Design of a Polymer-Based Hollow-Core Bandgap Fiber for Low-Loss Terahertz Transmission

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Abstract—We use numerical simulations to design a hollow-core microstructured polymer optical fiber (HC-mPOF) suitable for broadband, terahertz (THz) pulse transmission with relatively low losses and small dispersion. The HC-mPOF consists of a central large air-core surrounded by periodically arranged wavelength-scale circular air holes in a hexagonal pattern, embedded in a uniform Teflon matrix. The THz guidance in this fiber is achieved by exploiting the photonic bandgap (PBG) effect. In our low index contrast Teflon-air (1.44:1) hexagonal periodic lattice, the PBG appears only for a certain range of non-zero values of the longitudinal wavevector. We have achieved PBG over a broad spectral range (bandwidth ~400 GHz) ranging from 1.65 to 2.05 THz in the proposed HC-mPOF. The achievable loss coefficient in our designed HC-mPOF is <4 m^{-1} and the group velocity dispersion parameter is <±5 ps/THz·cm over a 300-GHz bandwidth (1.65~1.95 THz).

Index Terms—Microstructured fiber, photonic band-gap, polymer fiber, terahertz wave.

I. INTRODUCTION

IN RECENT years, terahertz (THz) frequencies (0.1 to 10 THz) [1], a range that falls in between the far-infrared and microwaves, have assumed considerable importance due to their potential applications in medical diagnostics, tomography, homeland security, identification of hidden objects, defense, sensing, astronomy etc. [1]–[7]. Moreover, THz waves are being considered for data transmission including wireless transmission for integration into the existing communication bands. Unfortunately, this apparently promising radiation suffers from high propagation loss in the atmosphere (mainly due to absorption by

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water), which tends to vary with daily weather, climate, and altitude [8]. However, in the case of local-area networks, THz-wireless communication has shown some promising results [9], [10].

A solution for integration of the THz technology into the communication band is to develop THz *waveguides*. However, this frequency range is not compatible with most conventional materials. Unlike optical waves, THz radiation suffers high absorption losses in conventional dielectric waveguides, whereas at the same time, unlike microwaves, THz radiation also suffers from high Ohmic losses and dispersion in metallic WGs [11]. Interestingly, though a THz wave suffers high losses in metal, glass, water, dust, fog, and cloud, it can penetrate deep into dry air, plastics, cloths, ceramics etc., which could potentially be utilized as a guiding medium for the THz radiation with appropriate engineering. Moreover, suitable THz WGs will also prove valuable for applications such as, remote sensing, medical endoscopy, diffraction-limited guidance, collimated beam delivery, long distance broad-band communication, and stronger light-matter interaction.

In the recent past several proposals for THz wave guidance have been explored using metallic or metal-dielectric based hybrid WG structures. Early THz WGs were composed of *planar* structures, where coplanar transmission lines, common for microwaves, were used to guide THz waves [12]. However, they suffer from high propagation loss (~ 20 cm^{-1}) at THz frequencies from the combined effects of Ohmic, diffraction and radiation losses. More recently, *non-planar* structures with both metals as well as few selective dielectric materials had been explored to design the THz WGs. The metallic WGs are the scaled-down version of microwave WGs, whereas the dielectric WGs are scaled-up version of the optical ones. Metallic non-planar WGs such as hollow core, parallel plate, metal sheet, single wire, two-wire structure, slit-WG etc. have also been reported [11], [13], [14]. Depending on the nature of the modes (TE/TM/TEM) and their confinement, the overall loss varies, and the dispersion increases drastically near the cut-off frequencies. In the case of dielectric-WGs also a trade-off exists between confinement and material loss. However, unlike the metallic WGs, dielectric WGs can take the form of an optical fiber, and the primary challenge is to find suitable materials for such a THz fiber. Dielectric polymers such as high-density polyethylene (HDPE), cyclic olefin copolymer (COC), polyethylene (PE), polytetrafluoroethylene (Teflon) are highly transparent and possess flat material dispersion over a wide THz band [11], [15]. Moreover, these polymers can be drawn in a fiber form [11], [16]. Different kinds of index-guided polymer fibers have already

