Numerical studies of 2D photonic crystals: Waveguides, coupling between waveguides and filters

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Abstract. In photonic crystals, light propagation is forbidden in a certain wavelength range, the bandgap. In a two-dimensional crystal composed of parallel high-refractive index rods in a low-index background a line defect can be formed by removing a row of these rods, which can act as a waveguide for frequencies in the bandgap of the crystal. In order to get more insight into the main features of such waveguides we have studied a number of properties, using simulation tools based on the finite difference time domain method and a finite element Helmholtz solver. We show conceptually simple methods for determining the bandgap of the crystal as well as the dispersion of a waveguide for wavelengths in this bandgap. For practical applications, it is also important to know how much light can be coupled into the waveguide. Therefore, the coupling of light from a dielectric slab waveguide into the photonic crystal waveguide has been examined, showing that a coupling efficiency of up to 83% can be obtained between a silicon oxide slab and a waveguide in a crystal of silicon rods. Finally, calculations on an ultra-compact filter based on reflectively terminated side-branches of waveguides (similar to tuned stubs in microwave engineering) are shown and discussed.

Key words: numerical modelling, photonic bandgap crystals, wavelength filter

1. Introduction

In order to integrate many photonic functions on a chip, it is necessary to make both the individual functional components and the interconnects as small as possible. Components based on dielectric waveguides are usually quite large, in the order of millimetres. For example, bends in waveguides introduce special problems, because the radius of curvature should be large (mm) in order to suppress radiation loss.

In the light of the above, photonic bandgap crystals are a promising class of structures for compact photonic integration. They consist of a regular lattice of dielectric materials with a high refractive index compared to the rest of the space. When the index contrast is high enough, a range of wavelengths exists for which propagation is forbidden in all directions, the so-called photonic band gap (Joannopoulos et al. 1995). Calculations show that it should be possible to make very tight bends in waveguides in these crystals, with a radius in the order of the wavelength, with (nearly) 100% transmission.
(Mekis et al. 1996; Baba et al. 1999). Other devices like ultra-compact wavelength filters are also possible (Sigalas et al. 1993; Fan et al. 1998; Mekis et al. 1998; Scherer et al. 1998).

This paper will focus on a particular 2-dimensional photonic crystal consisting of a square lattice of square rods of silicon in air. A simple method to determine the bandgap will be presented in Section 2.

A line defect that is formed when a row of rods is removed, can act as a waveguide (Benisty 1996; Sakoda et al. 1997; Centeno and Felbacq 1999), which we will call a crystal waveguide. For the considered lattice, such a waveguide is single-moded. The behaviour of such a mode is different from that in a dielectric slab. Consider a wave that is guided in the \( z \)-direction along a dielectric waveguide. Such a wave has a field distribution in the \( x-y \) plane (the mode profile), and a single effective index. On the other hand, modes guided along crystal waveguides show field profiles and phase velocities corresponding to the different Floquet modes. For such a mode an effective index corresponding to the first Brillouin zone can be determined numerically. From this wavelength dependent effective index the group velocity can be evaluated. Results of calculations on these quantities, and also on the effective modal width will be presented in Section 3.

In practical applications, the coupling efficiency between a photonic crystal waveguide and a conventional dielectric waveguide (e.g. an optical fibre) is an important issue. In order to gain some insight into this subject, we investigated the coupling between a dielectric slab and a crystal waveguide. The results are discussed in Section 4 of this paper.

In Section 5 we describe an ultra-compact filter that is obtained by coupling a cavity to a waveguide. When a row of rods is partially removed, so that a waveguide is formed that terminates in the crystal, a cavity is formed that acts as a resonator. If such a resonator is attached as a side-branch to a crystal waveguide, similar to a tuned stub in microwave engineering, a structure results that acts as a wavelength filter. (Danglot et al. 1998) have shown this effect for metallic photonic crystals in the microwave regime, but to our knowledge it has not been studied in dielectric photonic crystals. Increasing the quality factor \( Q \) of the cavity by not removing the rod directly adjacent to the crystal waveguide will result in a filter having a smaller bandwidth. Such high-\( Q \) cavities show a large field enhancement at resonance, which may be exploited for non-linear optics applications.

The paper ends with conclusions in Section 6.

2. Photonic crystal structure and bandgap calculation

We consider a crystal as shown in Fig. 1, consisting of a square lattice of silicon rods in air, having a lattice constant of 600 nm. The rods have a
150 × 150 nm square cross-section and a refractive index of 3.4 (assumed constant in the wavelength region of interest around \( \lambda = 1550 \) nm). For a very similar structure (Joannopoulos et al. 1995), a bandgap is known to exist around \( \lambda = 1.5 \) μm for TE polarisation (i.e. \( E \)-field parallel to the rods, perpendicular to the calculation window).

