Computational study of nanostructured composite materials for photonic crystal fibre sensors

Jincy Johny, Radhakrishna Prabhu, Wai Keung Fung
School of Engineering, Robert Gordon University
Aberdeen AB10 7GJ, United Kingdom
E-mail: r.prabhu@rgu.ac.uk

Abstract. Photonic Crystal Fibres (PCFs) developed using nanostructured composite materials provides special optical properties which can revolutionise current optical sensing technologies. The modal and propagation characteristics of the PCF can be tailored by altering their geometrical parameters and material infiltrations. A drawback of commercially available PCF is their limited operating wavelengths, which is mostly in the infrared (IR) spectral band. Nanostructured composite materials manipulates the optical properties of the PCF, facilitating their operation in the higher sensitivity near infrared (NIR) wavelength regime. Hence, there arises a need to closely investigate the effect of nanostructure and composite materials on various optical parameters of the PCF sensor. This paper presents a hexagonal PCF designed using COMSOL MULTIPHYSICS 5.1 software, with a nanostructured core and microstructured cladding. Propagation characteristics like confinement loss and mode field diameter (MFD) are investigated and compared with various geometrical parameters like core diameter, cladding hole diameter, pitch, etc. Theoretical study revealed that a nanostructured PCF experiences reduced confinement losses and also improved mode field diameter. Furthermore, studies are also carried out by infiltrating the cladding holes with composite materials (liquid crystal and glass). These simulations helped in analysing the effect of different liquid crystal materials on PCF bandwidth and spectral positions.

1. Introduction
The demand for optical fibres and fibre optic technologies increased considerably after the telecommunication revolution which ignited in the 1980’s. The exceptional characteristics of optical fibres such as structural versatility and enhanced sensitivity over current techniques make them a suitable candidate for sensing applications. They have many advantages such as immunity from electromagnetic interference (EMI), electrical isolation, small size, remote sensing ability, multiplexing capability, freedom from corrosion and ability to operate in extreme environmental conditions [1]. Despite the fact that conventional optical fibres offer remarkable performance in the communication industry, it doesn’t satisfy all the needs of sensing industry. The specific requirements of sensing industry include long distance real-time remote sensing with multi-point and multi-parameter sensing capability. Hence, studies are emerging on speciality fibres like fibre Bragg grating (FBG), photonic crystal fibres (PCF), doped fibres etc.
PCFs [2] are gaining popularity in recent years, owing to their specialized geometrical structure (core-air hole cladding) and unique properties, which include their guiding mechanisms and modal characteristics [3]. They produce lower optical transmission losses compared to standard optical fibres [4]. PCFs are more flexible than normal optical fibres, because it is possible to manage their
properties, leading to a freedom of design [5]. Propagation characteristics of PCFs can be tuned by altering different structural or physical parameters like core diameter ($\rho$), cladding hole diameter ($d$) and pitch ($\Lambda$) in combination with the choice of material refractive index and type of crystal lattice [5-6]. All these inherent capabilities of PCFs are being exploited for different sensing applications. However, new requirements of fibre optic sensors create a need for different materials and fibre structure which can provide special optical properties. Structuring greatly boosts the performance of the fibre sensors in specific applications. Nanostructured optical materials will provide special properties which can improve the capabilities of existing optical sensing technologies [7-8]. Nanostructuring of PCF air holes is expected to reduce the fibre confinement losses and also decrease its effective mode area, which in turn improves the fibre propagation distance and range of the fibre sensor. Furthermore, addition of composite materials (liquid crystal and glass) on to the cladding holes modifies PCF transmission and polarization properties, enabling them to operate within the photonic bands having highest sensitivities. The near infrared (NIR) wavelengths of the optical spectrum are of particular interest for fibre-optic sensing applications due to their improved sensitivity and accuracy compared to other spectral regions. Another advantage of material infusion is that the properties of the PCF can be modified even after the fabrication of the PCF. The PCF air holes filled with special materials like liquid crystals changes their optical properties in response to electric or magnetic fields or light intensity. Liquid crystal materials infused into the cladding holes creates a PBG (Photonic Bandgap) effect, restricting the modes within the core region rather than leaking, facilitating a stronger sensing signal.

2. Theory
PCFs normally have two modes of operation based on their light guiding technique– index guiding and bandgap guiding [9]. Index guiding PCFs operates similar to conventional optical fibres wherein light is confined within the high index core by modified total internal reflection (M-TIR) principle [10]. On the other hand, bandgap PCFs guides light in the low index core region by reflection from the photonic crystal cladding [11].

