MODELLING OF PHOTONIC CRYSTAL FIBRES

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Abstract: Different theoretical models for analysis of photonic crystal fibres are reviewed and compared. The methods span from simple scalar approaches to full-vectorial models using different mode-field decompositions. The specific advantages of the methods are evaluated.

1. Introduction

In 1987 it was suggested /1,2/ that the electronic bandgaps of semiconductors had an optical analogy in periodic dielectric structures (photonic crystals). However, the theoretical search for such photonic bandgaps (PBGs) was initially hindered by the lack of suitable theoretical models. Part of the reason for this lack must be found from the fact that only structures with a high refractive-index contrast are able to exhibit photonic bandgap effects (we here disregard so-called 1D photonic bandgap structures, which have been known for decades and are merely Bragg reflectors as known from e.g., multilayer films, gratings, etc.). Therefore, while scalar modelling of low-index contrast dielectric structures for the optical domain had been sufficient for most previous applications, the accurate modelling of photonic bandgap effects required fully vectorial models. Today, a wide range of theoretical models for general analysis of high-index contrast microstructures exist /3-6/ and photonic crystals are being extensively exploited.

One the most promising applicational areas where photonic crystals are finding use is in optical fibre technology. This specific field of research is today about five years old /7,8/, and it addresses the issue of periodically microstructured optical fibres with a high-index contrast (they typically consists of air holes in a silica background material). The fibres in question are often called Photonic Crystal Fibres (PCFs), and this new class of optical waveguides may conveniently be divided into two very different groups. The first is fibres having a high-index core (typically solid silica) surrounded by a two-dimensional photonic-crystal cladding-structure. These fibres have properties, which partly resembles those of conventional fibres due to the fact that the waveguidance is caused by Total Internal Reflection (TIR); the higher refractive index of the core compared to the effective index of the photonic crystal cladding allows for traditional index guiding. It is, therefore, important to notice that these fibres, which we shall name TIR-PCFs, do in fact not rely on PBG effects at all. Radically different to the TIR-PCFs are fibres, where the photonic-crystal-cladding structure is exhibiting PBG effect, and where this effect is utilised to confine light in the core region. These fibres, PBG-PCFs, show remarkable properties among which being the ability to confine and guide light along a core region having a refractive index below that of the cladding structure. While the TIR-PCFs were the first to be fabricated /9/, truly PBG-guiding fibres were only recently experimentally demonstrated /10/. In this presentation, we shall address both types of fibres and discuss the various theoretical tools employed for their modelling. Generally, the analysis of PBG-PCFs requires advanced fully vectorial models, whereas simple scalar models may in some cases be used for qualitative analysis of TIR-PCFs.

The presentations is organised in the following way; We will firstly describe a simple effective-index approach for modelling TIR-PCFs, and discuss a few properties of these fibres. Secondly, a so-called plane-wave method will presented, which is a very general method that may be applied to both TIR- and PBG-PCFs. The basic operational principle of PBG-PCFs will be described in more detail, and we will present two different methods for modelling PBG-PCFs. These methods both take basis in the plane-wave method but use different techniques to account for the core region.

2. Effective-index approach for TIR-PCFs

In order to establish a relatively simple numerical tool that could provide qualitative mode-propagation properties of the TIR- PCFs, Birks et al. /11/ in 1997 proposed a method, in which sequential use of well-established fibre tools was applied. The fundamental idea behind this work was first to evaluate the periodically repeated hole-in-silica structure of the cladding, and then (based on the approximate waveguiding properties of this cladding structure) replace the cladding by a properly chosen effective index. In this model, the resulting waveguide then consists of a core and a cladding region that have refractive indices n_{co} and n_{cl}, respectively. The core is pure silica, but the definition of the refractive index of the micro-structured cladding region is given in terms of the propagation constant of the lowest-order mode that could propagate in the infinite cladding material (the so-called Fundamental Space filling Mode, FSM, of the structure). This scalar effective-index method has also been used as a basis for the approximate dispersion and bending analysis presented in /12/.

The first step of the effective-index method is to determine the cladding mode field, Ψ, by solving the scalar wave equation within a unit cell centred on one of the holes (which are placed in a triangular lattice structure). The diameter of these unit cells equals the pitch, Λ, between the holes of the cladding structure. The hexagonal shapes of the cells are approximated by circular ones in order to make a general circular-symmetric mode solution possible. By reflection symmetry, the boundary condition at the cell edge (at radius $\Lambda/2$) is $d\Psi/ds = 0$, where s is the coordinate normal to the edge. The propagation constant of the resulting fundamental space-filling mode, β_{FSM}, is used to define the effective index of the cladding as $n_{eff} = \beta_{FSM}/k$ (where k is the free-space propagation constant of light with wavelength λ). It should also be noted that we in the calculation of this cladding field (together with the effective-index value) have assumed the normal weakly guiding field assumption /13/, although the index step between central hole (refractive index 1.0) and surrounding silica (refractive index around 1.45) actually is considerable. However, the hereby-introduced inaccuracy is considered to be less significant than the approximation of the guided-mode field in the effective-index fibre compared to the actual field in the PCF.

