Numerical Modeling of Photonic Crystal Fibers

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Abstract—Recent progress on numerical modeling methods for photonic crystal fibers (PCFs) such as the effective index approach, basis-function expansion approach, and numerical approach is described. An index-guiding PCF with an array of air holes surrounding the silica core region has special characteristics compared with conventional single-mode fibers (SMFs). Using a full modal vector model, the fundamental characteristics of PCFs such as cutoff wavelength, confinement loss, modal birefringence, and chromatic dispersion are numerically investigated.

Index Terms—Finite-element method, holey fiber, microstructured optical fiber, numerical modeling, photonic band-gap fiber, photonic crystal fiber.

I. INTRODUCTION

PHOTONIC crystal fibers (PCFs) [1]–[3], also called holey fibers or microstructured optical fibers, have been under intensive study for the past several years as they offer a number of unique and useful properties not achievable in standard silica glass fibers. PCFs fall into two basic categories. The first one, an index-guiding PCF [4], [5], is usually formed by a central solid defect region surrounded by multiple air holes in a regular triangular lattice and confines light by total internal reflection like standard fibers. The second one uses a perfect periodic structure exhibiting a photonic band-gap (PBG) effect at the operating wavelength to guide light in a low index core region, which is also called PBG fiber (PBGF) [6], [7].

Numerical simulations play an important role for the design and modeling of PCFs. So far, various modeling methods in which not only a full-vector model but also an approximate-scalar model is used have been developed such as effective index approach [5], [8], plane-wave expansion (PWE) method [9]–[12], localized-function method [13]–[16], multipole method (MM) [17]–[21], beam propagation method (BPM) [22]–[24], finite-difference method (FDM) [25], finite-difference time-domain method (FDTD) [26]–[28], boundary element method (BEM) [29], [30], and finite-element method (FEM) [31]–[54]. An approximate-scalar model is a valuable tool for aiding fabrication efforts because it is easy to use and provides good qualitative information. However, in order to model PCFs accurately, it is crucial to use a full-vector model. In particular, a complete vector model is necessary for predicting sensitive quantities such as dispersion and birefringence.

The choice of modeling tool can impact the computational time, required computational resources, and limitations of the methods, so it is important to explore the usefulness and limitations of each method.

In this paper, first, recent progress on numerical modeling methods of PCFs such as the effective index approach, basis-function expansion approach, and numerical approach is described. Next, using a full-vector mode solver based on the FEM with curvilinear hybrid edge/nodal elements [55] that can avoid spurious solutions and can accurately model curved boundaries of air holes in PCFs, fundamental characteristics of index-guiding PCFs such as cutoff wavelength, confinement loss, modal birefringence, and chromatic dispersion are numerically investigated.

II. ANALYSIS METHOD

A. Effective Index Approach

The cross section of a typical index-guiding PCF with sixfold rotational symmetry is schematically shown in Fig. 1, where $\Lambda$ is the hole pitch (center-to-center distance between the holes) and $d$ is the hole diameter.

The first approach developed for PCFs was the effective index approach [5], [8] based on a very simple scalar model using an effective cladding index. In this model, first, an effective index for the periodically repeated hole-in-silica structure is evaluated and then the microstructured cladding region is replaced by a uniform medium with a properly chosen effective index.
PWE involves defining the supercell over a restricted region and using periodic boundary conditions to extend the structure spatially, and therefore, the applicability to PCFs that do not need to be periodic is somewhat restricted. An alternative approach is the localized-function method (LFM) [15], [16]. As the guided modes in PCFs are localized in the defect core region, their modal fields are well described using localized Hermite–Gaussian functions. The LFM takes advantage of mode localization, and thus, a modest number of functions are required to accurately model the guided modes, resulting in less computational efforts, compared with the PWE. By decomposing the electromagnetic field (in LFM, as usual, three components of the electric field) and the index defect into localized Hermite–Gaussian functions, and the lattice of air holes using sinusoidal functions, each quantity can be represented efficiently and accurately without requiring the use of too many expansion terms [16]. Again, the wave equation is reduced to a matrix eigenvalue problem that is solved for the modal fields and their propagation constants. The LFM based on an approximate-scalar model is also available [13], [14].

