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MASTER

Photonic crystal properties of silicon oxide nitride

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PHOTONIC CRYSTAL PROPERTIES OF SILICON OXIDE NITRIDE

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Abstract

Photonic Crystal Properties of Silicon Oxide Nitride


The last few years have witnessed an ongoing search for periodic dielectric structures that give rise to a photonic band gap (PBG). Since these photonic crystals were introduced, various structures designs and device applications from microwave to optical frequencies have been proposed and realized. In this thesis, for the first time, the use of the relatively low index material silicon oxide nitride (SiON), has been investigated for photonic crystal purposes. Within a triangular lattice of circular dielectric rods, calculations show that a complete TM-gap exists between normalised frequencies 0.49-0.52. For a triangular lattice of circular holes a complete TE-gap exists between normalised frequencies 0.48-0.50. In addition it is shown from simulations, that it is possible to modify the dispersion relations in a predetermined manner by introducing refinements in the design of the photonic crystal. To further optimise the properties of these crystals, a novel technique to calculate the out of plane losses is presented. Also a new design to reduce the out of plane losses, the graded index profile, is introduced. Finally, straight waveguides, waveguide bends and coupled cavity waveguides, are investigated for their use within photonic integrated circuits.
# CONTENTS

Chapter 1 ............................................... .................................. ......................... 3
   Introduction ............................................................................................................. 3
   Outline of the thesis ......................................................................................... 4
Chapter 2 ........................................................................................................................ 6
   Theory ....................................................................................................................... 6
      2.1 Introduction ................................................................................................ 6
      2.2 The master equation ...................................................................................... 6
      2.3 Hermitian operator, the variational principle, symmetries and scalability ........ 8
      2.4 The photonic band gap in 1D and 2D ........................................................... 10
Chapter 3 ...................................................................................................................... 15
   Modelling .................................................................................................................. 15
      3.1 Introduction .................................................................................................. 15
      3.2 Dispersion relations and Density Of States .............................................. 18
      3.3 The Femlab program ................................................................................... 20
      3.4 Triangular lattice of holes .......................................................................... 25
      3.5 Optimising gap properties .......................................................................... 27
Chapter 4 ...................................................................................................................... 36
   Out of plane losses and waveguides ................................................................... 36
      4.1 Out of plane losses ..................................................................................... 36
      4.2 Straight waveguides ................................................................................... 41
      4.3 Waveguide bends ...................................................................................... 45
Chapter 5 ...................................................................................................................... 50
   Conclusions and recommendations .................................................................... 50
   Literature ............................................................................................................... 53
   Acknowledgements .............................................................................................. 56
   Bedankjes ............................................................................................................... 56
Chapter 1

INTRODUCTION

The search of controlling the optical properties of materials has probably started in 1946 when Purcell\(^1\) discussed the fact that the presence of an electromagnetic mirror can substantially alter the radiation properties of an electromagnetic dipole. This insight was further developed, by Yablonovitch\(^2\) and John\(^3\), and led to the concept of a photonic band gap. The basic idea consists in designing materials that can affect the properties of the photon, in much the same way that ordinary semiconductor crystals affect the properties of electrons, i.e. they create a situation whereby photons in a certain energy range cannot travel through the crystal and are reflected when impinging onto the crystal or are not allowed to propagate at all when generated inside the crystal. The analogy between electronic and photonic crystal becomes more transparent if one considers that the Maxwell's equation, in the absence of external sources and currents, can be casted in a form, which is reminiscent of the Schrödinger equation, namely

\[
\nabla \times \left( \frac{1}{\epsilon(r)} \nabla \times H(r) \right) = \frac{\omega^2}{c^2} H(r). \tag{1}
\]

Equation (1) represents a linear Hermitian eigenvalue problem whose solutions are determined entirely by the properties of the macroscopic dielectric function, the 'potential'. Therefore, if one were to construct a crystal consisting of a periodic array of macroscopic uniform dielectric, the photons could be described in terms of a band structure, as in the case of electrons.

The last few years have witnessed an ongoing search for periodic dielectric structures that give rise to a photonic band gap (PBG). Since these photonic crystals were introduced, various structures designs and device applications from microwave to optical frequencies have been proposed and realized\(^4\). For example: micron size Very Large Scale Integration (VLSI) components such as filters and low-loss waveguide...
bends, junctions and couplers; Micro cavity Light Emitting Diodes (MCLEDs) and photonic crystal based laser.

Our aim is to investigate the possibilities of the relatively low index material silicon oxide nitride (SiON) as a new photonic crystals material. SiON is a well-known amorphous material from the Si-IC technology. Recently the optical quality of deposition of SiON has been greatly improved and its losses are acceptable low for photonic integrated circuits (PIC) applications. If it can be adapted for photonic band gap structures, PIC manufacturing may profit from this very advanced Si-related technology. It is also suited for advanced optical purposes as its refractive index can be continuously tuned between 1.5 (SiO₂) and 2 (Si₃N₄) by controlling the nitrogen flow during deposition, which enables the control of a vertical index profile. Compared to lattice matched materials, SiON is easy to fabricate because it is an amorphous material. An additional advantage of the relative low index is that the dimensions of the photonic crystal in SiON are larger by a factor of two compared to high index materials such as InP or GaAs. Thus tolerances in etch conditions enable novel design possibilities. The obvious disadvantage of the low index is the smaller photonic band gap, which will limit the use of such material for photonic crystal based devices. The question at hand is of this reduction in band gap can be outweighed by the advantages.

In the literature, the use of low index materials (n<2.0) for photonic crystal purposes has never been studied in detail to our knowledge. Experimentally, it has been shown that Si₃N₄ has a complete gap. Therefore, modelling will be a key ingredient to understand and develop new insights in the behaviour of electromagnetic waves inside such low contrast photonic crystals. Furthermore, engineering and experimental work will have to show how we can make use of their novel properties as a functional building block in a variety of structures. In the next section an outline of this thesis is presented.

Outline of the thesis

Chapter 2 summarizes a general theory of photonic crystals. The Master equation will be derived from the macroscopic Maxwell equations. Also some properties of this
equation will be deduced in order to facilitate the modelling process. The photonic band gap and two structures will be briefly discussed.

Chapter 3 gives an extensive overview of the modelling process using a finite element method (Femlab 2.1). In particular it is shown that in SiON it is possible to modify in a predetermined way the dispersion relations by properly designing the position of dielectric material within the 2D-photonic crystal.

To optimise waveguiding properties of photonic crystals, in chapter 4 the out of plane losses will be calculated with a new technique within the Femlab program. Also the use of a graded-index profile is introduced instead of a slab structure to further decrease the out of plane losses. Finally the transmission properties of a variety of waveguides will be calculated and discussed. Coupled cavity waveguiding will be introduced within this discussion.

Conclusions and recommendations are given in Chapter 5.

Good introductions to the theory of photonic crystals, can be found in the following papers ref [6-8] and the excellent book by Joannopoulos et al9.
2.1 Introduction

In this chapter an outline of the basic theory is given. The purpose will be to give the reader an overview of the analytical and physical tools that can be used when modelling and engineering photonic crystals. It is not the intention to give a full overview of all the theoretical knowledge on photonic crystals. Only those parts that are of interest will be discussed, otherwise good references will be given to outline the theory.

