Study on HDPE-PCF evanescent wave sensor

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Abstract. The photonic crystal fiber (PCF) evanescent sensor has unique superior characteristics among the optical sensors, especially in terahertz (THz) wavelength range, PCF evanescent sensing will have huge application potentials. PCF characteristics and THz propagation characteristics in high-density polyethylene (HDPE) were combined. Finite element method was used to simulate and calculate THz-HDPE-PCF some parameters, at last the design considerations were given.

1. Introduction
As a new type of optical fiber, photonic crystal fiber (PCF) shows some of the unique characteristics compare to the traditional optical fiber (OF), such as unlimited single-mode, dispersion controllability, birefringence, can be designed for special mode field area, high non-linear, etc.\textsuperscript{1-6}. With the development of THz technology, THz play an important function in gas detecting and substance identify. Thus, in this paper we try to combine the PCF characteristics with THz characteristics in order to study and explore PCF sensing for finding a superior sensor.\textsuperscript{7-9}

2. The principle of THz-PCF evanescent sensing
The principle of THz-PCF evanescent sensing is that the part of THz frequency radiation is absorbed through the reaction of being measured substance and evanescent in PCF, then analyze substance by detected the THz radiation.
Total internal reflection-type PCF is characterized by guided-mode optical power concentrated at the center of the solid core defects, only a very small part of the optical energy (evanescent wave field) distribute in the surrounding air holes. The evanescent wave was absorbed by gas medium in the air, according to a Lambert Beer's law, the relationship between gas concentration and the optical intensity can be expressed as

\[ I(\lambda) = I_0(\lambda) \exp\left[ -\frac{\alpha(\lambda)}{C} \right] \]

(1)

To facilitate the analysis, the equation will be rewritten as

\[ C = -\frac{1}{r\alpha(\lambda)} \ln \frac{I(\lambda)}{I_0(\lambda)} \]

(2)

Where \( I \) and \( I_0 \) denote output light intensity and input light intensity of being tested gas respectively. \( \alpha(\lambda) \) for the gas absorption coefficient, \( \lambda \) for the length of the PCF as a probe, \( C \) is gas concentration, \( n_g \) for the gas refractive index, which is approximately equal to 1; \( n_e \) for guide-mode effective refractive index, \( r \) is the relative sensitivity coefficient, defined as:

\[ r = \frac{n_g}{n_e} \]

(3)

For the model to be determined, \( f \) is the ratio for the optical power to focus on the air holes divides the total power, through the Poynting's theorem:

\[ f = \frac{\int (E_x H_y - E_y H_x) dx dy}{\int (E_x H_y - E_y H_x) dx dy} \]

(4)

Equation, \( E_x, E_y, H_x, H_y \), express transverse electric and magnetic field model components.

By equation (2), we can see, if \( I, r, \) and \( \alpha(\lambda) \) were known, by detecting the \( I \) and can get the gas concentration \( C \) in PCF holes. And the longer of PCF, the better of the test, in general, for fiber-optic gas sensor, air chamber can be made longer. This PCF is used for gas sensing has a great advantage. In addition, you can change the PCF fiber mode field distribution the by changing structure, thus changing the relative sensitivity \( r \).

3. **THz-PCF structure shape of the clad holes influence to propagation constant**

Using finite element method to simulate total internal reflection-type transmission characteristics of THz-PCF evanescent wave, analyse the influence change of THz-PCF structural parameters on the evanescent wave. The background material is optical fiber of high-density polyethylene (HDPE), because of THz transmission losses are very small in plastic, also plastic is flexible comparing with silicon, it can be used hash environments.
So the HDPE material is selected to analyse THz–PCF evanescent wave sensing, the conventional silicon optical fiber material is not to be chosen.\cite{10-16}

In the whole, supposed the refractive index of HDPE $n=1.5$ in the THz band, a triangular arrangement air holes, and the whole calculation region size is $3.4\text{mm} \times 3\text{mm}$, in the process of meshing if a Yee's unit cell contains two kinds of different refractive index materials, use $\varepsilon = \varepsilon_a f + \varepsilon_b (1-f)$ to average them, $\varepsilon_a, \varepsilon_b$ is the dielectric constant of air and HDPE respectively. PML absorbing boundary conditions was placed around the calculation region, the outermost boundary is zero, The thickness of PML regions is 10% calculating region. Figure 1 is cross-sectional structure diagram of THz photonic crystal fiber, which the clad hole structure is circle.

![Cross-sectional structure diagram of THz photonic crystal fiber](image)

Fig. 1 Cross-sectional structure diagram of THz photonic crystal fiber

People used D-fiber optical fiber as evanescent wave gas sensors before\cite{17}, but the relative sensitivity is very low, only about 0.2% of the model energy can be used as a probe. The evanescent wave in PCF cladding air holes interact with the gaseous materials, it provides a new way. Monro, who verified the special PCF structure can be used as gas sensors, and pointed out from the theory that people can obtain high sensitivity gas sensor through the selection of suitable parameters\cite{18}.

