer bonding as new process step.** Supported membranes need a low-refractive index lower cladding. A common method is waferbonding to mount the membrane on a low-refractive index substrate. Precise alignment between the membrane and the support substrate is required to become a flat cleaved facet at the end.

- **Mechanical stability of the membrane.** Membranes can be realized by selective wet etching of the lower cladding after material etching. The quaternary core stays then free in the air. Such structures are mechanically fragile. Careful handling is required. Furthermore, the structure and especially the long access waveguides must be laterally supported by “arms” made of core material for complete membrane devices.

- **Electrical contacting.** Whereas the concept (not the processing) of electrical contacting is easy for the bulk-type PhC, a straightforward scheme for an electrical contact in a membrane-type PhC is still missing.

Membranes are the state-of-the-art for passive silicon devices, but they still require a lot of development to become useful for active electrically-pumped InP devices. However, if these challenges are mastered, we can profit from much lower losses in the PhC waveguides.
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Zürich, February 17, 2009, Patric Strasser
Appendix

A. **Energy density integration method**

A.1. **Proof of $P=rE$**

The basic equation for the use of *energy density detectors* is the linear relation between the power flux $P$ through a waveguide and the energy density $E$ integrated over the detector area across the waveguide according to equation (A.1).

$$P=rE, \quad (A.1)$$

where $r$ is an (unknown) proportional constant unequal to 0. The validity of this equation is proven in this section.

We demand single-mode operation of the waveguide to avoid beatings between modes with different k-vectors. The detector length $s$ parallel to the waveguide must be a multiple of the lattice constant of the photonic crystal (PhC) due to the sub-lattice-constant modulation $u_k$ of the field in the presence of the PhC. Without loss of generality, we assume a rectangle (in 2D) for the detector area, whereas the power flux is parallel to one side of the rectangle (Figure 106).

![Figure 106: Nomenclature.](image)

Arguing with photons (which makes the proof more intuitive), the photon flux through the side of this rectangle is

$$m = \frac{P}{h\omega}, \quad (A.2)$$

where $m$ is the number of photons per time crossing the boundary of the detector area, and $\omega$ the frequency of the light. If the rectangle has the length $s$ parallel to the photon flux, the time $t$ which the photon stays inside the area (and thus contributes to the energy density) is equal to

$$t = \frac{s}{v_{\text{photon}}}. \quad (A.3)$$

Let’s assume a homogenous power flux (stationary state). Then the number of photons $q$ in the detector area is then
Appendix

and the total energy in the detector area is

\[ E = q \cdot \hbar \omega, \]  \hspace{1cm} (A.5)

It should be noted that the energy distribution is not homogeneous in the waveguide, but modulated with a periodic function \( u_k \) with a periodicity of the lattice constant. As we have chosen the detector length \( s \) to be a multiple of the lattice constant, the condition (A.5) is fulfilled.

Now we can compose equations (A.2), (A.4) and (A.5), and we obtain equation (A.1):

\[ P = m \cdot \hbar \omega = \frac{q \cdot s}{v_{\text{photon}}} \cdot \hbar \omega = \frac{s}{v_{\text{photon}}} \cdot E. \]  \hspace{1cm} (A.6)

In the case of two counterpropagation waves, the contribution of both waves must be added, as the direction of the photon velocity is not relevant in the equation. The energy in the area is simply the sum of the individual energies carried by each wave. Furthermore, due to the same absolute value of the \( k \)-vector of the two counterpropagating waves, a beating between the two waves is not possible.

A.2. Calculation of the transmission

From the integrated energy density in the input- and output-values, we can directly calculate the transmission, including the reflections on the device. The transmission is calculated as follows

\[ T = \frac{P_{\text{transmission}}}{P_{\text{source}}}. \]  \hspace{1cm} (A.7)

\( P_{\text{transmission}} \), \( P_{\text{reflection}} \) and \( P_{\text{source}} \) denote the effective power fluxes, whereas \( P_{\text{input}} \) and \( P_{\text{output}} \) refer to the measured power fluxes or integrated energy densities in the input and output waveguide, respectively. In the output waveguide, the measured value is directly the transmission value, as long as we have no reflections from the end of the simulation domain. Therefore, the relation \( P_{\text{output}} = P_{\text{transmission}} \) holds. In the input waveguide, the contributions from the source and the reflections are added:

\[ P_{\text{input}} = P_{\text{reflection}} + P_{\text{source}}. \]  \hspace{1cm} (A.8)

The energy is conserved. We assume that the device is lossless and the energy can only propagate through the device or be reflected from the device:

\[ P_{\text{source}} = P_{\text{transmission}} + P_{\text{reflection}}. \]  \hspace{1cm} (A.9)

Using identities (A.8) and (A.9), we can deduce an equation for the transmission:
B. Loss determination with the fringe contrast method