2.2 The master equation

The equations governing all macroscopic electromagnetic phenomena, including the propagations of light in a photonic crystal, are the Macroscopic Maxwell equations\(^\text{10}\)

\[
\begin{align*}
\nabla \cdot D(r,t) &= \rho \\
\nabla \times H(r,t) - \frac{\partial D(r,t)}{\partial t} &= J(r,t) \\
\n\nabla \times E(r,t) + \frac{\partial B(r,t)}{\partial t} &= 0 \\
\n\nabla \cdot B(r,t) &= 0,
\end{align*}
\]

where \(E\) and \(H\) are the macroscopic electric and magnetic fields, \(D\) and \(B\) are the displacement and magnetic induction fields, \(\rho\) and \(J\) are the free charges and currents. Using the appropriate constitutive relations\(^\text{9}\) \(D(r) = \varepsilon(r)E(r)\) and \(B = \mu(H) = \mu H\), with \(\varepsilon(r)\) the relative position dependent dielectric constant (within this thesis it will be written as \(\varepsilon(r)\) and denoted as the dielectric constant), and in the absence of external sources and currents, the Maxwell equations become:
\[ \nabla \cdot \varepsilon_0 \varepsilon_x(r) E(r,t) = 0 \]
\[ \nabla \times H(r,t) - \varepsilon_0 \varepsilon_x(r) \frac{\partial E(r,t)}{\partial t} = 0 \]
\[ \nabla \times E(r,t) + \mu_0 \frac{\partial H(r,t)}{\partial t} = 0 \]
\[ \nabla \cdot \mu_0 H(r,t) = 0. \]  

(3)

Because (3) are linear equations, time dependence can be separated out by expanding the fields into a set of harmonic modes. Writing the mode as a certain field pattern times a harmonic time dependence \( e^{i\omega t} \) and inserting them into the two divergence equations of (3), gives

\[ \nabla \cdot H(r) = 0 \]
\[ \nabla \cdot D(r) = 0. \]  

(4)

These conditions give rise to a transversality requirement of the fields. In other words, there are neither sources nor sinks of the displacement and magnetic fields. Inserting the harmonic modes into the two curl equations gives,

\[ \nabla \times E(r) + i \omega \mu_0 H(r) = 0 \]
\[ \nabla \times H(r) - i \omega \varepsilon_0 \varepsilon_x(r) E(r) = 0. \]  

(5)

The master equation is now derived through decoupling (5) by dividing bottom equation of (5) by \( \varepsilon(r) \) and then taking the curl. Eliminating \( E(r) \) using the first equation gives the master equation,

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

(1)

where \( c \) is the light speed.

For a given \( \varepsilon(r) \) the master equation completely determines the magnetic field \( H(r) \). The electric field \( E(r) \) can now be computed with the use of the bottom equation of (5). In the next paragraph some properties of the master equation are studied.
2.3 Hermitian operator, the variational principle, symmetries and scalability

For optimising the photonic crystal properties it would be of great help to understand the behaviour of electromagnetic field inside a photonic crystal. The master equation completely governs this behaviour and for a given pattern of dielectric material the solution can be calculated. However, to understand some fundamental properties of this master equation, it would be beneficial to give first approximations without the need of rigorous calculations. Therefore some properties of the master equation will be discussed in this section.

Hermitian Operator

By defining operator $\Theta$ that takes the curl, then divides by $\varepsilon(r)$, and then takes the curl again; the master equation will obtain the apparent form of a linear Hermitian eigenvalue problem

$$\Theta H(r) = \frac{\omega^2}{c^2} H(r).$$

Proving that $\Theta$ is indeed a Hermitian operator is shown for example in ref. 9.

Generally, the most important properties of a linear Hermitian operator are: any linear combination of solutions is itself a solution, the eigenvalues are real, the eigenmodes are orthogonal and they can be catalogued by their symmetry properties. It will be shown in chapter 3 that using the orthogonality property will be of great value in the modelling process.

Variational principle

Another concept is the use, as in quantum mechanics, of the variational principle:

$$E_f \leq \langle H|\Theta|H \rangle = \langle \Theta \rangle.$$  \hspace{1cm} (7)

With $E_f$ the energy of eigenmode $f$ and $\Theta$ the linear Hermitian operator as defined in (6).
The method is to guess a plausible normalized mode function $H$ to represent the eigenmode of the ground state. If $H$ contains a variable parameter $\beta$, then the expectation value for $\langle \Theta \rangle$ depends on $\beta$. The variational method is to vary $\beta$ and find the minimum value of $\langle \Theta \rangle$. If there are sufficient variable parameters, the minimum is expected to be a close approximation to $E_0$, the energy of the ground mode. In addition, the eigenmode is now characterized as an analytical function. The method can be extended to obtain higher order modes, but is then more complicated, as it is necessary to make the trial mode function orthogonal to the eigenfunctions of all the lower modes. As a result, the variational principle is able to characterize the eigenmodes of $\Theta$.

Additionally, the variational principle is also able to give the physical insight that the displacement field $D$ is concentrated in regions of high dielectric constant when $E_j$ is minimized. This can be seen if (7) is rewritten in the form:

$$E_j \leq \int \frac{1}{\epsilon(r)} |\nabla \times H|^2 \, dr = \int \frac{1}{\epsilon(r)} |\omega D|^2 \, dr. \quad (8)$$

In other words, a harmonic mode will tend to concentrate its displacement field in regions of high dielectric constant, while remaining orthogonal to all the lower modes. This is a very important conclusion that together with the orthogonality requirement will be used to improve the properties of photonic crystals.

Symmetry

Following ref. 9 it is shown and proved that the common symmetry features from solid-state physics can also be applied to photonic crystal structures. I.e. discrete translational symmetry can be used, as in quantum mechanics, to introduce Bloch's theorem and the Brillouin zone\textsuperscript{12}. Taking into account rotational, reflection and inversion operations (the point group of the crystal), the Brillouin zone is reduced to the irreducible Brillouin zone. The irreducible Brillouin zone contains all nonredundant reciprocal lattice vectors $k$. This means that using only $k$ vectors for calculations that are within the irreducible Brillouin zone, will give a complete characterisation of the electromagnetic waves inside the photonic crystal. All other $k$
Vectors are essentially the same as those in the irreducible Brillouin zone and therefore are of no value in the calculations.

Finally, if there is mirror symmetry in a 2D-photonic crystal, there will be only two possible fundamental modes: Either the electric field is in plane, which will be addressed with Transverse Electric (TE), or the magnetic field is in plane, Transverse Magnetic (TM).

**Scalability**

Due to the fact that the Maxwell equations are scalable, the solutions of the problem at one length scale determines the solutions at all other length scales. Within a periodic lattice of circular dielectric rods or holes, it is possible to use normalised frequencies $\omega a / 2\pi c = a / \lambda$ and normalised radii $r / a$. With $c$ the light speed, $r$ the radius of the rod (or hole) and $a$ the lattice pitch.

All the calculations except when stated otherwise will use these normalised frequencies and radii.

### 2.4 The photonic band gap in 1D and 2D

In this last section of chapter 2 a one-dimensional and a two-dimensional photonic crystal are introduced to show, using knowledge build up in the previous section, how the photonic band gap arises. Some features of the crystals will be discussed.

**The multilayer film**

Consider the one-dimensional multilayer film (figure 1) where the propagation of light will be entirely at normal incidence, i.e. oblique to the stack of dielectric material.
If both materials have the same dielectric constant, the dispersion relation of the multilayer film is

\[ \omega(k) = \frac{ck}{\sqrt{\varepsilon}}, \]

the speed of light \( c \) reduced by the index of refraction. Introducing a dielectric contrast between the two materials will change the dispersion relation drastically. A frequency gap appears where no mode can exist regardless of \( k \) (figure 2).