If all the air holes are assumed to be circular, the modal fields can be expanded in cylindrical harmonic functions. This approach exploiting the local circular geometry is called the MM [17]–[21], which can describe the leaky nature of PCFs with a finite number of air holes. In the proximity of each air hole, the electromagnetic field (in MM, as usual, two longitudinal axial components of the electromagnetic field) is expressed in terms of Bessel and Hankel functions using local cylindrical coordinates. Inside each air hole, on the other hand, the axial electric and magnetic fields are expressed in terms of regular Bessel functions only. In order to obtain relations between all the expansion coefficients, boundary conditions on hole surfaces are used.

C. Numerical Approach

Although the basis-function expansion approach can accurately predict the modal properties such as dispersion and birefringence, it is difficult to apply it to more complicated fibers with noncircular air holes and/or longitudinally varying structures. Recently, published models utilize other direct numerical analysis techniques such as BPM [22]–[24], FDM [25], FDTD [26]–[28], BEM [29], [30], and FEM [31]–[54].

In the FEM, instead of solving the wave equation, the corresponding functional to which a variational method is applied is set up, where the fiber cross section is divided into the so-called elements, an equivalent discretized model for each element is constructed, and then all the element contributions to the whole fiber cross section are assembled, resulting in a matrix eigenvalue problem with nodal variables as unknowns, in contrast to the basis-function expansion approach taking expansion coefficients as unknowns. As a result, the matrices derived from the FEM and the basis-function expansion approach become sparse and dense, respectively.

For the characterization of longitudinally varying PCFs, the BPM is clearly the natural choice. Even the approximate-scalar BPM based on the fast Fourier transform (FFT-BPM) is able to describe some features of PCFs [22], [23]. This standard
Fig. 2. Transverse electric field vector distributions of (a) HE\textsubscript{x11} and (b) HE\textsubscript{y11} modes.

BPM splits the actual wave propagation into a propagation in a homogeneous medium, followed by a phase correction corresponding to the inhomogeneous index distribution in the fiber structure. The wave propagation in a homogeneous medium is efficiently carried out in the spectral domain using the FFT technique. In the FFT-BPM, however, a weakly guiding structure is assumed, so the polarization effect cannot be taken into account. Recently, the full-vector BPM based on the FEM (FE-BPM) [35] or the FDM (FD-BPM) [24] has been applied to compute the propagation constants and the modal profiles in high-contrast PCFs. The FE-BPM has been effectively applied to investigating the problem of leakage due to finite number of arrays of air holes in PCFs [35].

Although the BPM is currently the most widely used for the study of light propagation in longitudinally varying optical waveguides, it is difficult to take into account backward reflecting waves. One method used to study distributed reflection and diffraction at arbitrary angle is the FDTD technique. This technique is very powerful and versatile and has been introduced and adapted to PCFs [26]–[28]. Splice losses between a standard SIF and a PCF, and spot-size and numerical aperture conversion phenomena in a tapered PCF are numerically investigated [26], [27].

III. GUIDED MODES IN PCFS

In an index-guiding PCF, the core index is greater than the average index of the cladding because of the presence of air holes, and the fiber can guide the light by total internal reflection as a standard fiber does. That is, the guided light has an effective index \( n_{\text{eff}} \) that satisfies the condition

\[
\beta k_0 > n_{\text{FSM}}
\]

where \( \beta \) is the propagation constant along the fiber axis, \( n_{\text{co}} \) is the core index, and \( n_{\text{FSM}} \) is the cladding effective index of the FSM. In the case of a PCF made from pure silica, \( n_{\text{co}} \) is reduced to the index of silica.

Fig. 2 shows the transverse electric field vector distributions of the fundamental modes in a multimode PCF, where \( \Lambda = 2.3 \, \mu m \), \( d = 1.8 \, \mu m \), the background index of silica is assumed to be 1.45, and the operating wavelength is 0.46 \( \mu m \). The fundamental modes in Fig. 2 resemble the linearly polarized modes LP\textsubscript{01} in the conventional SIFs. As in the SIFs, the linearly polarized fundamental modes HE\textsubscript{x11} and HE\textsubscript{y11} are degenerate. The degeneracy in these two fundamental HE\textsubscript{11} states has already been confirmed by using the full-vector MM [17], the full-vector FEM [32], and the full-vector BPM [24]. Figs. 3–5 show the higher-order modes. By analogy with the SIFs, we call these guided modes TE, TM, HE, and EH. The higher-order modes in Figs. 3–5 look like the LP\textsubscript{11}, LP\textsubscript{21}, and LP\textsubscript{02} modes, respectively.