been proposed in the literature for THz guidance. Though they support broad-band transmission, their primary limiting factor is the material loss [11]. Dry air is perhaps the lowest transmission loss material for THz waves. From this perspective, a hollow-core fiber structure should be an effective solution provided that either a photonic band-gap (PBG) or an anti-resonance reflective (ARR) guiding mechanism can be used for confining the mode within the air-core. Recently several types of hollow-core THz fibers (Bragg fiber, microstructured fiber and ARR-guided structure) have been proposed with low dispersion and low loss [11], [17]–[19]. The primary drawback of these schemes is that their transmission window is limited by the PBG effect and to achieve low loss, the overall cross-section often exceeds tens of mm, which makes them bulky and inflexible.

In this letter, we report a numerically designed *hollow-core microstructured polymer optical fiber* (HC-mPOF) for low-loss guided transmission of THz radiation. The transmission loss is minimized by maximizing the confinement of the modal field within the air-core and reducing the overall fiber cross-section to improve its flexibility. The fiber cladding is made of Teflon with air holes in a hexagonal lattice structure. We have first examined the criteria for the existence of a PBG in such a structure and found after optimization that a PBG covering a wide band-width (> 400 GHz, ranging from 1.65 ∼ 2.05 THz) can be realized for the fundamental guided mode. We discuss the overall loss and dispersion characteristics of the designed structure in detail. Our designed parameters should be useful for motivating fabrication of THz transmission fiber.

II. NUMERICAL MODELING

In general, a PBG fiber is formed by introducing wavelength-scale periodic refractive index (RI) features over its transverse cross-section (say x-y plane) all along the fiber length (z axis). If we create a defect region in that otherwise periodic medium, the PBG-guided mode will be confined to that region (mimicking as a fiber core). In a two-dimensional (2-D) periodic lattice, the solution of Maxwell's equation can be written as [20]

$$\mathbf{H}_{(n,k_z,k_0)}(\mathbf{r}) = \mathbf{u}_{(n,k_z,k_0)}(\boldsymbol{\rho})e^{i\mathbf{k}_0\cdot\boldsymbol{\rho}}e^{i\mathbf{k}_z z} \qquad (1)$$

where, $\mathbf{H}$ is the magnetic field, $\mathbf{r}$ is the position vector, $\boldsymbol{\rho}$ is the projection of $\mathbf{r}$ on the x-y plane, $\mathbf{k}_0$ is the *in-plane* (x-y plane) wave-vector, lying inside the Brillouin Zone, k_z is the longitudinal (z) wave-vector, "n" is the band number and $\mathbf{u}(\boldsymbol{\rho})$ is a periodic function satisfying the relation, $\mathbf{u}(\boldsymbol{\rho}) = \mathbf{u}(\boldsymbol{\rho} + \mathbf{R})$, for any lattice vector, $\mathbf{R}$ in the x-y plane.

Though the PBG effect in 1-D periodic structures (e.g., Bragg fibers) can be studied analytically [21], a 2-D structure requires more complex analysis, and for accurate results, numerical modeling is inevitable. Full-vector *plane wave expansion* (PWE) is a popular numerical technique for calculating the band-structure of any complex geometry. However, it cannot handle losses and frequency dependent dispersion of the structure. In contrast, the *finite element method* (FEM) is more complicated numerically but it can handle both the loss and dispersion quite accurately. We employ both of these techniques. First, we employed the PWE method for locating the PBG in the periodic lattice, ignoring the loss and dispersion. After that, we defined a
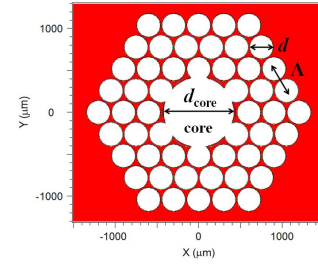