Figure 2. Dispersion relations for three different multilayer films. Left: each layer has the same dielectric contrast \( \varepsilon = 13 \). Middle: Layers alternate between \( \varepsilon = 13 \) and \( \varepsilon = 11 \). Right: Layers alternate between \( \varepsilon = 13 \) and \( \varepsilon = 1 \).

This frequency region is named the photonic band gap and is analogous to the semiconductor band gap between valence and conduction band. The photonic band gap can be understood by looking at the modes at the edge of the Brillouin zone. There are two possible orientations of standing waves at the edge of the Brillouin zone that obey the orthogonality requirement (figure 2 left figure shows indeed a two-fold degeneracy of the dispersion relation at the edge of the Brillouin zone).
mode can position its nodes in each low dielectric material (configuration \( n=1 \), dielectric band) or position its nodes in the high dielectric material (configuration \( n=2 \), air band). The energy of both waves will be different according to (8) when the two materials in the stack have different dielectric constants. The dielectric band will have its mode almost completely in high dielectric material, giving it a lower frequency; meanwhile the mode of the air band has its power concentrated in the low dielectric material, thus raising its frequency. At large dielectric contrasts, the power of the modes will be in both cases concentrated in the high dielectric material, but in different ways- the dielectric band more concentrated than the air band, because the position of the nodes (orthogonality requirement) has to be maintained. Figure 3 shows schematically the electric field inside the multilayer film in the three crystal configurations as mentioned in figure 2. The effects mentioned above can be clearly observed.

![Figure 3](image)

*Figure 3, schematic figure of the electric field inside each of the three multilayer films defined in figure 2. Grey region is the high dielectric region of the multilayer film. Solid lines denotes the dielectric \((n=1)\) band, dashed line the air \((n=2)\) band. Deduced from theoretical arguments and calculations performed in Femlab (Chapter 3).*

Changing the angle of incidence will destroy the complete (for all \( k \)) band gap because at off axis propagation there are no periodic dielectric regions to coherently scatter the light.

Triangular lattice of dielectric rods

A two-dimensional photonic crystal has to be periodic along two of its axis and homogeneous along the third. For example, consider a triangular lattice of infinite long dielectric columns (figure 4): For certain values of the column spacing, this crystal configuration can have a photonic band gap in the \( xy \)-plane, the plane
orthogonal to the rods. In contrast with the multilayer film this two-dimensional crystal has a photonic band gap for any in-plane direction of incident light. Furthermore if light is propagating strictly in the xy-plane, the system contains mirror symmetry, which will lead to separation of the modes in two distinct polarizations, TE or TM.

Figure 4. Triangular lattice of finite dielectric rods.

Analogous to the one-dimensional system, the band gap can be explained by looking at the modes at the edge of the Brillouin zone, but now for two individual directions instead of one, as was the case in the multilayer film. Figure 5 shows the Brillouin zone and the irreducible Brillouin zone with symmetry points Γ, M and K that define the two individual directions of the crystal, the Γ-M and Γ-K direction. Also the real space triangular lattice of holes from above is drawn. Remind that k-space and real space lengths are inversely proportional to each other.

Figure 5. Left figure shows the Brillouin- and the irreducible Brillouin zone (grey area). Right figure shows the triangular lattice of dielectric rods in air with the two symmetry directions.
Similar to the one-dimensional case, off-axis propagation (out-of-plane) will lead to the destruction of the complete band gap, because there are no periodic dielectric regions to coherently scatter the light.

Because of the major importance of a two-dimensional photonic crystal in very large scale integration, it shall be discussed in great detail in the next chapter.
Chapter 3

MODELLING

3.1 Introduction

To develop a further understanding of photonic crystals, it is essential to have a computational program that can solve the Maxwell equations numerically. There are two common computational approaches to study dielectric structures, either in time-domain or in frequency-domain. An outline of both methods can be found in ref. 13. In this thesis a two-dimensional finite element method, Femlab\textsuperscript{14} and a gap-map tracing program Translight\textsuperscript{15}, using a transfer matrix approach are used. Both programs are based upon the frequency-domain approach. Besides these two programs a Matlab program will be used to calculate the dispersion relations and the Density Of States of the various photonic crystals.

These programs will be used to optimise some photonic crystal properties as photonic band gap size, out-of-plane losses, waveguides and coupled cavity waveguiding structures which is the equivalent of impurity band conduction\textsuperscript{16} in semiconductor physics.

Before proceeding to optimise the photonic crystal properties it is shown by illustrative examples that the simulations of electromagnetic waves inside periodic dielectric material, are in agreement with the theory as derived in chapter 2.

Dielectric rods in air

To show the properties of a 2D photonic crystal, a triangular lattice of infinite dielectric rods in air is most illustrative. As mentioned in the previous chapter, only for certain column spacing this system has a complete band gap. To find the column spacing where there exists a band gap for the TE- and TM-mode in the Γ-M and Γ-K directions separately, the TRANSLIGHT\textsuperscript{15} program with normalised frequencies
and radii, is being used. Throughout this thesis the materials used in the simulations are air \( (n=1) \) and SiON \( (n=1.5) \).

Figure 6a. Transmission after eight rows of infinite dielectric rods in air as function of the normalised radius for the \( \Gamma\text{-}M \) direction. Left figure shows the ‘gap map’ for TE polarisation, right figure for TM polarisation. Blue indicates transmission 1, black indicates transmission below 0.001. See also colour scale.

Figure 6b. Transmission after eight rows of infinite dielectric rods in air as function of the normalised radius for the \( \Gamma\text{-}K \) direction. Left figure shows the ‘gap map’ for TE polarisation, right figure for TM polarisation. Blue indicates transmission 1, black indicates transmission below 0.001. See also colour scale.

Figure 6 shows the transmission signal after eight rows of infinite dielectric rods in air as function of normalised radii for \( \Gamma\text{-}M \) and \( \Gamma\text{-}K \) directions. The Translight program output is the transmitted part of the impinged electromagnetic wave in the explored direction. A few comments about these figures:

- Referring to chapter 2, the gaps will be larger for high dielectric materials such as GaAs or InP. This is because the electric and magnetic fields interact stronger
with the high index crystal than in the case of the low refractive index materials. Nevertheless these smaller gaps as will be shown, are still useful for several kinds of applications.

- Looking at figure 6 it is clear that the largest gaps occur for the TM-mode. This is an immediate consequence of equation 4 and 8. The TM-mode has its electric field parallel to the rods and according to equation 8 the energy will be reduced significantly because the field can easily penetrate the high dielectric regions without losing continuity (equation 4). In contrast, the TE-mode has its electric field perpendicular to the rods and can only penetrate the high dielectric regions where it is encountering them. Without losing continuity the TE-field must also penetrate the air regions. Therefore the reduction of its energy is less than in the case of the TM-mode. By the same argument connectivity of the high dielectric region is favourable for a TE-gap. In general terms, patches of high dielectric material are favourable for a TM-gap, and connectivity of high dielectric material is favourable for the TE-gap17.

- The gaps all decrease in frequency as $r/a$ increases. This is an expected feature, since the frequency scales as $1/\theta^{1/2}$ in a medium of dielectric constant $\varepsilon$, and as $r/a$ increases, the average dielectric constant of the medium steadily increases.