Numerical simulation using perfectly matched layer (PML) structure, when applied PML absorbing boundary conditions, the propagation constant will be a complex number, in fact, the real part for a phase constant, the imaginary part is related to the loss amount. Thus, the relationship of the mode effective refractive index will be\cite{19-21}

$$n_{\text{eff}} = \frac{\beta}{k_0} = n + \bar{n}i$$ \hspace{1cm} (5)

$$\alpha(\text{dB/m}) = \frac{20}{\ln 10} \text{Im}(\beta) = 8.686\bar{n}k_0$$ \hspace{1cm} (6)

$$\alpha(\text{cm}^{-1}) = 2\bar{n}k_0$$ \hspace{1cm} (7)

Where $n$ is real part of mode effective refractive index, $\bar{n}$ for the effective refractive imaginary part, $k_0=2/\lambda$ for the vacuum wave number (where $k_0$ unit is $\text{m}^{-1}$), $\lambda$ is the wavelength in vacuum, the $\alpha$ unit is $\text{dB/m}$, if the unit is $\text{cm}^{-1}$, formula (6) express the loss of expression (which $k_0$ unit of $\text{cm}^{-1}$).

Figure 2 shows the results by calculations in the THz band, the condition is the same area but different clad hole structure, we can be see from the figure, when the frequency is high, the effective refractive index changes slowly with frequency, indicating PCF cladding air column structure do not influence the effective refractive index. Under the same value in
0.1THz-2.5THz round, the relation is $n_{\text{ellipse}} > n_{\text{square}} > n_{\text{triangular}} > n_{\text{circle}}$, in the relation n represents real part effective refractive index.

![Graph showing the relationship between frequency(THz) and Re(n_eff) for different hole shapes](image1)

Fig. 2 The relationship between the fundamental mode effective index real part and the frequency with different clad hole structure

Figure 3 shows the relationship between the imaginary part of effective refractive index and the THz frequency as different clad hole structure with same area. The relationship are $n_{\text{ellipse}} > n_{\text{square}} > n_{\text{triangular}} > n_{\text{circle}}$, in the relation n represents imaginary part effective refractive index.

According to equation 6, the imaginary part of effective refractive index is related to the loss amount of PCF, so the circular hole structure denotes the smallest loss, ellipse hole structure denotes the biggest loss.

![Graph showing the relationship between frequency(THz) and Im(n_eff) for different hole shapes](image2)

Fig. 3 The relationship between the imaginary part of fundamental mode effective index and the terahertz frequency

4. The relationship between the structure parameters of clad hole in THz-PCF and the evanescent wave energy

Structure shapes of holes are changed, respectively circular, square, triangle and ellipse, under the conditions of holes distances are constant and hole areas are the same. Fig.4 shows evanescent wave energy of PCF changes with THz frequency (0.1THz-10THz). With the
frequency rising (2THz-10THz), fiber clad hole structure the THz-PCF sensor performance, while with the frequency decreasing (0.1THz-2THz), it is clear that the different clad hole structure of PCF has larger influence to transmission performance. Following relation were obtained: ellipse $\langle E_{\text{evanecent}} / E_{\text{total}} \rangle$ < square $\langle E_{\text{evanecent}} / E_{\text{total}} \rangle$ < triangular $\langle E_{\text{evanecent}} / E_{\text{total}} \rangle$ < circle $\langle E_{\text{evanecent}} / E_{\text{total}} \rangle$.

![Graph](image1.png)

Fig. 4 The evanescent wave energy with THz frequency with four different hole structure Shapes

![Graph](image2.png)

Fig.5 the fraction of power in air hole, as a function of $d/\Lambda=0.6$

From Fig.5 describes that $d/\Lambda$ equal constant, the fraction of power in air hole will increase with the frequency, at the same time, the bigger of hole diameter, the better of the result.
Fig. 6 the fraction of power in air hole $f$ as a function of $d/\Lambda$, at frequency=1THz

Choosing circle hole shape PCF, taking $d/\Lambda=0.4$, $d/\Lambda=0.6$ and $d/\Lambda=0.8$(Fig.6), the relationship between the fraction of power in air holes $f\%$ and $d/\Lambda$ is simulated by finite element method. From the simulation results it can be seen that increase the hole diameter with the same hole structure shape, evanescent wave energy as the sensing will be significantly increased, so as a PCF sensor, large diameter structure should be used.

5. The relationship between THz-PCF effective area of the fundamental mode and the evanescent wave energy

(a) $\nu=0.4$THz  (b) $\nu=0.8$THz  (c) $\nu=3$THz
Fig. 7 Fundamental mode field distributions with corresponding frequency are
0.4THz, 0.45THz, 0.8THz, 0.85THz, 3THz, 5THz

Taking f = 0.4THz, f = 0.8THz, f = 3THz with the three-dimensional mode field distribution, f = 0.45THz, f = 0.85THz, f = 5THz with two-dimensional mode field distribution. From Fig 7, we can see that the mode field diameter will increase when the frequency decrease, the reason is that the restrictive influence of air holes decreases to mode field along with the frequency decrease. Without taking into account the case of dispersion, SMF fiber core and the cladding refractive index does not change with the frequency changing, so the mode field diameter increases with the frequency reduced.