The cutoff wavelength of each higher-order mode is determined by using the effective cladding index \( n_{\text{FSM}} \). The cutoff of the higher-order mode occurs when its effective refractive index becomes equal to the value of \( n_{\text{FSM}} \). The accurate...
Fig. 5. Transverse electric field vector distributions of (a) HE$_{12}^1$ and (b) HE$_{12}^2$ modes.

Fig. 6. Effective index of the FSM for the PCF with different hole diameters.

The parameter $V$ for PCFs is frequently used in the design of conventional SIFs and is given by

$$V = \frac{2\pi}{\lambda} a \sqrt{n_{co}^2 - n_{cl}^2}$$  

(2)

that must be less than 2.405 for the fiber to be single mode, where $\lambda$ is the operating wavelength, $a$ is the core radius, $n_{co}$ is the core index, and $n_{cl}$ is the cladding index. Recently, it has been reported that the fundamental properties of index-guiding PCFs such as cutoff wavelength, mode field diameter (MFD), splice loss, and so on, can be easily estimated without the need for heavy numerical computations by appropriately defining the $V$ parameter [57]. By analogy with SIFs, the effective $V$ parameter $V_{eff}$ for PCFs can be defined as

$$V_{eff} = \frac{2\pi}{\lambda} a_{eff} \sqrt{n_{co}^2 - n_{FSM}^2}$$  

(3)

where $a_{eff}$ is the effective core radius. To adapt the concept of $V$ parameter to PCFs, the value of $a_{eff}$ should be determined. We have confirmed from the full-vector FEM analysis that

for small hole diameters, $d/\Lambda < 0.43$, the PCFs are endlessly single mode. Until now, various effective core radii have been proposed, such as $a_{eff} = \Lambda/2$, $a_{eff} = \Lambda - d/2$. When using these effective core radii, for the PCFs with hole diameter $d/\Lambda < 0.43$, the effective $V$ parameter $V_{eff}$ is not less than 2.405 at all wavelengths. So, to use the definition of the cutoff $V$ value as in conventional SIFs ($V = 2.405$), we have to choose the value of $a_{eff}$ to be $\Lambda/\sqrt{3}$ [34], [57]. Mortensen et al. proposed another effective $V$ parameter for PCF [58]. However, this definition is intrinsically different from the original $V$ parameter definition in SIF theory and corresponds to the normalized transverse attenuation constant $W$ parameter. So we adopt the $V$ parameter definition of (3). From (3) with $a_{eff} = \Lambda/\sqrt{3}$, the cutoff condition is given by $V_{eff} = 2.405$, as in conventional SIFs, and therefore the $V$ parameter in (3) enables us to apply the design principle for standard SIFs straightforwardly to PCFs [57].

Fig. 7 shows the relative cutoff wavelength $\lambda/\Lambda$ as a function of the effective core radius $d/\Lambda$. The calculated cutoff wavelengths obtained from (3) and $V_{eff} = 2.405$ agree well with the experimental results [59] and the results of direct numerical simulation based on the FEM. We can see that PCFs with relative hole diameters less than 0.43 can be endlessly single mode, and that even for large air holes single-mode operation is possible for wavelengths above a cutoff wavelength. If the value of $d/\Lambda$ is given, a given cutoff wavelength can be obtained by scaling the fiber structure. This allows for the development of single-mode fibers (SMFs) with very small or large MFDs, which are useful for highly nonlinear SMF application, high bit rate wideband data transmission, single-mode high power delivery, and so on.