- The first order gap (lowest $a/\lambda$) for the $\Gamma$-M direction is at a lower normalised frequency than for the $\Gamma$-K direction. This is a result of the change in lattice pitch for the two different directions. As depicted in figure 5 the $\Gamma$-M direction has a larger periodic lattice pitch than the $\Gamma$-K directions. Consequently the first gap for the $\Gamma$-M directions will be at a lower normalised frequency than that for the $\Gamma$-K direction.

- Finally, because only two $k$ vectors were explored in each polarisation instead of the complete irreducible Brillouin zone, it is doubtful to state if there is a complete band gap in this structure. Although there is an overlap between the gaps in the $\Gamma$-M and $\Gamma$-K direction this does not ensure that a complete gap is apparent. For example, there is also an overlap region in transmission gaps at
normalised frequency 0.90, but this is not a complete gap as will be derived. A dispersion relation that accounts for all \( \mathbf{k} \)-vectors within the irreducible Brillouin zone is needed. This can be obtained by using a position dependent dielectric constant combined with the plane wave method\(^8\). This method is well known and experiments show good agreement with the calculated dispersion relations. Therefore it will be used in the next section to calculate the dispersion relations and the Density Of States within several photonic crystals structures.

3.2 Dispersion relations and Density Of States

Using the normalised radius where the lowest transmission occurs (deduced from figure 6) \( r/a = 0.3 \), and using a Matlab program\(^9\) based upon ref. 18, the dispersion relations are obtained. Figure 7 shows the first four bands of the dispersion relations for both polarisations.

![Dispersion relations for triangular lattice of infinite rods for TE- (left figure) and TM-polarisation (right figure). Symmetry points M, \( \Gamma \) (depicted as 'G') and K are also depicted. The complete gap is depicted as the grey area in the TM-dispersion plot.](image)

The dispersion graph for TE-polarisation shows a gap between bands \( n=1 \) and \( n=2 \) for the \( \Gamma \)-M direction between normalised frequencies 0.48 and 0.53, but no gap for the \( \Gamma \)-K direction between these bands. This means that there is no complete photonic band gap for TE-polarisation in this photonic crystal, only a partial gap for the \( \Gamma \)-M direction. As expected, there is a complete gap for TM-polarisation between normalised frequencies 0.49 and 0.52, the overlap region of the gaps in \( \Gamma \)-K and \( \Gamma \)-
M-direction. Notice that no other branch of the dispersion relation crosses this normalised frequency region: therefore it is a complete gap.

By modifying the Matlab program used to calculate the dispersion relations, the density of states\(^{12}\) for the first five eigenvalues of approximately 22000 \(k\)-values chosen at equidistance points in the irreducible Brillouin zone, has been calculated.

![Graph showing the density of states for TE- and TM-polarisation.](image)

**Figure 8. Density of states for triangular lattice of dielectric rods in air for TE- (left figure) and TM-polarisation (right figure).**

To verify if the calculations are correct, the density of states for a known system from ref. 18 has been calculated with the modified Matlab program and compared with the density of states reported in ref. 18. A good agreement is found (see figure 9). Also the linear increase in density of states for low normalised frequencies is in agreement with theory, as the following derivation will show. At low normalised frequencies the dispersion relations are given by equation 9, thus \(\frac{dk}{d\omega}\). The change in number of available states \(N\) as function of a change in \(k\) is given by: \(dN = 2\pi kdk\). Which gives: \(\frac{dN}{d\omega} \sim \omega\). Therefore it is concluded that the calculations for SiON as shown in figure 8, are correct.
According to the discussion only a complete gap can exist for TM-polarisation. Figure 8 shows indeed zero density of states for TM-polarisation between normalised frequencies 0.49-0.52. For TE-polarisation there is a decrease in the density of states caused by the partial gap, but not to zero. The characteristic wobbles (spike followed by a dip in the density of states) in figure 8 are due to partial gaps and causes the transmission dips in figures 6a,b.

The two programs (Translight and the Matlab program) used in the above calculations are able to calculate transmission spectra and dispersion relations of perfect periodic crystals. Within these programs it is hardly possible to change the size or shape of one or more of the elements of the crystal. Furthermore the actual field distribution cannot be calculated with these programs. With these restrictions it becomes very difficult to optimise the crystal properties. Therefore a finite element method approach (Femlab\textsuperscript{14}), which allows flexible modelling and can calculate the field distribution, will be used.

3.3 The Femlab program

In this section the Femlab program will be discussed. Some previous calculations with the plane wave method will be compared with transmission calculations of the
Femlab program. Also some ambiguities in the transmission spectra will be briefly discussed. In the next paragraph the field distribution inside the photonic crystal will be studied and compared with theoretical results obtained in chapter 2.

Orthogonality and band gap

Figure 10 shows three typical output figures of the Femlab program. One with the displacement field distribution for TM polarisation at the edge of the Brillouin zone for the $n=1$ branch in $\Gamma$-$M$ direction, one in the band gap, and one for the $n=2$ branch. The source is a plain wave entering the system from the left boundary travelling to the right. Periodic boundaries conditions are applied on the top and bottom boundaries. This boundary condition ensures that the fields are equal at the top and bottom boundary and thus making the crystal infinite long in this direction.

According to the discussion in chapter 2 the dielectric band (top figure) will try to put its displacement field almost entirely inside the dielectric rods. Equation 8 shows that this will lower its energy. The air band field distribution (bottom figure) must be orthogonal to the displacement field of the dielectric band and therefore must have a node inside a dielectric rod (see figure 3). This will push the displacement field out of the dielectric rod into the air region. This will give rise to an increase of the energy according to equation 8. Between the dielectric band and the air band lies the band gap. In this region propagation of the field is not possible because there are no available states (see figure 8) and the field will decay exponentially. All these phenomena are clearly observed in figure 10.
Displacement field (Dz)

Figure 10. Displacement field at the edge of the Brillouin zone for the dielectric band (top), inside the band gap (middle) and for the air band (bottom). The source is a plane wave generated at the left side boundary of each figure. Red indicates positive values of the displacement field, blue negative values and green indicates no field. Periodic boundary conditions are applied at the top and bottom boundaries.

In the next section transmittance plots made with the Femlab program will be introduced and discussed briefly.

Transmission spectra

With the Femlab program it is possible to make a transmittance plot by calculating the energy outflow or to be exact the time averaged Poynting vector, at the right hand side boundary (see figure 10) as a function of the normalised frequency. Figure 10 shows, for normalised radii 0.30, both directions (Γ-M and Γ-K) and polarisations
(TE and TM) and for two different lengths (in propagation direction) of the crystal (10 and 20 rows), the transmittance using absorbing boundary conditions instead of periodic ones. (The use of different boundary conditions will have some influence on the transmittance plots as will be shown in upcoming paragraphs.) The transmittance is defined as the ratio between the calculated energy outflows at certain frequencies divided by the highest calculated energy outflow.

![Figure 11. Transmittance curves using absorbing boundary conditions for Γ-M direction (left) and Γ-K direction (right). In red TE-mode, in black TM-mode. Solid lines for a crystal with 10-rows and dotted lines for a crystal with 20-rows.](image)

Because the Femlab program uses a finite element method it is not possible to create an infinite number of rows in the propagation direction. Consequently the depicted transmission dips are not equal to zero, as they should. As showed in figure 11, increasing the number of rows has some influence on the band gap edges. It can be shown that a further increase in rows does not affect the position of the gap if one uses the normalised frequencies at a transmission of −10 dB (i.e. transmission 0.1). Therefore the gap edges are defined at normalised frequencies at −10 dB transmission.