A straightforward method for determining the bandgap is to calculate the transmission of a broad-band electromagnetic signal through the crystal for all directions in the reduced Brillouin zone. For that purpose, a 2-dimensional finite difference time domain (FDTD) scheme (Taflove 1995) is used. As shown in Fig. 2, a finite crystal of 8 rods width is defined. To the left of this, a dipole is oscillating at a central frequency corresponding to a wavelength of 1.5 μm; it is modulated with a pulse that is short enough (50 fs) that the resulting electromagnetic wave contains all wavelengths in the bandgap. This dipole will radiate in all directions. Taking the time-domain Fourier transform of the transmitted field at the right-hand side of the crystal for a range of propagation angles between 0 and 45°, covering the reduced Brillouin zone of the square lattice, yields the transmitted amplitude for a sufficiently wide wavelength range around the bandgap.

Fig. 3 shows a superposition of the graphs of the transmitted amplitude versus the wavelength, for 100 uniformly distributed propagation angles between 0 and 45°. In the wavelength range from \( \approx 1.3–1.7 \) μm, the transmission is nearly zero for all directions, revealing the photonic bandgap.

Although other methods (Joannopoulos et al. 1995), which use a single unit cell for the band-structure calculation, are more accurate, this method is fast and gives a good approximation of the total bandgap of the crystal, similar to the bandgap for the similar structure studied in (Joannopoulos et al. 1995).
Fig. 2. Configuration for determining the bandgap: a dipole radiator is positioned at the left-hand side of the crystal, while the transmission is determined along a vertical line at the right-hand side.

Fig. 3. Superposition of the transmission amplitudes across all relevant angles. The low area between approximately 1.3 and 1.7 is the bandgap for TE.
3. Crystal waveguides

Removing a row of rods creates a channel through which light can propagate, a so-called crystal waveguide. Such a waveguide can also be considered as two semi-infinite crystals brought into proximity. We have found from numerical calculations that this particular waveguide supports one symmetrical mode for all wavelengths inside the bandgap. In the calculations, the mode is excited through a thick Perfectly Matched Layer.

In integrated optics, waveguide modes are usually characterised by their effective index, which is directly related to the phase velocity along the waveguide. In order to determine the effective index of crystal waveguide modes, we applied two different calculation methods: finite difference time domain (FDTD) and a pandirectional finite element Helmholtz solver. Light is propagated through a waveguide with a length of about 25 lattice periods. In the Helmholtz solver, the effective index was calculated directly from the phase velocity. In the FDTD method, the waveguide was terminated by a number of rods, creating a mirror. From the interference pattern in the waveguide before the mirror, the effective wavelength can be determined and from that the effective index. Fig. 4 shows the result for both methods.

The effective index is lower than one, which means that the phase velocity is larger than the speed of light. In dielectric waveguides, the effective index is also lower than the index of the core layer. Since the core layer in a crystal waveguide is air, with a refractive index of one, this means that the effective index must be lower than one. This is also similar to the case of modes guided between parallel conducting plates.

![Fig. 4. Effective index of crystal waveguide, calculated by two different methods, as a function of the wavelength.](image-url)
In order to determine the group velocity, a third-order polynomial is fitted to the effective index values obtained from the FDTD calculations, and the following formula is used:

\[
\nu_{\text{group}} = \frac{\partial \omega}{\partial k_x} = \frac{c}{n_{\text{eff}} - \lambda \left( \frac{\partial n_{\text{eff}}}{\partial \lambda} \right)}
\]

This gives the group velocity graph shown in Fig. 5. The group velocity is smaller than the speed of light in vacuum and decreases with increasing wavelength.

Another important practical property of a waveguide mode, be it a crystal or a dielectric waveguide, is its effective width. This effective width is a useful quantity for assessing the coupling efficiency of light from free space or from another waveguide, since the overlap between the incoming field and the mode (and thus the coupling efficiency) is high when the effective widths are equal. For dielectric waveguides, this is calculated by taking into account the Goos–Hänchen shift on the interfaces (Kogelnik 1979).

The definition of the width of a crystal waveguide is not obvious, since the structure is not invariant in the propagation direction, and there is some arbitrariness in the choice of the location of the interface planes. An approximate effective width, however, can be defined for the lowest-order mode as:

\[
w = \frac{\lambda}{2 \sqrt{n_{\text{core}}^2 - n_{\text{eff}}^2}}
\]

Fig. 5. Group velocity of crystal waveguide mode, as a function of the wavelength.
corresponding to the width of a parallel-plate waveguide with perfectly conducting walls that supports a lowest order TE mode with the same effective index. The thus obtained effective width as a function of the wavelength is given in Fig. 6.