Fig. 1. Transverse cross section of the proposed HC-mPOF. Cladding is formed by the three hexagonally arranged rings of circular (shown in white) air holes (of diameter d and pitch Λ) embedded in Teflon (red background). The core at the center is formed by a circular air hole of bigger diameter, d_{core}.
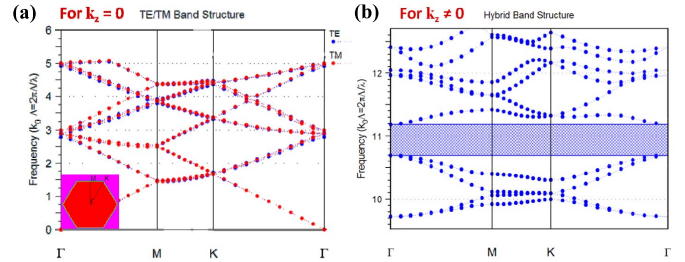

Fig. 2. Band diagram of air-Teflon hexagonal lattice for (a) $k_z = 0$, and (b) $k_z \neq 0$. The blue shaded region corresponds to lowest order band-gap. The inset in (a) shows the 1st Brillouin zone indicating co-ordinates of the k-vector.

super lattice structure, which includes both the defect core and surrounding microstructured cladding, and then, investigated the loss and dispersion characteristics of the PBG-guided mode via FEM.

III. PROPOSED FIBER DESIGN

The base material for the proposed fiber structure is chosen to be Teflon, as it is chemically inert to most chemicals, suitable for fiber drawing, transparent over a wide THz band and a relatively low cost material. The fiber's cross-section is composed of a uniform background of high index Teflon (RI about 1.44) with hexagonally arranged 4 rings of circular air holes (RI = 1) embedded in it. The diameter of air holes and their centre to centre separation are denoted as d and Λ, respectively. The central 7 air-holes are replaced by a bigger hole to create the defect hollow-core, which is then surrounded by a 3 periodic cladding rings. The cross-section of the proposed HC-mPOF is shown in Fig. 1. The RI of Teflon provides lower index contrast with air in comparison to other THz compatible polymers. Thus, the air-Teflon structure provides lower scattering loss at the dielectric boundaries (according to Ref. [22]). However, this low index contrast structure [$\Delta \approx (n_1 - n_2)/n_1 \approx 0.31$] cannot open a PBG for the *in-plane* wave-vector of either the TE or TM mode, at least in such a simple hexagonal geometry [cf. Fig. 2(a)]. Interestingly, a non-zero value of the longitudinal propagation constant (normalized value is $\beta_p = k_z n_{eff} \Lambda$, where n_{eff} is the effective index of the fiber mode) smoothens the band edges of *in-plane* (x-y) band-structure. As a result, a suitable range of β_p opens up one or more PBGs for such a 2-D structure [cf. Fig. 2(b)].

The cross-section of the HC-mPOF is optimized by investigating its band-structure by the PWE method using
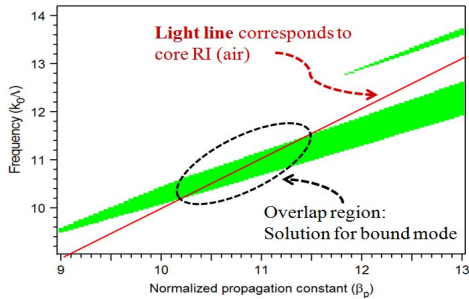
Fig. 3. Hybrid gap map (green shaded regions) for different β_p's. Solid line in red represents the light line corresponding to the core RI. Overlap region (indicated by the oval shape in black dash line) represents the solution for bound modes.

the commercially available software RSoft. Although higher values of d/Λ can yield a stronger band-gap effect, we cannot increase it arbitrarily as very high values of d/Λ pose difficulties in fabrication. By taking into consideration of these issues we have fixed it at 0.94, as several microstructured polymer fibers with such a large air-fraction has already been reported in the literature [23]. Thereafter we investigated scalability of this band-gap by varying the pitch (Λ). For smaller values of Λ, the band-gap effect becomes stronger so the gap-width increases; however, the mid-gap wavelength reduces due to a smaller periodicity. For further study, we have fixed the value of Λ at 300 μm, which provides us with a band-gap centered near 1.8 THz and with a band-width of more than 100 GHz.