According to the dispersion relations (figure 7) there should be a TM-gap between normalised frequency 0.44 and 0.52 in the Γ-M direction and a gap between 0.48 and 0.60 in the Γ-K direction. In good agreement with these results, the Femlab program shows a gap between 0.45 and 0.53 in Γ-M direction, and a gap between 0.47 and 0.59 for the Γ-K direction. Figure 12 shows the transmission spectra for these two directions in one plot where the overlap region of the two lines corresponds to the complete gap, which is between 0.48 and 0.53.
Using absorbing boundary conditions instead of periodic ones, the transmission spectra will be changed slightly. Figure 13 shows the transmission spectra for the triangular lattice of rods using absorbing boundary conditions (red line) and periodic boundary condition (black line). At normalised frequency 0.47 the transmission for the absorbing boundary condition is higher than for the periodic ones. This can be explained by the fact that the absorbing boundary condition breaks the symmetry of the crystal. Therefore, modes that would be absent in a perfect crystal (when applying periodic boundary conditions) can still exist and can propagate freely within the crystal. As a consequence, the partial gap between normalised frequencies 0.44 and 0.49 in the Γ-M direction will have a higher transmission (shoulder) than in the case of a perfect crystal.

There is also a difference in transmission for normalised frequencies above 0.70. Because this area of normalised frequencies is of no importance for the work presented in this thesis, no attention is paid to it.

Figure 13 also shows that the first order gap for periodic boundary conditions has shifted to lower normalised frequencies by 0.01. The gap lies between normalised frequencies 0.44 and 0.52, which is in exact agreement with the plane wave method. Nevertheless, the more practical absorbing boundary condition will be used for further calculations.
Figure 13. Transmittance spectra of dielectric rods in air in Γ-M direction when using absorbing boundary conditions (red line) and periodic boundary conditions (black line).

Concluding: The Femlab program is able to calculate the position of the gaps in agreement with the plane wave method and thus will be suitable to use for further modelling work on photonic crystals.

In the next section another basic design will be examined, the triangular lattice of holes.

3.4 Triangular lattice of holes

According to the discussion in chapter two it is expected that in a triangular lattice of holes a complete TE gap due to the connectivity of the dielectric material can be present. Figure 14 shows a figure of a triangular lattice of holes.

Figure 14. Triangular lattice of holes.
In figure 15 the dispersion relation of this particular system is shown for (optimal) normalised radii 0.37. Figure 16 shows the density of states.

**Figure 15.** First four bands of the dispersion relations of the triangular lattice of holes for TE-polarisation (left) and TM-polarisation (right). Symmetry points $M$, $\Gamma$ depicted as 'G' and $K$ are also shown. Grey area within left figure denotes the complete gap.

**Figure 16.** Density Of States for both polarisations; TE left figure, TM right figure.

Evidently there is only a complete gap for TE-polarisation between normalised frequencies 0.48 and 0.50.

Figure 17 shows the transmission spectra obtained with the Femlab program, for $\Gamma$-$M$ and $\Gamma$-$K$ direction. Again the number of rows is varied and absorbing boundary conditions are being used. Both polarisations are calculated.
Figure 17. Transmission of triangular lattice of holes for Γ-M (left) and Γ-K (right) direction, TE- and TM-polarisations. Solid lines denote crystals with 10 rows, dashed lines crystals with 20 rows.

The Femlab program shows indeed a large TE gap and the gap positions are in agreement with the dispersion relations. In figure 18 the TE-gap for both directions is plotted. The overlap region corresponds to the complete gap, which is between normalised frequencies 0.47 and 0.51 in good agreement with the plane wave method.

Figure 18. Transmission of triangular lattice of holes in Γ-K and Γ-M direction for TE-polarisation. Overlap region between the two lines corresponds to the complete TE-gap.

3.5 Optimising gap properties

It would be interesting to see if it is possible to make a larger (less transmission when using the same number of rows) gap. This would be of great significance because a larger gap will definitely lead to better performances of devices where photonic crystals are used. This increase of the gap can be achieved by varying the shape of the
holes or rods, using the knowledge of chapter 2. In this section a start towards an optimum design will be presented.

The advantage of using relatively low index materials such as SiON, over high index materials is that the crystal dimension are increased by a factor two. This means that the etching has less stringent conditions, and thus it may be possible to introduce smaller features within the structures that are beneficial for the properties of the crystal. In the literature Cox and Dobson have shown (for the square lattice case) that the dispersion relations can be modified by changing the unit cell filling\textsuperscript{20,21}. Their results depend highly on small features within the unit cell and therefore are of high interest for low index material system such as SiON. In this section it will be shown that by using the theoretical arguments of chapter two it is possible to modify the dispersion relations in a predetermined manner by introducing refinements in the designs.

**Triangular lattice of rods**

As explained in chapter 2 and showed in figure 10, the fields of the n=1 and n=2 bands of the dispersion relations are orthogonal to each other. From equation 8 it is learnt that lowering and raising the energy can be done by 'putting' the displacement field in high or low dielectric material, respectively. With this knowledge it is possible to adjust the band structure in a specific way by changing the shape of the rod. The aim is to make a larger gap in a certain direction. This means that an improved design for the Γ-M direction does not ensure that the dispersion relation in the Γ-K direction is improved as well, more likely it is worsened. This shall be discussed in greater detail throughout this section. The overall idea is to search for special optical features by particular design details.

To start, figure 19 shows the displacement field (TM polarisation) of a single rod for the n=1 and n=2 branch of the dispersion relation in Γ-M direction at the edge of the Brillouin zone. Notice that the fields are orthogonal to each other and are in agreement with the predictions of figure 3.
Figure 19. Displacement field of rods in air at edge of Brillouin zone for n=1 (left) and n=2 (right) in Γ-M direction for TM-polarisation. Red indicates positive values for the displacement field, blue negative ones.

The n=1 branch shows that the displacement field tends to escape from the rod at the top and bottom. Elongating the rod would improve the confinement of the field and thus lowering the energy. I.e. the n=1 branch will move to lower normal frequency. For the n=2 branch a same argument can be made. In this case a larger gap can be made by moving the n=2 branch to a higher frequency. Repelling the displacement field from the rod by removing the left and right side of the rod will do the job. The field is then pushed in low dielectric material (air) and therefore increases its energy (see figure 20 for improved the design). Of course these adjustments will also counter affect each other, i.e. removing the left and right side of the rod will have negative consequences for the n=1 branch, and also elongating will have negative consequences for the n=2 branch.

Two important remarks have to be made; First, these refinements only work for the Γ-M directions. In the Γ-K directions, by the same arguments, probably more harm is done than good. A Bragg reflector would be ideal, but then there would be no gap at all in any other directions, see chapter 2. Therefore, the presented designs are only based upon one direction, but without ignoring completely the other direction. At the end of this section a procedure will be proposed to develop structures that improve the dispersion relations in any directions based upon the same line of arguments to improve the gap in one direction.

Second remark, changing the size of the rod does change the effective dielectric constant and moves the gap to higher or lower normalised frequency. The goal is to
keep the same effective index, which can be achieved by keeping the amount of
dielectric material in the crystal constant. Figure 20 shows the result for improved
dielectric rods in air for the Γ-M direction.

![Figure 20. Transmission spectra for circular rods (black) and improved design (red) for triangular lattice in Γ-M direction.](image)

Evidently the procedure is successful, the gap has widened by 20% and becomes
deeper by a factor of nine. Figure 21 shows the fields within the improved design for
n=1 and n=2.