Next, to evaluate the MFD, we introduce the Marcuse formula [60] as

$$\frac{w}{a_{eff}} = 0.65 + \frac{1.619}{V_{eff}^2} + \frac{2.879}{V_{eff}^6}$$  

(4)

where $w$ is the half MFD and is called the effective modal spot size. In Fig. 8, calculated MFD results are shown as a function of wavelength for different hole sizes. The experimental results for two PCFs fabricated by Crystal Fiber A/S [61], namely, LMA-5 ($\Lambda = 2.9 \mu m$, $d/\Lambda = 0.44$) and LMA-8 ($\Lambda = 5.6 \mu m$, $d/\Lambda = 0.49$), are also shown. The results of (3) and (4) are in
good agreement with measured data [61]. Knowledge of MFD is an important starting point in the context of nonlinearities. Due to the high index contrast between silica and air, the PCF technology can offer a smaller MFD compared to standard fiber technology, which is useful for broadband supercontinuum generation, soliton pulse transmission, nonlinear optical loop mirror, optical signal processing, and so on. In addition, PCFs have a large potential for single-mode large-mode-area optical fibers with low nonlinearity because of their endlessly single-mode properties combined with large MFDs.

With the modal spot size, Gaussian beam propagation theory states that the splice loss $L_s$ between a PCF and a SMF is given by

$$L_s = -10 \log_{10} \left( \frac{2w_{SMF}^2}{w^2 + w_{SMF}^2} \right) \exp \left( -\frac{2\delta^2}{w^2 + w_{SMF}^2} \right)$$

(5)

where $2w_{SMF}$ is the MFD of the SMF that is also calculated with (4) and $\delta$ is a transverse offset. In evaluating the splice losses, we assume that the SMF is an SM28 fiber. Fig. 9(a) and (b) shows the splice losses between the PCF and the SM28 fiber as a function of hole pitch $\Lambda$ for $d/\Lambda$ from 0.25 to 0.55 with $\delta = 0$ and as a function of offset $\delta$, respectively, where an operating wavelength is 1.55 $\mu$m. For comparison, the measured results [62] and the numerical results obtained by use of the FEM [62] are also plotted. The results based on (5) agree approximately with the measured and numerical results.

V. CONFINEMENT LOSS AND EFFECTIVE MODE AREA IN PCFS

The losses in PCFs occur for a number of reasons, such as intrinsic material absorption loss, structural imperfection loss, Rayleigh scattering loss, confinement loss, and so on. Fabrication-related losses can be reduced by carefully optimizing the fabrication process [63]. Confinement loss is an additional form of loss that occurs in single-material fibers. PCFs are usually made from pure silica, and so the guided modes are inherently leaky [18] because the core index is the same as the index of the outer cladding without air holes. This confinement loss can be reduced exponentially by increasing the number of rings of air holes that surround the solid core, and is determined by the geometry of the structure. It is important to know how many numbers of rings of air holes are required to reduce the confinement loss under the Rayleigh scattering limit for practical fabrication process.

Fig. 10 shows the normalized confinement loss of the fundamental mode in PCFs with finite cross sections as a function of the normalized effective area, taking the ratio of hole diameter to pitch ratio $d/\Lambda$ as a parameter, where $N$ is the number of rings of air holes and the background silica index is assumed to be 1.45. The effective area of the fiber core $A_{eff}$ is defined as [64]

$$A_{eff} = \frac{\int \int \int_{S} |E_t|^2 \, dx \, dy}{\int \int \int_{S} |E_t|^4 \, dx \, dy}$$

(6)

where $E_t$ is the transverse electric field vector and $S$ denotes the whole fiber cross section. As expected, increasing the air-hole size, the mode becomes more confined, and thus the effective area and the confinement loss are both reduced. Also, increasing the number of rings of air holes, the confinement loss is significantly reduced. On the other hand, the effective area is almost independent of the number of hole rings. We can see that the confinement loss contributes significantly to the loss of PCFs when the hole pitch $\Lambda$ is small. Fig. 10 is a general map of the effective area that can be used for designing various PCFs, such as ultralow nonlinearity PCFs and high nonlinearity PCFs with desired confinement loss properties. If, for example,
the operating wavelength is given, the effective area and the confinement loss can to a large extent be tailored via the choice of hole pitch, hole size, and number of hole rings.