IV. RESULTS AND DISCUSSION

The band-structure of the proposed periodic cladding structure is shown in Fig. 2(b) for a fixed value of β_p. However, we have also varied the z-component of the wave-vector to produce a complete map of band-gap (mainly for the lowest order band-gap) as a function of β_p, as seen in Fig. 3. The green shaded regions are the gap map, which are gradually increasing in width for higher values of β_p as it flattens the band-edges more. The *light line* corresponding to the core RI is also superposed on the figure (solid line in red). For our proposed air-core structure the *light line* is essentially a straight line with unit slope in the frequency vs wave-vector plane. The bound modes of interest, which are basically the defect states of the transverse periodic lattice, must confine inside the hollow-core, and hence its dispersion relation must follow (more or less!) this *light line*. The encircled region with dashed line (c.f. Fig. 3) indicates the range of β_p (10.2 $\sim$ 11.5) and frequency for which the bound modes can exist. This range can be understood physically as follows: smaller values of β_p are not sufficient to open up the PBG for bound modes, whereas, for larger values of β_p, the fields of modes become more confined in the high RI region, which reduces overlaps among them and as a consequence the PBG disappears.

At the next step we study the bound modes (PBG guided modes) by considering a *supercell* geometry. The *supercell*, consists of multiple unit cells including the defect core at the center, now becomes the new unit cell. However, the size of this new cell must be large enough to sufficiently isolate the defect core for accurate results. The core size is chosen carefully to eliminate the unwanted *surface states* [20], which are generally a big hindrance to achieve low transmission
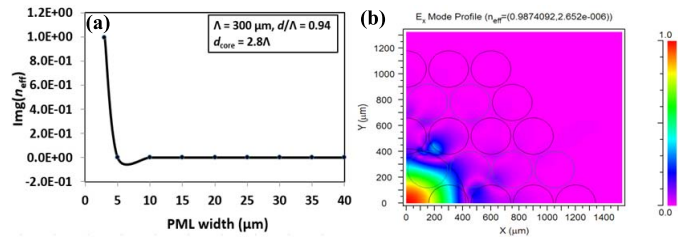

Fig. 4. (a) Variation of the imaginary part of the effective index as a function of PML width. (b) 2-D mode field profile (x component of the E-field) of the fundamental mode; only 1st quadrant is plotted owing to an obvious symmetry in the structure.
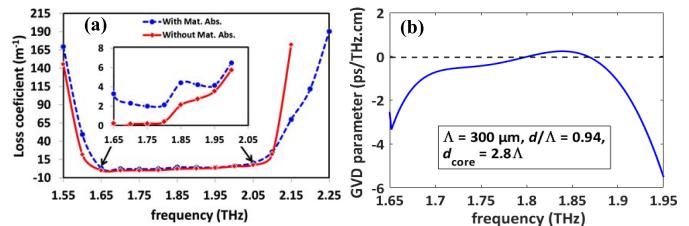

Fig. 5. (a) Variation of transmission loss [with (blue dashed) and without (red solid) material absorption] and (b) GVD parameter as a function of THz frequency for the fundamental mode of the proposed HC-mPOF. The inset in 'a' shows an expanded view of the two loss spectra.

loss in PBG fibers. By comparing the performance between different core diameters (d_{core}), we chose $d_{core} = 2.8\Lambda$, which resulted in a non-uniform core-surface boundary. As a consequence, the *surface states* get eliminated significantly and the confinement loss is minimized.

To calculate the loss and dispersion of the fundamental bound mode, we employed the FEM in a commercially available FEMSIM module in RSoft software. In the FEM analysis, we have employed an appropriate *perfectly matched layer* (PML) and optimized its width along with the FEM element size to yield a converging solution. A fine triangular element of size $= \Lambda/64$ is considered throughout the FEM analysis. In this context, we have scanned the imaginary part of the mode's effective index [Img(n_{eff})] as a function of PML width [see Fig. 4(a)], which reveals that, converging solution can be obtained for PML widths > 10 μm. As a precautionary measure, we have fixed its value at 30 μm for rest of the analysis. The mode profile of the fundamental PBG guided mode at 1.7 THz is plotted in Fig. 4(b), where only the 1st quadrant of simulation domain is shown owing to the structural symmetry of our fiber. The figure clearly reveals a strongly confined fundamental mode (nearly Gaussian in shape) in the proposed HC-mPOF. We may mention that a higher order mode also coexists with the fundamental one. However, its confinement loss is larger by a factor of 1000, indicating that it would leak away after a short distance of propagation.