![Figure 21. Displacement field improved design at edge of Brillouin zone for n=1 (left figure) and n=2 (right figure) branch. Red indicates positive values for the displacement field, blue negative ones.](image)

This same method will be used to optimise the design for the Γ-K direction, starting
with circular rods again. Figure 22 shows the displacement field for n=1 and n=2 at
the edge of the Brillouin zone for TM-polarisation.
Figure 22. Displacement field for rods in air at edge of Brillouin zone for \( n=1 \) (left) and the two fold degenerate \( n=2 \) branch (right) in \( \Gamma-K \) direction. Red indicates positive values for the displacement field, blue negative ones.

In agreement with figure 7 (dispersion relations) there are actually two possible modes with the same energy that are orthogonal to the lower mode. The field distributions are calculated just above and below the degenerate normalised frequency. Optimising the design for \( \Gamma-K \) directions becomes a bit of a fluke when using the same arguments as in the \( \Gamma-M \) direction. But in agreement with the \( \Gamma-M \) direction it can be seen, by merging the two possible states, that every rod shows the typical dipole state as was also observed in the \( \Gamma-M \) direction. Therefore the same design as for the \( \Gamma-M \) direction will be used to improve this design.

Figure 23 shows the result for the improved design in \( \Gamma-K \) direction.
As can be seen from figure 23 the improved design does not show any improvements compared to the original design. It is very likely that this is caused by the degenerations of the \( n=2 \) branch. Again this only shows that in this direction nothing has changed. Impinging the crystal from another direction (\( \Gamma-M \)) will presumably have some negative effects. To overcome these problems it is proposed that the rotational symmetry of the modified rods must agree with the rotational symmetry of the crystal. Thus, the improved designs should have six-fold rotational symmetry. This ensures that the two individual directions within the crystal (\( \Gamma-M \) and \( \Gamma-K \)) are also the two individual directions within modified rod. This also gives the possibility to improve the design in one direction and make further modifications within the other direction. The result would be an omni-directional improved design with a larger complete gap.

**Triangular lattice of holes**

The optimising procedure for the triangular lattice of rods can also be done for the triangular lattice of holes but now for TE-polarisation. Figure 24 shows the norm (absolute value) of the displacement field at the edge of the Brillouin zone for \( n=1 \) and \( n=2 \).
Figure 24. Norm of the displacement field for triangular lattice of holes, left figure \( n=1 \) right figure \( n=2 \) branch. Red indicates positive values blue indicates no field.

The left figure of figure 24 shows that the fields has to linger between the holes. Removing part of the sides of the holes would increase the number of displacement field inside the high dielectric material and therefore lower its frequency. At the \( n=2 \) branch it is clear that between the holes in \( \Gamma-K \) direction the displacement fields pile up. Making a smaller hole (elliptical) between the large holes would increase the amount of displacement field in low dielectric material and thus increase the frequency. Figure 25 shows the transmission of the improved design (see figure 24) for TE-polarisation in the \( \Gamma-M \) direction.

![Figure 25. Transmission for circular holes (black) and improved design (red), for triangular lattice in \( \Gamma-M \) direction.](image)

It can be seen from figure 25 that the gap has increased considerably. It has broadened by 20% and become deeper by a factor of nine. Especially the \( n=1 \) branch is affected by the improved design. Figure 26 shows the norm of the displacement field within the new design at the edges of the Brillouin zone for \( n=1 \) and \( n=2 \).
Figure 26. Norm of displacement field for improved design at $n=1$ (left figure) and $n=2$ (right figure) for TE-polarisation and $\Gamma$-$M$ direction. Red indicates positive values blue indicates no field.

In the $\Gamma$-$K$ direction the dispersion relation is also degenerated at the $n=2$ branch just like the dielectric rods. The optimisation procedure for this direction may not work, but figure 27 shows that in the $\Gamma$-$K$ direction the dispersion relations do not significantly change when using the same improved structure as for the $\Gamma$-$M$ direction.

Figure 27. Transmission for circular holes (black) and improved design (red), for triangular lattice in $\Gamma$-$K$ direction.

The six-fold symmetry argument, introduced in the previous section can of course also be applied in this case. But, it is also possible to improve the dispersion relations by calculations in k-space. Within the Matlab program that is used to calculate the dispersion relations the position dependent dielectric constant (position of holes or rods) is Fourier transformed. Small changes in the second and third order Fourier coefficients will results in different shapes of the holes and rods. By calculating the affect in width of the complete gap for every change in Fourier coefficient, an optimal design can be achieved.
In conclusion, it is shown that using simple arguments it is possible to create better performing gaps in certain directions, which may be beneficial for certain applications. A method based upon the same arguments but starting from a six-fold rotational symmetry design and a more rigorous calculations method are proposed. These results can be useful for many kind of devices, but certainly for waveguide bends as shall be discussed in the next section.
Chapter 4

OUT OF PLANE LOSSES AND WAVEGUIDES

One of the most promising functional devices for photonic crystals are waveguides and waveguide bends. The size of all optical chips depends mostly on curvature of the bends. This implies that making use of photonic crystals instead of normal ridge waveguides, the size of chips can be reduced significantly. Although recent results are promising, the losses caused by out of plane losses are reducing the efficiency of the waveguides. In the next section, novel 2-dimensional calculations for out of plane losses will be made for three types of structures within the system of triangular lattice of holes.

4.1 Out of plane losses

Confinement in the z-direction, parallel to the holes or rods, within a 2-dimensional photonic crystal occurs by effect of total internal reflection and or by guidance of a higher index material in the core of a slab waveguide (double hetero structure). Whenever an electromagnetic wave is not within a higher index region compared to air, it is not guided at all. Therefore when an electromagnetic wave crosses an etched hole in a photonic crystal, out of plane losses (in z-direction) occur. This shows that it is very important to understand the out of plane loss mechanism. The following 2-dimensional calculations within three different structures: (a) A structure without guiding properties, (b) a double hetero structure (slab) and (c) a novel graded index design based on properties of the SiON material, will show some features of this loss mechanism. The novel design will be discussed briefly before continuing to the calculations.

Within SiON it is possible to make use of a graded index profile instead of a double heterostructure that is normally used to guide the light in the z-direction. This graded index profile can be realised by controlling the nitrogen flow during deposition of the SiON layer. The design can be compared with graded index fibres and has the same advantages. It does not suffer from intermodal dispersion and the average angle of
waves that reflect by total internal reflection from the cladding is reduced. For low index materials the last advantage is very important because the critical angle for total internal reflection is much smaller than that for high index material. Within the Femlab program this graded index profile has been simulated with 10 layers of different dielectric contrast in the range of 1.5 - 1.57. Figure 28 shows schematically the three designs.

Figure 28. Three designs for studying out of plane losses. (a) no waveguide, (b) double hetero waveguide, (c) novel graded index waveguide. Grey scale denotes schematically the index, white low index, and black high index.

At the left side of the design a plane wave is launched into the core of the structure. At this boundary (where the wave is launched into the design) the time-averaged Poynting vector is calculated as function of normalised frequency. This flow accounts for the inflow minus reflections at the holes (outflow at the entrance), i.e. the net inflow. Also the time averaged Poynting vector at the exit (at the right core
boundary) has been calculated. This energy flow is equal to the net inflow minus the out of plane losses. With this, the normalised out of plane losses are given by:

\[
LOSSES \propto 1 - \frac{OUTFLOW}{NET INFLOW}.
\]  

Figure 29 shows the transmission and losses as function of normalised frequency for each of the three structures with an aspect ratio, the ratio between hole depth and diameter of the hole, of 4.