VI. Modal Birefringence

One of the interesting characteristics of PCFs is their strong birefringence. Using PCFs, highly birefringent fibers can be easily realized because the index contrast is higher than conventional fibers and the fabrication process permits the formation of the required asymmetric microstructure near the fiber core. One possible use of highly birefringent PCFs is as polarization maintaining fibers (PMFs) that can stabilize the polarization state in the fiber. So far, various highly birefringent PCFs have been reported [65]–[67] as shown in Fig. 11. The configurations of Fig. 11(a) and (b) [65], [67] have different air-hole diameters along two orthogonal axes near the core region and Fig. 11(c) has two defects in the hole arrangement [66].

Fig. 12(a) shows an image generated from the scanning electron micrograph of the first reported highly birefringent PCF [64]. To estimate the birefringence of this fiber with noncircular air holes irregularly arranged around the core, it is necessary to carry out the real-model simulation [51], so the full-vector FEM is used here. The transverse electric field vector distributions of the two different polarization modes called the slow-axis and fast-axis modes are, respectively, shown in Fig. 12(b) and (c). The effective index of the slow-axis mode is slightly larger than that of the fast-axis mode. Fig. 13 shows the modal birefringence as a function of wavelength. The birefringence obtained by using the real-model simulation is $3.66 \times 10^{-3}$ at $\lambda = 1.54 \mu m$ and is in good agreement with the measured value of $3.7 \times 10^{-3}$ [65]. The birefringence of the order of $10^{-3}$ is one order of magnitude larger than that of conventional PMFs.

Highly birefringent PCFs have possibilities of realizing a single-polarization single-mode (SPSM) fiber [68], [69], which guides only one polarization state of the fundamental mode.
The SPSM fiber can eliminate both polarization mode coupling and polarization mode dispersion. Fig. 14 shows an example of SPSM-PCF structure [50], [70], where $\Lambda$ is the hole pitch and $d$ and $d'$ are the diameters of the small and large air holes, respectively. The design principle of SPSM fiber is to have the cutoff wavelengths of the fundamental modes polarized along the slow axis (slow-axis mode) and the fast axis (fast-axis mode) longer and shorter than the operating wavelength, respectively. The cutoff of either polarization occurs when its effective refractive index becomes equal to the cladding effective index of the FSM. In order to reduce the confinement loss of the slow-axis mode, eight of the central air holes are enlarged. Fig. 15 shows the wavelength dependence of the confinement loss for the single-polarization PCF with ten rings of air holes, where $\Lambda = 2.2 \, \mu m$, $d/\Lambda = 0.5$, and $d'/\Lambda = 0.95$, and the background index of silica is calculated through the Sellmeier equation. Within the wavelengths ranging from 1.48 to 1.6 $\mu m$, the confinement loss of the slow-axis mode is less than 0.1 dB/km and the fast-axis mode is unguided. From these results, a low-loss SPSM-PCF can be realized with the highly birefringent PCF in Fig. 14. The SPSM-PCF is expected to be used in various optical devices as the pigtails of polarization-sensitive optical components.
Theoretically, in the PCF structure with sixfold symmetry, the two linearly polarized fundamental modes are degenerated. Small imperfections in the PCF structure that are produced during the fabrication process, however, create asymmetries that break the degeneracy and lead to birefringence. Small irregularity, such as the variation of the hole size or the position, results in the perturbed PCF from the sixfold rotational symmetry structure. Since PCFs with the small hole pitch and the large hole diameter cause large perturbation from the perfect structure [71], [72], the PCFs with the large hole pitch and the small hole diameter have the advantage for suppressing the birefringence induced by the structural irregularity.

VII. CHROMATIC DISPERSION TAILORING

PCFs possess the attractive property of great controllability in chromatic dispersion. The chromatic dispersion profile can be easily controlled by varying the hole diameter and the hole pitch. Controllability of chromatic dispersion in PCFs is a very important problem for practical applications to optical communication systems, dispersion compensation, and nonlinear optics. So far, various PCFs with remarkable dispersion properties have been investigated both experimentally and numerically.