Total transmission loss is a combined effect of three major sources of loss: confinement loss (α_c), material absorption loss (α_m) and scattering loss (α_s). Since the RI contrast is relatively small for our structure, α_s would be relatively low, and hence we have neglected it in the calculation of transmission loss. The α_c arises from the finite number of air hole rings in the cladding and can be calculated from the Img(n_{eff}) component of the corresponding mode. We have calculated the transmission loss with and without material absorption, and the results are shown in Fig. 5(a). A fixed value of material

loss for Teflon (0.8 cm^{-1}) was used in our calculations [24]. The figure reveals that the material loss of Teflon has relatively small effect on the overall loss spectrum. This is because the mode is strongly confined within the hollow core and has very little overlap with the Teflon structure. As a result, a loss of less than 0.04 cm^{-1} can be achieved in our proposed fiber over a wide range of $1.65 \sim 2.05$ THz (bandwidth 400 GHz) even after including the material loss. We note that it can be reduced even further by increasing the number of air hole rings. An expanded view of loss spectrum is shown in the inset of Fig. 5(a). For optical pulses propagating through an optical fiber, *group velocity dispersion* (GVD) plays a crucial role as it leads to distortion of pulse shape and pulse broadening. It is thus important to consider the GVD of our designed fiber for THz frequencies. Fortunately, as the mode is strongly confined inside the hollow-core, it experiences very low dispersion within the band-gap; however, similar to any other PBG-guided structure, the dispersion increases sharply near the band-edges. We have calculated the GVD parameter (β_2) from the frequency dependence of the real part of the mode effective index [Re(n_{eff})], and the results are shown in Fig. 5(b). The GVD is anomalous ($\beta_2 < 0$) except for a small frequency window ($1.8 \sim 1.87$ THz), where it becomes normal ($\beta_2 > 0$). However, the amplitude of β_2 remains below 5 ps/(THz.cm) over the band-gap regions, which is indeed quite low, and it blows up at both the band-edges.

V. Conclusion

In this letter, design of a PBG fiber is proposed for possible application in THz wave transmission. Through a detailed numerical analysis, a HC-mPOF is optimized to yield a PBG around 1.8 THz. The primary aim was to maximize the THz transmission window while minimizing both the loss and dispersion, and reduce the overall fiber cross-section for a compact design. The cross-section of the proposed HC-mPOF consists of a hollow-core (defect region), surrounded by hexagonally arranged 3 rings of air holes embedded in a uniform higher index material (Teflon). The size of the fiber core is deliberately chosen larger from rest of the holes and its diameter is optimized to 2.8 times the lattice periodicity to achieve PBG for out of plane propagation and to eliminate the unwanted lossy *surface-states* with sufficient mode confinement. The structure is first optimized through the *plane wave expansion* method to locate the band-gap and study its scalability. After optimizing the cross-section, a *finite element method* is employed to thoroughly investigate the loss and dispersion characteristics of the PBG guided mode. Our results reveal that just 3 air-hole rings in the cladding are enough to establish single mode guidance with extremely low confinement loss. The calculated PBG extends over almost 400 GHz (range $1.65 \sim 2.05$ THz) band-width with very low transmission losses (≤ 4 m^{-1}) and low GVD ($\beta_2 < \pm5$ ps/THz.cm) over $1.65 - 1.95$ THz. The nearly Gaussian shaped fundamental mode is strongly confined inside the hollow core. Though in general, the fabrication of hollow-core fibers is difficult, recently reported modern fabrication technologies [11], [16], [18], [19], [23], [25] show lot of promise to realize such complex fiber structures in practice. Our proposed HC-mPOF should be a good candidate for high-power, low-loss, low-dispersion pulse propagation in the THz regime and may prove valuable for a multitude of applications.

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