Numerical modeling of photonic crystal fibers using the finite element method

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Abstract. Propagation constants and amplitudes of eigenwaves of photonic crystal fibers are calculated numerically using an algorithm based on combination of the exact nonlocal boundary conditions method and the finite-element method. The design of fibers has a central large core filled with nematic liquid crystal. We investigate the influence of radii of the cladding air holes and their number as well as radius of the central liquid crystal on the spectral characteristics of fibers. Our results strongly suggest that radius of the crystal in contrast to the size and the number of capillaries has a significant influence on eigenwaves and propagation constants. Varying this radius we control the number of solutions of the problem for a fixed wavelength.

1. Introduction
Spectral problems of the theory of photonic crystal fibers (PCF) attract a lot of attention (see, for example, [1], [2]). PCF having a central large core filled with nematic liquid crystal (NLC) is a modern component of micro-devices used in photonics and laser technology [3]. The development of efficient numerical methods for accurate and stable computations of spectral characteristics of NLC-PCF is essential for designing and optimizing of such devices. Mesh methods, namely, various modifications of the finite-element method (FEM, see, for example, [3], [4]) and the finite-difference method (see, for example, [5], [6]) are used extensively to solve these important applied problems. Often the authors concentrate on the algorithm's features and physical interpretation of the numerical results rather than on fundamental mathematical aspects, including correctness of used models.

The original problems for eigenwaves of open dielectric waveguides, particularly, NLC-PCF, are formulated on the whole plane. From the mathematical point of view, the main difficulty in applying the mesh methods to solve such problems is the transfer of radiation conditions from infinity to the boundary of the finite mesh domain. This obstacle was overcome in two different manners by the method of exact nonlocal boundary conditions in [7] and [8]. The original problems were reduced to problems on a bounded domain (on a circle) through the use of the nonlocal boundary operators defined by the Fourier series. This approach allows us to give a new correct formulation of the problem for eigenwaves of NLC-PCF as a generalized spectral problem with a nonlinear dependence on the spectral parameter, which is applicable for the numerical solution. A more convenient for the numerical solution formulation of the spectral problem for open dielectric waveguides was proposed in [9]. It is also a problem in a bounded domain and is formulated as a generalized eigenvalue problem for self-adjoint operators in a Hilbert space, but the spectral parameter enters into it linearly. The latter property significantly simplifies the numerical solution of this class of problems and allows us to
develop efficient numerical methods. An algorithm for the numerical solution of such problems based on the finite-element approximation was proposed in [9]. The convergence of this method was proved in [10].

In the presented paper, using mentioned above algorithm, we calculate numerically propagation constants and amplitudes of eigenwaves of NLC-PCF and investigate the influence of radii of the cladding air holes and their number as well as radius of the central liquid crystal on the spectral characteristics of the fibers. Our results strongly suggest that radius of the crystal in contrast to the size and the number of capillaries has a significant influence on eigenwaves and propagation constants. Varying this radius we control the number of solutions of the problem for a fixed wavelength.

2. Problem statement and the exact nonlocal boundary conditions method

In this section, following [3], we state the problem for the TE-eigenwaves of NLC-PCF. We use Cartesian coordinates and assume that the generating line of the fiber is parallel to Ox axis. Figure 1 shows a schematic diagram of the investigated NLC-PCF. All the cladding air holes have the same radius \( r \) and are arranged with a hole pitch \( L \). The big central hole has a radius \( r_0 \) and is infiltrated with NLC material. We assume that the refractive index \( n \) of this material is equal to \( n_0 = 1.5024 \). The structure of all capillaries \( \Omega \) is surrounded by silica with the refractive index \( n_s = 1.45 \). As usual, the refractive index of air is one and the magnetic permeability of all dielectric materials is equal to the magnetic constant \( \mu_0 \). Note that our consideration is true for a much more general case, namely, if the refractive index is a sufficiently smooth function of the transverse coordinates and \( \Omega \) is a bounded domain with a piecewise smooth boundary \( \gamma \).