Now having determined the cladding- and core-index values, the approximate propagation properties of the PCF may be calculated as for a step-index fibre with core index n_{co}, core radius $\Lambda/2$, and cladding index $n_{cl} = n_{eff}$. As an extension to the cladding-mode model originally described in /11/, it was in /12/ added that the refractive index for silica was wavelength dependent. This was done through the introduction of the generally applied Sellmeier formula /14/. The effective-index approach should primarily be seen as a rapid method for gaining a qualitative impression of the waveguiding properties of TIR-PCFs, and it has (as such) only been applied on fibres with a triangular cladding index structure.

Despite their resemblance with conventional optical fibres, the TIR-PCFs persist a number of unusual properties. The main reason for this is attributed to the very strong frequency dependence of the effective refractive index of the cladding structure. As the frequency is increased (moves towards shorter wavelengths) in TIR-PCFs, the field of the cladding modes are expelled from the air holes. Thus, the mode-index of both the cladding modes, and the core modes approach the index of silica (as well as that of each other), and a low-wavelength bending-loss edge appears. For longer wavelengths, the mode field will spread into the holes of the cladding structure, and consequently average out the refractive index regions, resulting in an ordinary upper bending-loss edge. It is actually these bending-loss properties, which eventually may limit the spectral operational range of the TIR-PCFs and not so much their additional unusual features, namely their possibility of being (nearly) endlessly single mode /11/. The TIR-PCFs have also been predicted to show a remarkably high dispersion /12/, and their novel dispersion properties has also demonstrated TIR-PCFs as potentially useful for wide bandwidth generation of visible light through non-linear effects in the low-loss waveguide /15/.

It is, therefore, obvious that the TIR-PCFs allows for new and highly interesting waveguiding properties. However, the next fundamental step towards a new dimension in optical waveguiding appears when the PBG effect is brought in effective use /10/. However, for this step to be taken, more complex numerical tools had to be developed, and we will address these in the following paragraphs.

3. Basic plane-wave method

In 1990, the first method for finding PBGs in photonic crystals was described /3/. The method was closely related to methods used for calculating electronic bandgaps in semiconductor crystals, in that it described the magnetic field **H** as a plane wave multiplied by a Bloch function **U** with the periodicity of the photonic crystal:

$$\mathbf{H}(\mathbf{k},\mathbf{r}) = e^{\mathbf{k}\cdot\mathbf{r}}\,\mathbf{U}(\mathbf{k},\mathbf{r}) \qquad (1)$$

For a two-dimensionally periodic structure, the periodicity of the photonic crystal may be described by the two primitive lattice vectors $\mathbf{R_1}$, $\mathbf{R_2}$. Then:

$$\mathbf{H}(\mathbf{k},\mathbf{r}) = \sum_{\mathbf{G}}\sum_{j=1}^{2} h_j(\mathbf{k}+\mathbf{G})\,\mathbf{e}_j(\mathbf{k}+\mathbf{G})\,e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \qquad (2)$$

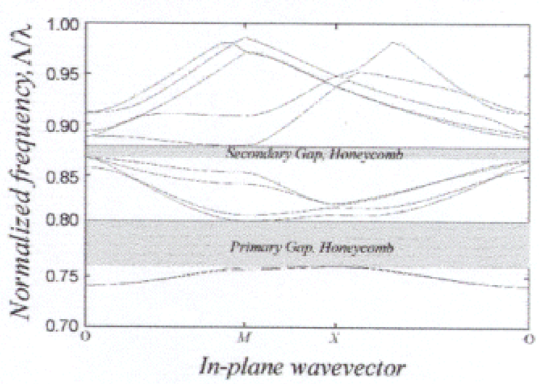
Where $(\mathbf{k}+\mathbf{G})$, $\mathbf{e_1}(\mathbf{k}+\mathbf{G})$, $\mathbf{e_2}(\mathbf{k}+\mathbf{G})$ form a triad (since the magnetic field is transverse). The sum is over all possible reciprocal lattice vectors defined by $\mathbf{G}\cdot\mathbf{R} = N2\pi$, where **R** is any one of the primitive lattice vectors. Basically, (2) is a Fourier transform of the magnetic field. We may, therefore, insert this form into Maxwell's equation:

$$\nabla \times \left(\frac{1}{\varepsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{k},\mathbf{r}) \right) = \left(\frac{\omega}{c} \right)^2 \mathbf{H}(\mathbf{k},\mathbf{r}) \qquad (3)$$

By Fourier transforming the dielectric function of the structure $\varepsilon(\mathbf{r})$, equation (3) may be formulated as an eigenvalue problem, which may be solved for a truncated number of shortest reciprocal lattice vectors.