Loss determination is a key technique for the characterization of photonic crystals (PhC) or ridge waveguides. Most easily, the cutback method is used where (PhC) waveguides of different lengths are fabricated and their absolute transmission is measured. By comparing waveguide length against absolute power transmission and fit a linear regression line into it, the slope directly delivers the loss figure. However, the cutback method requires waveguides of different length. To extract loss figures from a single structure, the fringe-contrast method \cite{71} is preferred.

\[
T = \frac{P_{\text{transmission}}}{P_{\text{source}}} = \frac{2 \cdot P_{\text{output}}}{2 \cdot P_{\text{source}}} = \frac{2 \cdot P_{\text{output}}}{P_{\text{input}} + P_{\text{output}}} = \frac{2 \cdot P_{\text{output}}}{P_{\text{source}} + P_{\text{reflection}}} + \frac{2 \cdot P_{\text{output}}}{P_{\text{source}} - P_{\text{reflection}}} 
\]

(A.10)

In the case of losses, equation (A.9) is not valid. It must be changed to

\[
P_{\text{source}} = P_{\text{transmission}} + P_{\text{reflection}} + P_{\text{losses}} 
\]

(A.11)

\(P_{\text{losses}}\) cannot be removed from equation (A.10), and appears in the final equation (A.12) for the transmission through a device. If this value is (as usually) unknown, it leads to an overestimation of the transmission through the device.

\[
T = \frac{2 \cdot P_{\text{output}}}{P_{\text{input}} + P_{\text{output}} + P_{\text{losses}}} 
\]

(A.12)

It is difficult to obtain \(P_{\text{losses}}\) from the simulation. If they are included in the simulation by the \(\varepsilon^\prime\)-model, this value cannot be calculated. However, if the losses are caused by another channel(s) in which an area-detector can be placed, \(P_{\text{losses}}\) are obtained in the same way as \(P_{\text{output}}\).

\[\text{Figure 107: The waveguide cavity.}\]

The fringe contrast method uses a cavity formed by the waveguide to be measured and the two mirrors with reflectivity \(R_1\) and \(R_2\) at both sides. The situation is depicted in Figure 107. The usual realization is a waveguide between two cleaved facets of the chip. The transmission measurement shows fabry-perot fringes. They can be used to determine the losses. This method is widely used in Chapter 5 to obtain the waveguide losses of the access waveguide structures.
B.1. Theory

The transmission measurement can be described by a transfer matrix method.

\[
\begin{pmatrix}
T \\
0 \\
R
\end{pmatrix}
= M \cdot 
\begin{pmatrix}
S \\
\end{pmatrix}
\tag{B.1}
\]

The transmission matrix \( M \) set the input beam \( S \) and the reflected beam \( R \) into relation with the transmitted light \( T \). The matrix \( M \) has the form (Ref. [186], p. 72 or Ref. [56], p. 254)

\[
M = \begin{pmatrix}
M_{11} & M_{12} \\
M_{21} & M_{22}
\end{pmatrix} = \begin{pmatrix}
\frac{t}{t_i} & \frac{r}{t_i} \\
\frac{r}{t_i} & \frac{t}{t_i}
\end{pmatrix} \cdot \begin{pmatrix}
e^{-ikl} & 0 \\
0 & e^{ikl}
\end{pmatrix} \cdot \begin{pmatrix}
\frac{t}{t_i} & \frac{r}{t_i} \\
\frac{r}{t_i} & \frac{t}{t_i}
\end{pmatrix},
\tag{B.2}
\]

whereas we assume identical interfaces on both sides with reflection coefficient \( r \) and transmission coefficient \( t \). The propagation in the cavity is described by \( e^{\pm ikl} \), whereas \( l \) is the cavity length. Solving equation (B.1) for \( T \) gives

\[
T = M_{11} \cdot S - \frac{M_{12} \cdot M_{21}}{M_{22}} \cdot S = \frac{\text{det}(M)}{M_{22}} \cdot S.
\tag{B.3}
\]

The determinant of \( M \) is equal 1, as we easily can see:

\[
\text{det}(M) = \text{det}\left(\begin{pmatrix}
\frac{t}{t_i} & \frac{r}{t_i} \\
\frac{r}{t_i} & \frac{t}{t_i}
\end{pmatrix}\right) \cdot \text{det}\left(\begin{pmatrix}
e^{-ikl} & 0 \\
0 & e^{ikl}
\end{pmatrix}\right) \cdot \text{det}\left(\begin{pmatrix}
\frac{t}{t_i} & \frac{r}{t_i} \\
\frac{r}{t_i} & \frac{t}{t_i}
\end{pmatrix}\right)
\]

\[
= \frac{1 - R_2}{|t_2|^2} \cdot \frac{1 - R_1}{|t_1|^2} = \frac{T_2}{|t_2|^2} \cdot \frac{T_1}{|t_1|^2} = \frac{1}{n} \cdot \frac{n}{1} = 1
\tag{B.4}
\]

here we used the relationships \(|t|^2 = R\), \( T = \frac{n}{n_i} |t|^2 \) for normal incidence from medium \( b \) into medium \( a \), and \( R + T = 1 \) (Energy conservation).