The effective width of the crystal waveguide mode is calculated to be between 0.95 and 1.22 μm, which is quite different from the seemingly natural physical width of 0.6 μm, equal to the lattice constant since a single row of rods is removed.

Crystal waveguide modes share many properties with those of standard dielectric waveguides. The effective index is smaller than the index of the core material, and, of course, the group velocity is smaller than the speed of light. If the width of the crystal waveguide is defined as the lattice constant, it is smaller than the effective modal width, as is the case in dielectric waveguides. As mentioned in the introduction, in contrast to the case of a conventional dielectric waveguide, the transverse field distribution in a crystal waveguide varies periodically (with the lattice period) along the propagation direction.

4. Coupling from a dielectric waveguide to a crystal waveguide

In this section, the coupling of light from a normal dielectric waveguide to a crystal waveguide will be investigated. The structure is given in Fig. 7. We will only consider the central wavelength of the bandgap, \( \lambda = 1.5 \) μm. For this wavelength, the effective width of the crystal waveguide as calculated in the previous section is 1.05 μm. We chose to investigate two different materials for the input waveguide: one with a refractive index of 1.45, and one

![Fig. 6. Effective modal width of crystal waveguide mode, as a function of the wavelength.](image-url)
with a refractive index of 1.8. These values have been chosen to study the
effects of both Fresnel and overlap losses, which are anticipated to be both
different for the two considered index values (see below).

Fig. 8(a) and (b) show the total coupling loss and the theoretical Fresnel
losses of both structures. In Fig. 9, the effective modal width of the incoming
waveguides is given. In approximation, the difference between the Fresnel
losses and the total coupling loss is the extra loss caused by the mismatch of
the modal field. It is difficult to draw conclusions from these results. For the
waveguide with the high refractive index, the extra loss is smallest around
d = 0.6 μm. The effective modal width of the dielectric guide is around
1 μm, which is close to the effective modal width of the crystal waveguide
according to Equation (2). This suggests that the effective modal width as
calculated in the previous section is a useful tool when analysing the coupling
from other waveguides or free space into crystal waveguides. However, the
other waveguide, with the refractive index of 1.45, does not fully comply with
this theory; the extra coupling loss is lowest at a width of around 0.6 μm,
where the effective modal width is not closest to the effective width of the
crystal waveguide mode.

Apparently, the simple modal width picture is not sufficiently accurate
to understand the coupling of dielectric waveguides to crystal waveguides.
This may be because the crystal mode is not the same at the entrance of
the photonic crystal as it is deeper into the waveguide; the surface distorts
the mode. It will be very interesting to examine how this coupling loss
may be further minimised. The following are possibilities for improve-
ments:
– Changing the refractive index of the dielectric waveguide to a value between 1.45 and 1.8
– Moving the end of the dielectric waveguide into the crystal guide
– Changing the size or the index of the rods near the entrance of the crystal waveguide

5. An ultra-compact wavelength filter

Several examples of wavelength filters in photonic bandgap materials, based upon resonant cavities can be found in literature. Most of these filters transmit a small range of wavelengths while reflecting the larger part of the
spectrum (Sigalas et al. 1993). Also, an add-drop filter has been shown in which the index or the size of single rods must be tuned to achieve proper operation (Fan et al. 1998). We will show a filter based upon waveguide side-branches, which transmits most wavelengths, while reflecting a number of small wavelength ranges, also known as a notch filter.

The first observation of a filter function arises when a single rod directly adjacent to the crystal waveguide is removed. This defect will start acting as a cavity; for a certain wavelength, all light will be reflected into the incoming channel. The filter characteristic is shown in Fig. 10. Increasing the side-branch length to 3 rods, as shown in Fig. 11, gives a narrower filter char-

![Fig. 9. Effective modal width for dielectric waveguides at 1.5 μm wavelength, as a function of the physical waveguide width.](image)

![Fig. 10. Filter characteristic of a crystal waveguide with 1 missing rod adjacent to the waveguide.](image)
acteristic, as shown in Fig. 12: this is to be expected, since the free spectral range decreases while the finesse of the cavity remains more or less constant.

The filter function can be explained by means of scattering matrix theory (Haus 1982). The spot where the branch connects to the main waveguide is a node with three input and three output ports, as drawn in Fig. 13. Light coming in from an input port will be distributed across the three output ports according to the following matrix:

Fig. 11. Crystal waveguide with a 3-rods-deep side-branch.

Fig. 12. Filter characteristic of a crystal waveguide with a 3-rods-deep side-branch; transmission as a function of the wavelength.
with

\[ S = S^T = S^{-1} \]  

in which the vectors contain the amplitudes of the incoming and outgoing modes. Due to the symmetry of the system, some of the elements of the matrix are equal.