For the two-dimensional photonic crystal structures of interest in the fibres, the plane wave vector **k** may have a non-zero longitudinal component k_z /16/, which will remain unchanged due to the uniformity of the structure in the z-direction. This out-of-plane wave vector relates to the propagation constant, β, from standard optical fibres. An example of the photonic bandgaps that may be exhibited by a full two-dimensionally periodic array of air holes in a silica-background material is illustrated in Fig.1. The calculation is for a k_z-value equal to $1/\Lambda$, where Λ describes the minimum center-to-center spacing between two air holes. An important aspect to be aware of is that the refractive-index contrast between silica and air is to low to provide a PBG effect for waves propagating strictly in the periodic plane, i.e. with a k_z-value equal to zero. However, in the case of out-of-plane propagation, i.e., non-zero k_z -values, full PBGs may be found to form in the silica/air photonic crystals.

Fig. 1: Band structure diagram for a honeycomb-lattice structure consisting of air holes in a silica-background material. The air-filling fraction is 30%. Two so-called out-of-plane photonic bandgaps are indicated. Notice that a minimum frequency limit exists below which no mode solutions exists. The minimum frequency relates to the fundamental space-filling mode of the structure.



The out-of-plane photonic bandgaps illustrated in Fig.1 indicates how a periodic cladding structure may prevent transverse power dissipation, and thereby be used to form a waveguide. However, in order to do so, a fibre core region has to be included; By locally breaking the periodicity of a photonic crystal, a spatial region with optical properties different from the surrounding bulk photonic crystal can be created. If such a defect region supports modes with frequencies falling inside the forbidden gap of the surrounding full-periodic crystal, these modes will be trapped at the defect. This is the principle on which the operation of the PBG guiding fibres relies, namely a complete out-of-plane 2D bandgap exhibited by the photonic crystal cladding, and a correctly designed defect, forming a spatial region to which very strong transverse confinement can be achieved.

4. An efficient plane-wave method and super-cell approximations

The method based on the solution of equation (3) is well suited for calculating the PBGs of a periodic dielectric structure, since it describes the field and the structure as a Bloch function /17/. However, to include a core, one has to impose an artificial periodicity, which is handled numerically by creating a supercell with periodically repeated core-defects. This yields correct guided solutions, if the supercell is much larger than the guided mode-area /18/. Such a supercell approach requires a high number of plane waves, which initiated an interest in models capable of handling a large number of eigenvalues.

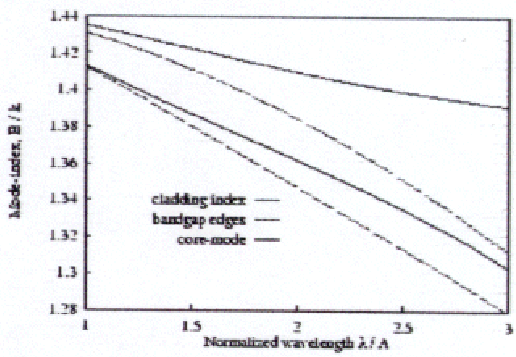
The eigenvalue equation (3) is Hermitian /19/. Therefore, fast iterative schemes for finding the eigenvalues by a Rayleigh quotient method exist /20/. If one has a guess of the weights $h_j(\mathbf{k}+\mathbf{G})$ in (2), then the curl of the magnetic field is quickly found (it scales linearly with the number of plane waves). By using a FFT to find the curl in real space, we may create a situation, where we may easily divide by the dielectric function in (3). We may then use the FFT to transform the result back into Fourier space, which makes it easy to take the last curl in (3). Since the FFT scales like NlogN, where N is the number of plane waves, we may solve equation (3) for a large number of plane waves using this method /18/, by applying a suitable preconditioning /20/. When only finding the lowest eigenvalues as in TIR fibres, this method solves the problems extremely fast. However, the memory demands and the calculation time increases, if a large number of eigenvalues must be found, and this is typically the situation in analysing PBG-PCFs.

5. Basic properties of PBG-PCFs

For the illustration in Fig.2, we have employed the above-described supercell approximation to calculate the bandgaps of a PBG-PCF with a honeycomb cladding structure and an extra, centrally placed defect hole (more details on the Honeycomb PBG-PCF may be found in /21/ and /22/).