2.1. Confinement loss
Confinement or leakage loss [12] expressed in dB/km is given by:

$$ L = \frac{20}{\ln 10} \left(\frac{2\pi}{\lambda}\right) \text{Im}(n_{\text{eff}}) $$

(1)

Where $\text{Im}(n_{\text{eff}})$ is the imaginary part of the effective refractive index, $n_{\text{eff}}$ and $\lambda$ is the propagating wavelength.

2.2. Effective mode area
Effective mode area [13] of the PCF is given by the equation:

$$ A_{\text{eff}} = \left[\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |E(x,y)|^2 \, dx \, dy\right]^2 / \left[\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |E(x,y)|^4 \, dx \, dy\right] $$

(2)

Where $E(x,y)$ is the optical mode field distribution.

Also, effective area is related to mode field diameter (MFD) by the equation:

$$ A_{\text{eff}} = k_n \left(\frac{\pi}{4}\right) \text{MFD}^2 = k_n \pi w^2 $$

(3)

Where $k_n$ is the correction factor and spot size, $w = \text{MFD}/2$ [14].

Mode Field diameter is approximated as,

$$ \text{MFD} \approx \frac{2}{\sqrt{\pi}} \sqrt{A_{\text{eff}}} $$

(4)
3. Nanostructured PCF Design
Current studies are carried out by changing the size (nano size holes in the core and micro size holes in the cladding), shape (circular, elliptical) and distribution of PCF air holes. In the previous study carried out, the designed solid core PCF exhibited limited operating wavelengths [15]. Hence, inorder to achieve spectral shifting and bandwidth enhancement, core nanostructuring and also the effect of different liquid crystal materials infiltrations within the cladding holes are being investigated. PCF parameters such as confinement losses, effective area and MFD are studied as a function of normalized frequency (\(\Lambda/\lambda\)). MFD and effective area is associated with the electric field distribution within the fibre. Analysis of these parameters gives a better insight of the propagation characteristics of the PCF.

**Figure 1.** Cross section of: (a) step-index SMF, (b) solid core PCF, (c) designed nanostructured PCF and (d) nanostructured core zoomed view

Figure 1 (a) and (b) shows the cross sectional view of the structural difference between a standard step-index single mode fibre (SMF) and a solid core PCF with microstructured cladding. During the fibre modelling, the only physical parameter that needs to be taken into account in the case of SMF is the core diameter. On the other hand, while modelling a PCF, three geometrical parameters are to be considered, core diameter, cladding hole diameter and also the pitch (hole to hole distance). Figure 1 (c) and (d) shows the cross section of the designed nanostructured PCF with a four ring hexagonal lattice of circular air holes in the cladding and a five ring array of elliptical air holes in the core. Simulations were conducted on a hexagonal PCF designed using the wave optics module of COMSOL MULTIPHYSICS 5.1. The geometrical parameters of the nanostructured PCF comprises of: pitch (\(A\))
which is the cladding hole center to center distance; \(d_1\) is the diameter of the cladding air hole; \(d_2\) and \(d_3\) are the length of major axis and minor axis of the elliptical air holes within the core and \(\Lambda'\) is the hole to hole spacing between the elliptical air holes of core.

4. Simulation Results and Discussion

![Figure 2](image)

**Figure 2.** (a) Electric field mode profile of the nanostructured PCF, (b) Zoomed view of electric field mode profile in PCF core

Figure 2 (a) and (b) shows the electric field profile of the fundamental mode obtained for the designed nanostructured PCF. From table 1 we can see that the mode confinement wavelengths can be brought down from the infrared (IR) to the near infrared (NIR) wavelengths by tuning the physical parameters of the core and cladding air holes. NIR lower cut off wavelength of 925 nm was achieved for the nanostructured PCF with design parameters: \(\Lambda = 1\mu m\), \(d_1 = 0.8\mu m\), \(\Lambda' = 100nm\), \(d_2 = 60nm\), \(d_3 = 20nm\).

