

Characterization and optimization of photonic crystal fiber evanescent wave sensor for gas explosives detection in terahertz wave

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Some gas explosives spectrum resonance absorption peaks is in terahertz wave, the relative sensitivity of evanescent wave solid core PCF sensor used for their sensing detection is simulated and calculated by finite element method (FEM). The relative sensitivity of PCF increases rapidly with the growth of operating wavelength, for the same operating wavelength, the larger the cladding d/λ is, the higher the relative sensitivity is. Moreover, the relative sensitivity of several different fiber core structure PCF is also compared when d/λ is set be 0.8, the relative sensitivity will increase with both the fiber core holes number and holes radius increase in the premise of not changing guide light principle. By simulating, the symmetric fiber core nine holes arranged square lattice PCF what holes radius is $50\mu\text{m}$ is the best choice for sensing detection application.

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1. Introduction

Recently monitoring of explosives which have a potential threat for our body healthy and life safety is increasingly receiving a significant attention. Some explosives, such as DNT(2,4-Dinitrotoluene), passivated RDX, HMX and TNT(2,4,6-Trinitrotoluene), is familiar with us, what absorption spectrum is within the rang of terahertz wave^[1]. Photonic crystal fibers (PCF) play a crucial role in sensing application, air holes arranged periodically running along the entire length of the fiber in cladding provide tremendous degree of freedom in PCF design^[2], which has been used for making various different-function device, especially PCF sensor based evanescent wave is one of the most interests. Terahertz radiation, which lies in the crossing areas of Rf microwave technology and photonics technology, with wavelengths from 0.03 to 3 mm and the frequency is between 0.1THz and 10THz, has allowed for the label-free detection of proteins, explosives, pharmaceutical drugs and the hybridization of DNA, for low frequency vibration and rotational energy level of biological macromolecules is included in terahertz wave, so it has obvious fingerprint feature. In addition, THZ radiation is strongly absorbed by water and silicon medium, high-density polyethylene (HDPE) is almost transparent to terahertz wave transmission, both materials absorption loss and dispersion is very low, so HDPE is introduced as PCF terahertz

waveguide. Moreover, the structure parameter of the THZ-PCF is in the magnitude of mm, compared to the counterparts in visible and infrared wave, THZ-PCF is more easily to be prepared and filled for measurands^[3]. Therefore, combination of THZ and PCF is a best choice for sensing application in gas explosives.

Relevant study based PCF evanescent wave sensor emerge constantly. In 2008, X.Yu put forward a idea of adding a small hole with the center of solid core PCF, the percentage of the evanescent intensity with the total intensity increase from original 0.03 % to 0.37 %^[4]. Jiyoung Park etc have researched PCF with ring-core hollow-defect for evanescent wave chemical sensing, compared to the counterparts center with a hole and traditional solid core, the relative sensitivity this hollow-defect doped ring structure PCF improve obviously in near infrared wave in 2009^[5]. But it is merely appropriate for gas sensing what absorption spectrum is in visible or infrared light and the relative sensitivity is lower. In 2011, Haixia Cui conducted a study on HDPE-PCF evanescent wave sensor fundamental characteristics, proofed that PCF with a circular clad hole structure shape is superior to that of other shape and fundamental mode can get relatively high power density and be suitable for evanescent sensing^[6]. Once J.B.Jensen used photonic band-gap fiber (PBF) for evanescent sensor, light is evidently guided through the silica in the entire cladding, with the intensity peaking in the core-like structures if

light within band gap is selected^[7]. In this way evanescent wave can interact with all holes measurands and relative sensitivity enhance rapidly. However, PBF has stringent requirement for an accurate control on periodicity of the holes so that increasing the fabrication tolerances, besides they have narrower spectral band propagation.

On the basis of above discussion, This paper makes a simulation and calculation for the relative sensitivity of evanescent wave solid core HDPE-PCF for gas explosives sensing detection in terahertz wave by finite element method (FEM) and compares the relative sensitivity of five modified fiber structure, providing a theoretical reference for the future design of THZ-PCF sensor.

2. The principle of THZ-PCF evanescent wave sensing

2.1 The principle of evanescent wave

Evanescent wave is an electromagnetic field which has an exponential decay form sharply when meeting total internal reflection conditions in two different refractive index material interface. here evanescent field is produced at HDPE-air holes interface. This field has an exponential decay form is given by^[8]:

$$E(z) = E_0 \cdot \exp(-z / d_p) \tag{1}$$

Where d_p is the penetration depth is given by

$$d_p = \frac{1}{k_0 \sqrt{n_2^2 \sin^2 \theta - n_1^2}} \tag{2}$$

2.2 The principle of THZ-PCF evanescent wave sensing

The principle of THZ-PCF evanescent wave sensing is that the fraction of THZ radiation is absorbed by the interaction of being measured substance and evanescent in PCF holes, and then analyze measurands kinds or concentration by output THZ radiation intensity.