Inside the bandgap, we observed a single defect-mode traversing the bandgap from approximately $\lambda/\Lambda = 1$ to 3. This mode is caused solely by introducing a defect air hole in the honeycomb structure. For the full periodic structure, we find exactly the same PBGs (with no modes inside) with identical boundaries to those of the crystal including the defect. This defect-mode is strongly localised to the core region (albeit this is a low-index region), and does not couple to cladding modes in the PCF, (since the mode is falling inside the bandgap of the photonic-crystal cladding). Loss-less guidance may, therefore, in principle, be achieved over long lengths. Although not illustrated, most of the field of the defect mode for this particular PBG-PCF is distributed in the silica. Also included in the Fig.2 is the effective cladding index defined using the lowest-frequency allowed mode in the full periodic structure. Above this cladding-index line is a semi-infinite 'bandgap', where no modes exist. This is the region in which all TIR-PCFs operate, since a high-index defect causes at least one mode to appear above this line. Such index-guided modes are not featured by low-index core PBG-PCFs.

Fig. 2: Illustration of the first bandgap of a honeycomb-based PBG-PCF as a function of the normalised wavelength λ/Λ. Within the primary bandgap, the extra air hole in the core of the fibre causes a single degenerate mode to appear. This 'defect' mode is localised around the core of the fibre, and does not couple to the cladding structure (as it is here forbidden due to the photonic bandgap effect). For a fibre with $\Lambda = 1.0\ \mu m$, the core mode falls within the bandgap in a wavelength range from approximately to 1.0 µm to well above 3.0 µm. Leakage-free, single mode waveguidance is thus obtained over this wavelength range. A supercell size of 5x5 simple honeycomb cells and 16384 plane waves were used for the calculation.



The supercell approach for inclusion of the PBG-PCF core in the model may for many analyses imply very high demands on computer memory. Consequently, a number of researchers have been developing alternative methods, in which the localised nature of the guided mode fields of the PCFs is utilised /23-25/. In the following section, the idea behind this approach is discussed.

6. Method based on localised functions

The eigenvalue equation (3) is quite general, in that it is also valid for anisotropic materials. However, since silica is isotropic, we may choose to exploit this by choosing the well-known vectorial transverse eigenvalue equation:

$$\left[\nabla + n^2k^2 - \beta^2\right]\mathbf{e}_t = -\nabla_t\left(\mathbf{e}_t \cdot \nabla_t \ln\left(n^2\right)\right) \qquad (4)$$

In this formulation, the transverse wavevector k is scalar. Therefore, this formulation is suitable for finding guided solutions (which in principle are the same for all **G**-vectors (2)). Such formulations, therefore, avoid the supercell formulation of the core. One may then describe the cladding by a Fourier formulation (cosines), while the core-defect and the transverse electric field is described by localised functions /23/. The eigenvalue equation may then be recast into a Hermitian matrix eigenvalue problem /23/, where the matrix elements are found from overlap integrals, which may be found analytically.

Since there is no supercell, the number of cosines needed to describe the cladding is limited for TIR-PCFs. This is important since each basis function, used to describe the structure, adds an extra overlap integral to each matrix element. The size of the eigenvalue matrix on the other hand is determined by the number of localised basis functions used to describe the field.

One solves equation (4) by choosing a k-value, and then finding the eigenvalues, β. Thus one obvious advantage of the (4) over the (3) formulation, is that material dispersion is more easily introduced. Further, it has been reported that relatively few basis functions are needed to describe the solutions accurately /23/.

As previously described, an efficient modesolver exist for the plane-wave method. However, to our knowledge no quick method (as an FFT analogy) exist for finding the overlap integrals in /23/. In a sense, we are forced to choose between an efficient mode-solver and efficient basis functions. When making this choice, it should be remembered that the operator based plane-wave method is relatively more efficient, when a limited number of eigenvalues are needed (TIR-PCFs), while the localised function approach is relatively more efficient, when many eigenvalues are required (PBG-PCFs). Also, notice that (4) becomes particularly simple in the scalar case, which may be applied to TIR-PCFs with small air holes /24/. In this case, the gradient becomes a simple differentiation, while the terms on the right side vanish.

7. Conclusions

In conclusion, it should be noted that the appearance of the new class of optical waveguides represented by the photonic crystal fibres not only have opened up for new waveguiding properties, but it has also placed new and stronger demands on fibre modelling. Where most problems previously could be address by a well-developed scalar theory, an accurate description of both TIR-PCFs and PBG-PCFs generally requires a full vectorial mode solver. This naturally becomes very important, keeping in mind that a large part of the fundamental understanding of conventional fibres does not directly apply for PCFs. We, therefore, have to develop a complete range of new theoretical understanding of a novel type of waveguides, and in this process the numerical modelling is going to play a central role.

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