Fig. 16 shows the chromatic dispersion property of PCF with perfect hexagonal symmetry shown in Fig. 1 as a function of wavelength for \( d/\Lambda \) ranging from 0.2 to 0.9 in steps of 0.1, where the material dispersion given by a Sellmeier formula is included directly in the vector FEM calculation. The chromatic dispersion \( D \) of a PCF is easily calculated from the effective index of the fundamental mode \( n_{\text{eff}} \) versus the wavelength using

\[
D = -\frac{\lambda^2}{c} \frac{d^2 n_{\text{eff}}}{d\lambda^2} \tag{7}
\]

where \( c \) is the velocity of light in a vacuum. When the hole diameter to pitch ratio is very small and the hole pitch is large, the dispersion curve is close to the material dispersion of pure silica. As the air-hole diameter is increased, the influence of waveguide dispersion becomes stronger. We can see that it is possible to shift the zero dispersion wavelength to visible to near-infrared (IR) regions by appropriately changing the geometrical parameters such as hole pitch and hole diameter [73], [74] and that a PCF with a very small hole pitch and a large air-hole diameter has large normal dispersion in the 1.55-\( \mu \)m wavelength range [48]. In addition, Fig. 16(c) points out that a PCF with \( \Lambda \approx 2.5 \) \( \mu \)m and \( d/\Lambda \approx 0.25 \) exhibits nearly zero dispersion-flattened behavior [75], [76].

The cladding structure of typical PCFs is usually formed by air holes with the same diameter arrayed in a regular triangular lattice shown in Fig. 1. However, using a PCF with all of the same air-hole diameter in the cladding region, it is difficult to control both the dispersion and the dispersion slope in a wide wavelength range. In index-guiding PCFs, since the periodicity in the cladding region is not essential to confine the guiding light into the high-index core region, it has been reported that various effective refractive index profiles can be obtained by varying the hole diameter of each air-hole ring along the radius [43].

Fig. 17 shows two examples of PCFs and their effective refractive index profiles, where \( d_i \) (\( i = 1 \) to \( n \)) is the hole diameter of the \( i \)th air-hole ring and the air-hole diameters are \( d_1 > d_2 = \cdots = d_n \) in Fig. 17(a) and \( d_2 < d_1 = d_3 = \cdots = d_n \) in Fig. 17(b). The effective refractive index in the cladding...
region increases with decreasing air-hole diameter, and the effective refractive index in the cladding region decreases with increasing air-hole diameter. By optimizing the air-hole diameters $d_i$ and the hole-to-hole spacing, both the dispersion and the dispersion slope can be controlled in a wide wavelength range.

Fig. 18 shows an example of nearly zero dispersion-flattened PCF with ten air-hole rings designed by using this design principle, where $\Lambda = 1.6 \, \mu m$ and the air-hole diameters are $d_1 = 0.47 \, \mu m$, $d_2 = 0.71 \, \mu m$, $d_3 = 0.74 \, \mu m$, $d_4 = 0.62 \, \mu m$, $d_5 = \cdots = d_{10} = 0.65 \, \mu m$. It is possible to decrease the effective refractive index in the cladding region along the radius by increasing the air-hole diameters along the radius. It is also possible to realize flattened dispersion by using the effective refractive index profile in Fig. 18(b) with small hole pitch.

Fig. 19 shows the chromatic dispersion and effective area as a function of wavelength for the PCF in Fig. 18(a). The wavelength range for which the PCF dispersion remains between 0.1 and 0.3 ps/(km·nm) is from 1.41 to 1.68 µm. The confinement loss of the fundamental mode is less than 0.1 dB/km in the wavelength range shorter than 1.7 µm. In short wavelength range, this PCF supports the second order mode; however, the confinement loss of the second-order mode is larger than 1000 dB/m in the wavelength range over 1.0 µm and the effective refractive indices of the second-order mode are quite different from those of the fundamental mode, so this PCF effectively operates as an SMF in the telecommunication window. The PCF with nearly zero flattened-dispersion and small effective area is attracting interest because it can offer high nonlinearity over a wide wavelength range [77], [78].

VIII. CONCLUSION

Analysis methods for numerical modeling of photonic crystal fibers (PCFs) were reviewed in detail. Through the full-vector finite-element method (FEM), the fundamental characteristics of PCFs such as normalized frequency, cutoff wavelength, confinement loss, modal birefringence, and chromatic dispersion have been numerically investigated. The numerical method used here can be applied to designing not only index-guiding PCFs but also photonic band-gap fibers (PBGFs). Numerical modeling techniques have great potential for designing profitable PCFs.

REFERENCES