Mode effective area is defined as

\[
A_{\text{eff}} = \frac{\left( \iint_{-\infty < x < \infty, -\infty < y < \infty} |E(x, y)|^4 \, dx \, dy \right)^{1/2}}{\iint_{\text{NLR}} |E(x, y)|^4 \, dx \, dy} \tag{8}
\]

In the equation, E (x, y) is the electric field distribution of mode field; NLR is non-linear waveguide region, for this thesis, NLR is the fiber background region besides the air-hole. Fig. 8 shows the relationship between effective area of fundamental model and frequency with four different clad hole structure shape.

The relationship between fundamental effective area and the THz frequency at four different clad hole structure shape is: affective area (ellipse) > affective area (square) > affective area (triangular) > affective area (circle). Because the effective area and the energy density distribution of evanescent wave inverse, so the evanescent wave energy density distribution should be: ellipse \( \left( \frac{E_{\text{evanescent}}}{E_{\text{total}}} \right) \) < square \( \left( \frac{E_{\text{evanescent}}}{E_{\text{total}}} \right) \) < triangular \( \left( \frac{E_{\text{evanescent}}}{E_{\text{total}}} \right) \) < circle \( \left( \frac{E_{\text{evanescent}}}{E_{\text{total}}} \right) \).
Fig. 8 The fundamental mode effective area with THz frequency at four different hole structure shape

6. The relationship between mode field distribution and evanescent wave energy in THz-HDPE-PCF

The circle clad hole structure shape is selected with hole period 500µm, d/Λ=0.6, Fig.9 shows the relation between mode field distribution of the fundamental mode and second-order mode with frequency. The changes of mode effective area with a circular clad hole at the THz frequency range is shown in figure 10. The proportion is shown in figure 11, which is the energy of fundamental mode and second-order model with frequency changing.

Fig9 Mode field changes of fundamental mode and second-order mode with the THz frequency

(a) - (c) represent frequency at 0.33THz, 0.25THz and 0.15THz, corresponding area: 1.70 mm², 9.67 mm² and 29.2 mm²; (d) - (f) represent frequency 1.2THz, 1THz and 0.93THz, corresponding area: 0.56mm², 8.6 mm² and 12.1mm²;
Fig. 10 The mode effective area of a circular hole structure shape with the THz frequency

Fig. 11 The proportion of the energy of fundamental mode and second-order mode with THz frequency

The two ratio curve is almost coincident that the evanescent wave field energy of fundamental mode HE11 and second-order mode TE01 in the THz region. The second-order mode can not find in the low frequency. Further more fundamental model can get relatively high power density, so in evanescent wave sensing, it is much better using the fundamental mode as sensing than second-order mode. Single-mode operation was shown in Figure 12. The conclusions of figure 11 and figure 12 consistent with reference literature [22].
Fig. 12 Phase diagram of single-mode operation

In figure 12, the dotted line represents cutoff frequencies of the second-order mode, solid line represents boundaries with the Non-confined mode, so three parts can be obtained: multi-mode area, single-mode area and the non-restricted-mode area. Only the structure in the middle can achieve single-mode optical fiber transmission.

7. Conclusion

THz-HDPE-PCF evanescent wave sensor is a very important direction of development, this sensor play an important function in gas detecting and substance identify. At the same time, THz transmission losses in plastic small, flexibility is good, it can work in harsh environments, THz-HDPE-PCF evanescent wave sensors is a superior sensor. Following conclusions can be obtained.

a. The principle of THz-PCF evanescent sensing is that part of THz frequency radiation is absorbed through the reaction of being measured substance and evanescent in PCF, then analyse substance by detected the THz radiation.

b. THz transmission losses in plastic is very small; also plastic is flexible comparing with silicon. It can be used at harsh environments. So the HDPE material is selected to analyse THz–PCF evanescent wave sensing, the conventional silicon optical fiber material is not to be chosen.

c. Corresponding propagation constant relationship is Re(\text{n}_{\text{eff}})(\text{ellipse}) > Re(\text{n}_{\text{eff}})(\text{square}) > Re(\text{n}_{\text{eff}})(\text{triangular}) > Re(\text{n}_{\text{eff}})(\text{circle}) with the same area, different clad hole shape structure. THz-PCF effective index is different with different propagation constant, result different electromagnetic fields transmission in PCF.

d. At low frequency (0.1THz-2THz) with four different clad holes structure shape, the evanescent wave energy ratio in total energy is shown: ellipse (E_{\text{evanescent}}/E_{\text{total}}) < square (E_{\text{evanescent}}/E_{\text{total}}) < triangular (E_{\text{evanescent}}/E_{\text{total}}) < circle (E_{\text{evanescent}}/E_{\text{total}}). In 0.1THz-2THz sensing, sensing performance with a circular clad hole structure shape is superior to the other three shape of THz-PCF sensor.

e. To get a better sensing performance in THz-HDPE-PCF, to use large aperture single-mode operation PCF to be used.
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