![Figure 1. The structure of the suggested NLC-PCF and the decomposition of the coordinate plane \( R^2 \).](image)

The original problem is formulated as follows: find pairs of the numbers \((\beta,k) \in \Lambda\) and nonzero real-valued vanished at infinity functions \( u \) satisfying the equation

\[-\Delta u + \beta^2 u = k^2 n^2 u, \quad x \in R^2 \setminus \gamma,\]

and the boundary conditions

\[u^+ = u^-, \quad \frac{\partial u^+}{\partial \nu} = \frac{\partial u^-}{\partial \nu}, \quad x \in \gamma.\]  

Here \( x = (x_1, x_2) \), \( \nu \) is the unit outward normal vector for the curve \( \gamma \), \( k = (\varepsilon_0 \mu_0)^{1/2} \omega \) is the longitudinal wavenumber, \( \varepsilon_0 \) is the vacuum permittivity, \( \omega \) is the angular frequency, \( \beta \) is the propagation constant, \( u \) is the amplitude of the longitudinal component of the electric field, \( \Lambda = \{ (\beta,k) : \beta / n_0 < k < \beta / n_s, \beta > 0 \} \). If \((\beta,k) \in \Lambda\), then the transverse wavenumber
\[ p = (\beta^2 - k^2 n^2)^{1/2} \]  

(3)

is real and positive. Equation (1) has the form

\[ -\Delta u + p^2 u = 0 \]  

(4)

on the domain \( \Omega_x = \mathbb{R}^2 \setminus \bar{\Omega}_x \), and \( p \) defines the rate of decay of \( u \) at infinity, namely (see [11], for example),

\[ u = \exp(-p|x|)O\left(1/\sqrt{|x|}\right) \text{ as } |x| \to \infty. \]

We can solve the original problem as the parametric eigenvalue problem, where the parameter is either \( \beta \) or \( k \), but let us introduce the new pair of the unknown parameters \( (p, \beta) \) and the set

\[ K = \{ (\beta, p) : \beta > 0, \ 0 < p < \sqrt{(n_0^2 - n^2)/n_0^2} \beta \}. \]

It is easy to see that formula (3) defines the one-to-one correspondence between the sets \( \Lambda \) and \( K \). Let us consider the new problem: find pairs of the numbers \( (\beta, p) \in K \) and nonzero real-valued vanished at infinity functions \( u \) satisfying the following equation on \( \mathbb{R}^2 \setminus \gamma \):

\[ -\Delta u + p^2 \sigma u = \beta^2 (\sigma - 1)u, \quad \sigma = n^2 / n_0^2, \]  

(5)

and transparency conditions (2). Using (3), we see that equation (5) transforms to equation (1). The converse is also true. Therefore the two problems are equivalent in the following sense: \( (\beta, k, u) \) is a solution of (1) if and only if \( (\beta, p, u) \) is a solution of (5). Now we reduce problem (5) to a problem posed on a circle.

We assume that the origin belongs to \( \Omega_x \). Let \( B_{R_0} = \{ x : |x| < R_0 \} \) be the circle of the minimal radius \( R_0 \) such that \( \Omega_x \subseteq B_{R_0} \). We choose a number \( R \) that more or equal to \( R_0 \) and put \( \Omega = B_R, \quad \Gamma = \partial \Omega, \quad \Omega_x = \mathbb{R}^2 \setminus \bar{\Omega}_x \) (see Fig. 1). Each solution of problem (5) satisfies equation (4) on \( \mathbb{R}^2 \setminus \bar{\Omega}_x \), hence it is smooth on this domain. By \( u_p (u) \) we denote its restriction to the domain \( \Omega_x \). Then the function \( u_p \) satisfies equation (4), and for \( x \in \Gamma \) the following equalities hold:

\[ u_p = u, \quad u_{\nu \nu} = u_\nu. \]

Here \( \nu \) is the unit outward normal vector for the curve \( \Gamma \), \( u_\nu \) is the derivative of \( u \) in the direction of \( \nu \). The function \( u_p \) is the solution of the exterior boundary value problem

\[ -\Delta u_p + p^2 u_p = 0, \ x \in \Omega_x, \quad u_p = u, \ x \in \Gamma. \]  

(6)

Using separation of variables, we easily get

\[ u_p = \sum_{n=0}^{\infty} \frac{K_n(pr)}{K_n(pR)} a_n(u)e^{in\phi}, \quad a_n(u) = \frac{1}{2\pi} \int_0^{2\pi} u_p \left| r e^{-i\phi} \right| d\phi. \]  

(7)

Here \( (r, \phi) \) are the polar coordinates of \( x \) in the system where the pole is the center of \( B_R \), \( K_n(r) \) is the modified Bessel function of the second kind of order \( n \). Thus, we see that \( (\beta, p, u) \) satisfies the following equation on the circle with the nonlocal boundary condition:

\[ -\Delta u + p^2 \sigma u = \beta^2 (\sigma - 1)u, \ x \in \Omega, \quad u_\nu + S_p (p)u = 0, \ x \in \Gamma. \]  

(8)
Here,
\[
S_r(p)u = -u_{p,v} = \frac{1}{R} \sum_{n=-\infty}^{\infty} K_n(Rp) a_n(u) e^{i p u}, \quad K_n(r) = -\frac{1}{\rho} \frac{K_n'(r)}{K_n(r)}.
\]  (9)

The operator $S_r(p)$ is the mentioned above nonlocal boundary operator. Problem (8) is the desired problem on the bounded domain. In [12] we investigated the generalized solvability of problem (8) and proved its equivalence to the original problem, in [9], [10] we proposed and theoretically investigated a numerical method for problem (8) based on FEM. We solve problem (8) as the parametric eigenvalue problem for $\beta^2$, where $p > 0$ is the parameter. In the next section we describe the numerical results obtained using this method.