![Figure 29](image)

Figure 29. Relative out of plane losses (defined by equation 10) for the three structures presented in figure 28 with aspect ratio 4.

The broad peak in figure 29 denotes that the relative out of plane losses are high when the frequency is within the gap of the grating. (The existence of the gap in the structures can be compared with the gap in a multilayer film or within an antireflection coating.) For normalised frequencies below the gap the graded index has lower relative losses than the other two structures, but for higher normalised frequencies the relative losses are almost equal. The expected feature that a slab has fewer relative losses (better guiding in the z-direction) than a structure without waveguide is clearly observed especially for low normalised frequencies (below the gap), but again for higher normalised frequencies the difference is marginally. These effects, the differences between low and high normalised frequencies, can be explained by the fact that part of the mode propagates within the sub-core region.
Figure 30. Electric field distribution at normalised frequency 0.63 for slab structure with aspect ratio 4.

Figure 30 shows the field distribution for the slab structure at normalised frequency 0.63. Part of the wave can pass through the sub-core region and can re-enter the core after the region of the holes. This will influence the calculations and a quantitative comparison between the structures cannot be made. Therefore the same calculations are done but now for a structure with deeper holes so that the wave cannot travel through the sub-core but has to travel through the holes. This will suppress the possibility that part of the wave can propagate in the sub-core region. Also in the literature is shown that increasing the aspect ratio will reduce the out of plane losses. Figure 31 depicts the result for a design with aspect ratio 7.

Figure 31. Transmission of the three structures presented in figure 28 but now with an aspect ratio of 7.
The losses have decreased by almost a factor two in the frequency region outside the gap. Within the gap the losses have decreased by approximately 30%. From figure 31 it can also be seen that the structure without guiding has higher losses than the slab structure at all normalised frequencies, which is in agreement with the discussion in the previous paragraph. Therefore the results obtained for the graded index are more trustful. As shown in figure 31 the graded index performs better at high normalised frequencies and has the same relative losses as the slab structure for frequencies below the gap. Within the gap the losses are larger. This suggests that this first design does not have the optimal index profile in the z-direction. Therefore the losses can be further reduced by optimising this graded index profile in the z-direction. Figure 32 shows the electric field within the graded index structure at normalised frequencies 0.63 which can be used to improve the index profile within the design.

![Figure 31](image31.png)

**Figure 32, electric field for graded index profile at normalised index 0.63 and aspect ratio 7.**

From figure 32 it can be seen that the wave expands in the holes. Hence, to reduce losses to the substrate, it is important that between the holes within the dielectric region, the wave is tapered to the core region in such a way that within the next hole the expansion of the wave is limited to the depth of the hole. This can be accomplished by not only applying the graded index to the core region, but also to the sub-core region.

Remark: In 2-dimensional computation for waveguides the out of plane losses can be modelled with an imaginary part of the dielectric constant, as was shown by
H. Benisty et al\textsuperscript{25}. The Femlab program is able to use imaginary dielectric constant, but it would be too difficult to imply this within this thesis. Therefore the calculations of waveguiding properties of SiON will be done without taking the out of plane losses into account.

4.2 Straight waveguides

In this section the waveguiding properties of SiON will be studied. By removing one, two or three rows of holes within a triangular lattice of holes a line defect appears. Within this line defect it is possible to guide the light\textsuperscript{6}. In the first three waveguides that will be presented, the transmission properties of these waveguides will be studied. It is of no interest to explore the system of dielectric rods in air. The waveguide in this system would be air, without any guiding properties in the vertical direction.

Figure 33 shows the transmission of waves within the three waveguides denoted with W1 (waveguide 1 row missing, etc.), W2 and W3 describing system with one, two and three missing rows respectively. The rows are removed in the $\Gamma$-$K$ directions.

![Figure 33](image)

Figure 33. Transmission of three waveguides, W1, W2 and W3. Vertical dotted lines denote the band gap region. The designs are also schematically depicted.

A plane wave is generated at the entrance of the waveguide (left side of the design). At the end of the waveguide the time averaged Poynting vector has been calculated. The structures are schematically depicted in figure 33.

The dominant feature for guiding the light in these structures is index guiding. Only between the dotted lines also guiding by the photonic band gap occurs. Apparently,
the transmission maximum is not within the band gap region. This, and other features within figure 33 will be discussed in the next paragraphs.

Figure 33 shows dips in the transmission around normalised frequency 0.37 and 0.47 for the three waveguides. This is caused by the following effect: The electromagnetic wave in the waveguide will have a smaller wavelength (due to the higher effective index in the region of the waveguide) in the waveguide than in the crystal. When the wavelength in the waveguide is twice the length of the lattice pitch (generally: \( n\lambda = 2a \)), a transmission dip occurs because the sidelobes of the electromagnetic wave encounters the crystal periodically. Therefore the transmission is reduced. The same line of argument can be made for the second gap. Figure 34 shows the field at normalised frequency 0.37. As can be seen the wave has a wavelength that is equal to twice the lattice pitch of the crystal.

*Figure 34. Magnetic field at normalised frequency 0.37. A transmission dip occurs because the wavelength is twice the lattice pitch.*

In the W1 case the second transmission gap at normalised frequency 0.48 is reducing the transmission, therefore it is not suitable for a waveguide. W2 and W3 don't suffer from this gap any more.

Figure 35 shows a typical figure for waveguiding through a straight (W3) waveguide with normalised frequency within the photonic band gap and a figure of the same waveguide but now for a normalised frequency outside the band gap. It can be seen that there are no waves within the crystal when the normalised frequency is within the band gap (left figure). On the contrary, for frequencies outside the band gap free propagation of modes is possible (right figure and see also figure 34).
Figure 35. Magnetic field distribution in a W3 waveguide at normalised frequency 0.50 within the band gap (left picture) and at normalised frequency 0.40 outside the band gap.

Figure 33 shows also that the transmission maximum does not occur as expected within the band gap region. This is a direct consequence of the increased reflectivity of the crystal at normalised frequencies within the band gap region. As a consequence, the backwards reflection (negative consequences for transmission) are obviously reducing the transmission within the band gap region. It will be shown that within a 60-degree bend index guiding is not the dominant guiding factor anymore and the transmission maximum is then as expected, within the band gap region.

Another way to guide electromagnetic waves inside a photonic crystal is by coupled cavity waveguiding. This can be compared with impurity band conduction within semiconductors. In the SiON the evanescent wave is much larger than in higher refractive index materials, due to the low dielectric constant. This should be beneficial for coupled cavity waveguiding because the cavities are better connected by this larger evanescent wave. Figure 36b gives the transmission spectra for four coupled waveguiding structures, which are shown in figure 36a. (W1 B1 stands for Waveguide 1 row missing and Barrier of 1 hole between the cavities.)
Each cavity has its eigenmodes. Effective waveguiding can only occur when an eigenmode of the cavity lies within the band gap of the crystal and a lossless cavity exists. From figure 36b it can be seen that the W1 cavity does not have an eigenmode in the normalised frequency range 0.48-0.50, the photonic band gap range of the crystal. It has a monopole mode at normalised frequency 0.40 and a dipole mode at normalised frequency 0.55. On the contrary, the W2 cavity does have an eigenmode (dipole) inside the photonic band gap as shown in figure 36b.
Figure 37 gives the field patterns of monopole and dipole cavity modes, at normalised frequencies 0.42 and 0.51 respectively for the two structures with the W2 B3 cavity.