| Design | Core dimensions | Cladding dimensions | Confinement wavelengths |
|--------|----------------|-------------------|------------------------|
| 1      | \(\Lambda' = 0.1\Lambda = 0.22\mu m = 220nm\) | \(\Lambda = 2.2\mu m\) | \(\geq 1950\) nm |
|        | \(d_2 = 0.6\Lambda' = 0.132\mu m = 132nm\) | \(d_1 = 0.8\Lambda = 1.76\mu m\) | |
|        | \(d_3 = 0.2\Lambda' = 0.044\mu m = 44nm\) | | |
| 2      | \(\Lambda' = 0.1\Lambda = 0.2\mu m = 200nm\) | \(\Lambda = 2\mu m\) | \(\geq 1775\) nm |
|        | \(d_2 = 0.6\Lambda' = 0.12\mu m = 120nm\) | \(d_1 = 0.8\Lambda = 1.6\mu m\) | |
|        | \(d_3 = 0.2\Lambda' = 0.04\mu m = 40nm\) | | |
| 3      | \(\Lambda' = 0.1\Lambda = 0.15\mu m = 150nm\) | \(\Lambda = 1.5\mu m\) | \(\geq 1450\) nm |
|        | \(d_2 = 0.6\Lambda' = 0.09\mu m = 90nm\) | \(d_1 = 0.8\Lambda = 1.2\mu m\) | |
|        | \(d_3 = 0.2\Lambda' = 0.03\mu m = 30nm\) | | |
| 4      | \(\Lambda' = 0.1\Lambda = 0.1\mu m = 100nm\) | \(\Lambda = 1\mu m\) | \(\geq 925\) nm |
|        | \(d_2 = 0.6\Lambda' = 0.06\mu m = 60nm\) | \(d_1 = 0.8\Lambda = 0.8\mu m\) | |
|        | \(d_3 = 0.2\Lambda' = 0.02\mu m = 20nm\) | | |
Figure 3. Confinement loss vs normalised frequency for: (a) $\Lambda = 2.2 \mu m$; (b) $\Lambda = 2 \mu m$

Figure 4. MFD vs normalised frequency for: (a) $\Lambda = 2.2 \mu m$; (b) $\Lambda = 2 \mu m$

Figure 3 depicts the variation in confinement loss (in dB/km) with respect to normalized frequency ($\nu = \Lambda / \lambda$) for different pitch or cladding hole spacing. It can be observed that confinement losses decreases with normalized frequency or in other words confinement losses increases with wavelength. Another advantage of bringing down the mode confinement wavelengths from the IR to NIR wavelengths is a reduction in confinement losses. Figure 4 shows the changes in MFD (in $\mu m$) with respect to normalized frequency for different pitch values. From the graph it is clear that MFD decreases with normalized frequency, or MFD experiences an increase for longer wavelengths and a decrease for shorter wavelengths. This is because, at lower wavelengths, the power density of the electric field propagating through the fibre would be higher, intensity would be lower and hence the effective mode area and MFD would be smaller. From table 2 we can see that by infiltrating different liquid crystal materials on to the cladding holes, a shifting and broadening of the spectral bands can be observed. Mode confinements in the NIR wavelengths were achieved by infiltrating the holes with liquid crystal material Cat No. 1550. To sum up, PCF nanostructuring and liquid crystal material infiltrations, reduces its losses and enhances the PCF sensor transmission distance and coverage.

Table 2. Confinement wavelengths of PCF filled with different liquid crystal materials

| Sl No. | Liquid crystal material | Refractive index | Confinement wavelengths |
|--------|------------------------|------------------|------------------------|
| 1      | K21                    | 1.732            | 1650 -2000 nm          |
| 2      | PCH-5                  | 1.6049           | 1200-1650 nm           |
| 3      | Cat No. 1550           | 1.522            | 825-1100 nm            |
5. Conclusion
The computational study carried out by nanostructuring the PCF core and by changing the size, shape and distribution of the PCF holes resulted in a shift in its spectral band, accompanied with a reduction in confinement losses and MFD. It was found that the PCF confinement wavelengths and losses are a strong function of its structural parameters. Further simulations carried out by varying the liquid crystal material infiltrations within the PCF holes resulted in a wavelength shift from IR to NIR. Moreover, altering refractive index of the liquid crystal material filled into the cladding holes of PCF caused a shifting and broadening of the photonic bands. Through these simulations it was identified that the spectral positions and bandgaps can be tuned by nanostructuring the PCF holes and changing its material infiltrations. Hence, nanostructuring and composite material infiltrations makes it possible to have different designer wavelengths for the PCF sensors. In addition, low confinement losses and MFD improves the signal power of the sensor, which in turn enhances its range and propagation distance.

6. References
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