This leaves us with the evaluation of the matrix element \( M_{22} \), or the square of it, as we measure the transmitted intensity:

\[
\frac{1}{|M_{22}|^2} = e^{-2 \alpha l} \cdot \frac{(1 - R_1) \cdot (1 - R_2)}{(1 - e^{-2 \alpha l} \cdot \sqrt{R_1 \cdot R_2})^2 + 4 \cdot e^{-2 \alpha l} \cdot \sqrt{R_1 \cdot R_2} \cdot \sin^2(\beta)}
\tag{B.5}
\]

The yet unknown parameter \( \beta \) can be eliminated by defining the power ratio (fringe contrast) \( u \):

\[
u = \frac{P_{\text{min}}}{P_{\text{max}}} = \frac{\left(1 - e^{-2 \alpha l \sqrt{R_1 \cdot R_2}}\right)^2}{\left(1 - e^{-2 \alpha l \sqrt{R_1 \cdot R_2}}\right)^2 + 4 \cdot e^{-2 \alpha l \sqrt{R_1 \cdot R_2}}},
\tag{B.6}
\]

Equation (B.6) can be solved for \( \alpha \):
With equation (B.7), the losses can be obtained from a single optical measurement. The cavity length $d$ can be determined by fabrication and is known, the fringe contrast $u$ is obtained from the optical measurement, and the reflection coefficients can be calculated from the refractive indices of the waveguide and the surrounding air.

C. **Notations**

- Electric field $\vec{E}$
- Magnetic field $\vec{H}$
- Electric displacement field $\vec{D}$
- Magnetic induction $\vec{B}$
- Free electric charge density $\rho$
- Free current density $\vec{j}$
- Magnetic permeability of the vacuum $\mu_0 = 4\pi \cdot 10^{-7} \text{ H/m}$
- Magnetic permeability $\mu$
- Electric permittivity of the vacuum $\varepsilon_0 = 8.85419 \cdot 10^{-12} \text{ F/m}$
- Electric permittivity $\varepsilon$
- Speed of light $c = 299792458 \frac{\text{m}}{\text{s}} = \sqrt{\varepsilon_0 \cdot \mu_0}$
- Frequency $\nu$
- Reduced frequency $\omega = 2 \cdot \pi \cdot \nu$
- Angular frequency $\omega = 2\pi \cdot \nu$
- Reduced Planck constant $\hbar = \frac{\hbar}{2 \cdot \pi} = 1.055 \cdot 10^{-34} \text{ Js}$
- Atomic unit (do not confuse with the reduced frequency) $u = 1.67 \cdot 10^{-27} \text{ kg}$
- Reduced frequency $u = a / \lambda$

D. **Mathematical functions**

- Real part of a complex function $\mathfrak{R}(\cdots)$
• Nabla-operator
\[ \nabla = \begin{pmatrix} \partial_x \\ \partial_y \\ \partial_z \end{pmatrix} \]

• Time-deviation
\[ \dot{x} = \frac{\partial x}{\partial t} \]

• Divergence
\[ \text{div}(\vec{x}) = \nabla \cdot \vec{x} \]

• Curl
\[ \text{rot}(\vec{x}) = \nabla \times \vec{x} \]

• In Dirac-notation for the mode \[ \overline{\psi} \] is the complex conjugated field

• Average of a variable (continuum)
\[ \bar{x} = \frac{\iiint x \cdot dx \cdot dy \cdot dz}{\Omega} \]

• Average of a variable (discrete)
\[ \bar{x} = \frac{\sum_{i=1}^{n} x_i}{n} \]

• Standard deviation
\[ \sigma = \frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n - 1} \]

• RMS roughness (continuum)
\[ \text{rms} = \sqrt{\frac{\iiint (x - \bar{x})^2}{\Omega}} \]

• RMS roughness (discrete)
\[ \text{rms} = \sqrt{\frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n}} \]

E. Definition of the polarization
In this work, the following definition for the polarization is used:

• Transversal electric (TE) polarization: The H-field is perpendicular to the slab waveguide plane, \( \vec{H} = H \cdot \hat{z} \) and \( \vec{E} \cdot \hat{z} = 0 \).

• Transversal magnetic (TM) polarization: The E-field is perpendicular to the slab waveguide plane, \( \vec{E} = E \cdot \hat{z} \) and \( \vec{H} \cdot \hat{z} = 0 \).

Note that the separation into TE and TM modes in a PhC is only obtained for a symmetric substrate. As our slab waveguide is asymmetric, the modes are not completely separated into these polarizations. Still, we can distinguish between TE-like and TM-like modes [41].
Curriculum vitae

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