![Magnetic field](image)

Figure 37. Magnetic field for monopole and dipole cavity modes for the W2 B3 cavity. Notice that the monopole mode is leaky and thus not suitable for coupled cavity waveguiding.

The monopole mode is leaky because it is not within the photonic band gap. The dipole mode is within the gap, and photon tunnelling allows propagation of the wave. These coupled cavity waveguides are a new and interesting area for research. They can be used for compact on-line filtering. Also for low-loss bend waveguides coupled cavity waveguiding is very promising.

### 4.3 Waveguide bends

In order to reduce the size of optical integrated chips, small radius waveguide bends are needed. Photonic crystal structures are investigated as building blocks for such compact bends. In a triangular lattice bends of 60 degrees can be made. In figure 38 the transmission of two (W1 and W3) 60-degree bends is shown, also schematically the designs are depicted in figure. The transmission has been calculated in the same way as done for straight waveguides.
As expected, the guidance is best around the photonic band gap of the crystal. As already mentioned. However a look at the magnetic field shows that the electromagnetic wave becomes multi-mode after the bend, as depicted in figure 39.

Optimising these structures can be done by smoothening the bend by turning twice over 30 degrees. This can be done by removing holes at the inner side and add holes at the outer bend in such a way that the wave is initially travelling in the $\Gamma$-$K$ direction then in the $\Gamma$-$M$ direction and finally back to the $\Gamma$-$K$ direction again. Figure 40 shows the transmission spectra for the two smooth bend designs with three and six extra holes in the outer bend of the W3 60-degree bend. The designs are schematically shown in figure 40.
Figure 40. Energy outflow for 60-degree bend and for two optimised bends as function of normalised frequency. Designs are shown on the right.

In figure 41 the field distribution is given at normalised frequency 0.50, the maximum transmission frequency for the optimised design with 6 extra holes.

As can be seen from figures 40 and 41, the transmission is increased by a factor of two for the W3 bend 6 rods design. On the contrary the design W3 bend 3 rods, does not show any improvement at normalised frequency 0.50. This is caused by the change in waveguide width, which is a direct consequence of the change in direction. Therefore it would be better to put only three holes at the outer bend without removing three holes from the inner bend. Within the second improved design this problem has been taken into account and only three holes were removed from the
inner bend and six holes added in the outer bend to ensure better continuity of the waveguide width in the bend.

Figure 41 shows indeed that the fundamental mode is better transmitted as compared to figure 39. This implies that by smoothening the bend even further, a single-mode bend might be possible.

It is without doubt that implementation of the improved designs as found in the previous sections, is beneficial for the properties of the waveguide bend. This requires further research into improved bending design.

As already mentioned, coupled cavity waveguiding might be very promising for waveguide bends. In the next paragraphs some topics will be briefly discussed.

The cavities calculated for the straight waveguides show that only the W2 structure has an eigenmode within the photonic band gap of the crystal. Therefore only this structure will be used for calculations. Figure 42 shows the energy outflow for two designs.

![Figure 42](image)

*Figure 42. Transmission for coupled cavity bend waveguiding. Designs are also shown.*

Figure 43 shows the field distribution at normalised frequency 0.50, the transmission maximum for the W2 B1 barrier.
From figure 43 it can be seen that the field and cavity alignment is changed. The normal dipole mode has vanished and a second node is present in the cavity. This can be explained by the fact that the cavity only accepts a mode that is present in the crystal and is an eigenmode of the cavity. Because the cavity is turned, the cavity will most likely accept another mode, as the field is still a plane wave from the left. In this case a mode with an extra node. As a consequence the second cavity after the bend does not accept the field because the field is not aligned with the cavity. This also explains why the configuration W2 B3 bend does not work. Therefore it is suggested that cavities with symmetry comparable to the lattice should be used. Also the use of different cavities before and after the bend might be interesting.
CONCLUSIONS AND RECOMMENDATIONS

This chapter contains the conclusions of this work and some recommendations for future work.

The purpose of the research was to investigate the possibilities for SiON as a new photonic crystal material. A brief overview over the entire scope of relevant topics has been made to find out if SiON is indeed a useful material for photonic band gap applications.

It is shown that:

1. SiON has a complete band gap for a triangular lattice of holes for TE-polarisation between normalised frequencies 0.48 and 0.50, and also a complete gap for a triangular lattice of rods for TM-polarisation between normalised frequencies 0.48 and 0.53.

2. The modified Matlab program can calculate the density of states correctly.

3. The simulation program Femlab which uses the finite element method algorithm, is capable of calculating transmission spectra that are in agreement with conventional calculations methods such as the plane wave method or the transfer matrix method.

4. Dispersion relations can be modified in a predetermined way by modifying the shape of the rods and holes (based upon the orthogonality requirement and the variational principle). Improved designs for rods show a 15% broader- and nine times stronger gap for the Γ-M direction. The improved design for holes show a 20% broader and a nine times stronger gap for the Γ-M direction (see recommendations).
5. A novel modelling technique for out of plane losses has been presented. It is shown that for small aspect ratios the out of plane losses are larger than for large aspect ratios. Also for small aspect ratios it is shown that the electromagnetic wave can propagate within the sub-core region. For the first time the use of a graded index has been suggested as waveguiding layer within photonic crystals. This first graded index design shows less out of plane losses for normalised frequencies above the band gap, larger losses within the gap region and comparable losses with the slab waveguide for frequencies below the band gap.

6. Straight photonic crystal waveguides are possible within the SiON material system for W2 (waveguide made out of the removal of two rows of holes) and W3 and are not possible for the W1 waveguide.

7. Straight-coupled cavity waveguiding is possible when using the W2 cavity and is not possible for the W1 cavity.

8. A conventional bend W1 and W3 suffer greatly from reflections in the bend. Therefore an optimised, double 30-degree bend, is proposed. Transmission of the optimised structure is enhanced with a factor of two. Also the fundamental mode is better transmitted.

9. Coupled cavity waveguiding for bends is possible if field-cavity alignment can be maintained after the bend.

10. Based upon these conclusions SiON is a very promising new photonic crystal material, also for reasons of simplicity in fabrication.

The following recommendations for further research can be made:

1. The line of arguments used to improve the gap in one direction can also being used omni-directional by starting with a six-fold rotational symmetry design.

2. Rigorous calculations in k-space by changing second- and third order Fourier coefficients, for omni-directional optimisation of the shape of
holes and or rods, can be used to further improve the photonic crystal properties of SiON. This can be done with the Matlab program used to calculate the dispersion relations.

3. The calculations done on the novel graded index waveguide should be extended to fully 3-dimensional calculations. This can be done analytically with the Matlab program that can calculate the dispersion relations for each individual layer of the graded index profile. A scattering matrix method, well known from semiconducting physics, can be used to couple the different modes in each region. Also it is possible to improve the graded index profile in the z-direction within the 2-D calculations, to reduce the losses further.

4. Waveguide bends are one of many applications that can be useful for novel devices. Therefore further research in optimising the double 30-degree band has to be made.

5. Promising are the coupled cavity waveguiding systems that can be used for many different purposes. Finding cavities that possess eigenmodes within the band gap are crucial. Also the use of different cavities in one device is interesting.

6. The abnormal dispersion relations of photonic crystals can be used in many different ways. Therefore the focus should not only be on telecommunication purposes but should be extended to many different areas where light manipulation is needed.


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