When a perfect mirror with a wavelength-dependent phase-shift is introduced at the output of port 3, while only having input into port 1, the input of port 3 can be calculated as follows:

\[ A_{3}^{\text{in}} = \exp(i\varphi(\lambda))A_{3}^{\text{out}} \]  

\[ A_{3}^{\text{in}} = \exp(i\varphi(\lambda))A_{3}^{\text{in}} s_{1} \left(1 + r_{3}\exp(i\varphi(\lambda)) + r_{3}^{2}\exp(2i\varphi(\lambda)) + \cdots\right) \]

\[ = \frac{\exp(i\varphi(\lambda))A_{3}^{\text{in}} s_{1}}{1 - r_{3}\exp(i\varphi(\lambda))} \]  

so, using (3) and (6), the output amplitude of port 2 is:

\[ A_{2}^{\text{out}} = t_{1}A_{1}^{\text{in}} + s_{1}A_{3}^{\text{in}} = A_{1}^{\text{in}} \left(\frac{t_{1} - t_{1} r_{3}\exp(i\varphi(\lambda)) + s_{1}^{2}\exp(i\varphi(\lambda))}{1 - r_{3}\exp(i\varphi(\lambda))}\right) \]

Using the fact that \( S^{*} = S^{-1} \), it may be proved that:

\[ -t_{1} r_{3} + s_{1}^{2} = t_{1}' \equiv t_{1} \exp(i\theta(\lambda)) \]  

Hence
So, for certain values of $\lambda$, the numerator of this formula becomes zero, yielding zero transmission and full reflection.

This configuration is similar to a transmission line with a parallel short-circuited stub.

The device as described above has a filter characteristic with dips in the transmission (and peaks in the reflection) that are too wide for some applications. The bandwidth of the filter is directly related to the finesse of the resonating cavity, which is dependent on the reflection coefficients on either side of the cavity. At the far side of the cavity, the reflection is 100%; at the junction, it is only approximately 33%. By moving the cavity down one rod and introducing an extra rod as shown in Fig. 14, the reflection coefficient at the junction increases dramatically, while still retaining the symmetry of the system. This leads to the response curve in Fig. 15. Using the same arguments as before, the transmission can be shown to be zero for certain wavelengths.

A high-$Q$ resonator like this builds up a high intensity in the cavity. This high intensity could be used for nonlinear applications, without the need for a high input power. In this cavity, the intensity is about 20 times larger than the input intensity.

\[ A_{2}^{\text{out}} = A_{1}^{\text{in}} \frac{1 + \exp(i\varphi(\lambda) + \theta(\lambda))}{1 - r_{3} \exp(i\varphi(\lambda))} \tag{9} \]
6. Conclusions

This paper shows the results of some calculations on waveguides in a 2-dimensional photonic bandgap crystal. For such a configuration to be practical, the light will have to be confined in the third dimension, which might be hard to achieve. However, the authors feel that the concepts described here can be used in the description, calculation and design of general photonic crystal devices.

The used photonic crystal is a square lattice of silicon rods in air. A simple method was used to determine the bandgap. Removal of a row of rods creates a monomodal crystal waveguide for all wavelengths in the gap. The effective index of these modes is lower than one; but, as it should the group velocity is lower than the speed of light in vacuum. An effective modal width is introduced, which is found to decrease with increasing wavelength. The effective modal width may play an important role in the losses on coupling dielectric waveguides to crystal waveguides. It is shown that, for the considered photonic structure, such coupling losses can be as low as approximately 15%. The Fresnel losses, caused by the effective index difference between the dielectric waveguide mode and the crystal waveguide mode, are an important factor; in the coupling from a waveguide with a higher refractive index, these losses are the dominant part of the total loss.

In normal waveguide-to-waveguide coupling, the effective modal width is a powerful design parameter, which can be used to roughly minimise the coupling loss. Our results indicate that this picture holds only approximately for coupling to a crystal waveguide, and that the physics is probably too complicated to describe the coupling only in terms of effective modal widths and the Fresnel losses.
When a single rod is removed next to a waveguide, this will create a filter characteristic, which means that for some wavelengths no light will be transmitted. As a consequence, waveguides in photonic crystals are quite sensitive to technological imperfections of this kind. One can use this phenomenon to design an ultra-compact filter. The wavelength characteristic of the filter is determined by the length of the side-branch (which affects the free spectral range) and the reflection coefficients of the junction point. We have shown a filter that blocks a wavelength range of approximately 4 nm. Cavities of this kind may be used for intensity enhancement.

References