**Figure 2.** Variation of the propagation constant $\beta$ with the transverse wavenumber $p$ for the fiber without cladding air holes.

**Figure 3.** Variation of the propagation constant $\beta$ with the transverse wavenumber $p$ for the fiber with 36 cladding air holes.

**Figure 4.** The fundamental mode of the fiber without cladding air holes.

**Figure 5.** Variation of the effective index $n_{eff}$ of the fundamental mode with the wavelength $\lambda$ for a rank of number $m$ of cladding air holes.

### 3. Numerical results and discussion

Figure 2 shows the variation of the propagation constant $\beta$ with the transverse wavenumber $p$ for the fiber without cladding air holes and core radius $r_c = 1.7 \mu m$. This structure satisfies the classical optical fiber. It is well known that the fundamental modes of such fibers have no cut-off values, i.e. the fundamental (propagating) mode can propagate for any positive wavelength $\lambda$ (see [12], for example). The bottom curve starting at (0,0) is the dispersion curve of the fundamental mode, its diagram
for $\lambda = 7.7148\mu m$ is presented in Fig. 4. The variation of the effective index $n_{\text{eff}} = \beta / k$ of the fundamental mode with $\lambda$, for this fiber is presented in Fig. 5 by the blue line.

If the core is surrounded by the cladding air holes, then the fundamental mode has a cut-off value. Figure 3 shows the variation of the propagation constant $\beta$ with the transverse wavenumber $p$ for the NLC-PCF having 36 cladding air holes with radius $r_L = 0.4L$ and the hole pitch $L = 2.9\mu m$, where $r_0 = 1.7\mu m$. The bottom curve of the fundamental mode starts from the cut-off value. Variation of the effective index $n_{\text{eff}}$ of the fundamental mode with the wavelength $\lambda$ is presented in Fig. 5 by the azure line. We see that it has the cut-off value. There are not any solutions of the problem with $\lambda$ more than $2.378\mu m$. The diagram of the fundamental mode for $\lambda = 2.3775\mu m$ is presented in Fig. 7.

We investigated the influence of radii of the cladding air holes and their number as well as radius of the central liquid crystal on the fundamental mode. It is interesting that the size and the number of capillaries have no significant influence on the mode diagrams and the propagation constants (see Figs. 5-9).

We investigated the influence of radius of the central liquid crystal on the spectral characteristics of the fibers. Our results strongly suggest that radius of the crystal in contrast to the size and the number of capillaries has a significant influence on eigenwaves and propagation constants (see Figs. 10, 11).
Varying this radius we can control the number of solutions of the problem for a fixed wavelength (see Fig. 11).

4. Conclusions
The exact nonlocal boundary conditions method together with the finite-element method gives the reliable tool for numerical modeling of PCF. The future development of these methods is urgent to calculate leaky modes of PCF.

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References
[1] Obayya S 2011 Computational Photonics (John Wiley and Sons)
[2] Coldren L, Corzine S, and Mashanovitch M 2012 Diode Lasers and Photonic Integrated Circuits (John Wiley and Sons)
[3] Hussein R A et al 2015 Opt. Quant. Electron. 47 2993-3007
[4] Pintus P 2014 Optics Express 22 15737-15756
[5] Kowalezyk P et al 2011 Optics Express 19 19354-19364
[6] Monfared Y et al 2013 Optik 124 7049-7052
[7] Joly P and Poirier C 1999 Math. Meth. Appl. Sci. 22 389-447
[8] Dautov R Z and Karchevskii E M 2002 Computational Mathematics and Mathematical Physics 42 1012-1027
[9] Dautov R Z and Karchevskii E M 2005 Computational Mathematics and Mathematical Physics 45 2119-2134
[10] Dautov R Z and Karchevskii E M 2016 Lobachevskii Journal of Mathematics 37(5) 610–625
[11] Kartchevski E M, Nosich A I and Hanson G W 2005 SIAM Journal on Applied Mathematics 65(6) 2033-2048
[12] Dautov R Z and Karchevskii E M 2009 Integral Equation Method and Exact Nonlocal Boundary Conditions in the Theory of Dielectric Waveguides (Kazan University Press)