We consider here the total internal reflection PCF where most of the guided light power is confined within the solid core defects with a fraction (evanescent field) of power extending into the surrounding holey region, the evanescent field is absorbed by the gas explosives in the air holes. According to a Lambert Beer's law, gas concentration can be obtained from the optical intensity attenuation:

$$I(\lambda) = I_0(\lambda) \exp[-r\alpha(\lambda)lC] \tag{3}$$

where I and I_0 denote output and input light intensity of being detected gas explosives respectively. $\alpha(\lambda)$ is absorption coefficient and is a function of wavelength, l is the length of the PCF used for a probe (interaction Length),

C is gas concentration and r is the relative sensitivity coefficient, defined as:

$$r = (n_r / n_e) f \tag{4}$$

Among them n_r for the gas refractive index, which is approximately equal to 1.0, n_e for fundamental-mode effective refractive index, f is the ratio for the optical power which focus on the air holes divides the total power. For a particular fiber mode f can be calculated through the Poynting's theorem:

$$f = \frac{\int_{holes} (ExHy - EyHx) dx dy}{\int_{total} (ExHy - EyHx) dx dy} \tag{5}$$

Ex, Ey and Hx, Hy are the transverse electric and magnetic fields of the mode respectively^[9].

From formula (3), once $l, r, \alpha(\lambda)$ is certain, we can get measurands information by detecting I . The length of PCF is interaction length which can be made longer, which is one of PCF advantages than the traditional optical fiber what reaction area is outside the fiber. In addition, we can change the PCF fiber mode field distribution by varying fiber structure, thus improving the relative sensitivity.

3. Evanescent wave THZ-PCF cladding d/λ influence on the relative sensitivity and confinement loss

FEM is a powerful numerical tool that can cope with any kinds of mathematics and physics problems based on variational principle, mode field distribution of PCF of any irregular section shape and refractive index under any combination material can be successfully analyzed by FEM which be performed by COMSOL Multiphysics in a higher calculation accuracy. Here we consider the fundamental mode of PCF which consists of hexagonal lattice arrangement of five ring holes in cladding, quarter of the cross-section of which as shown in Fig. 1.

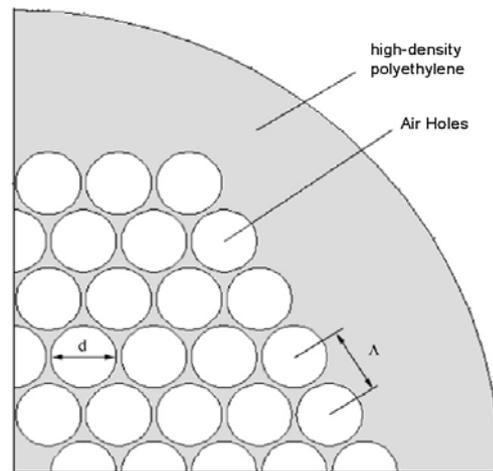


Fig. 1. Quarter of the cross-section of original THZ-PCF.

In order to make transmission wavelength of PCF waveguide covers the rang of absorption spectrum of above explosives, the structure parameter is set as follows: pitch of holes Λ is 0.6 mm, high-density polyethylene materials refractive index is 1.5, air in holes refractive index is 1.0. The relative sensitivity of PCF what various d/λ is from 0.6 to 0.9 in steps of 0.1 is simulated as shown in Fig. 2.

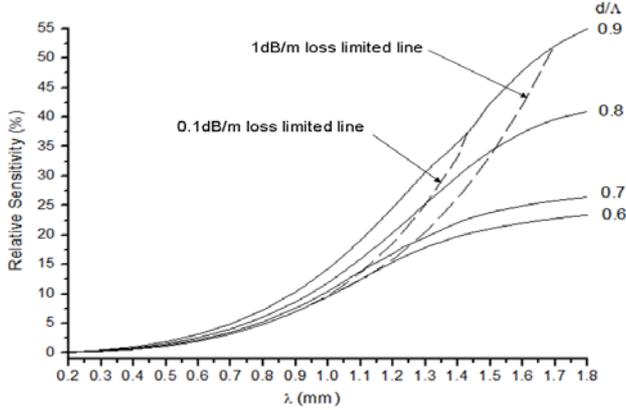


Fig. 2 Relative sensitivity of THZ-PCF versus wavelength for different d/λ .

It can be seen that the relative sensitivity of PCF increases with the growth of operating wavelength, for the same operating wavelength, the larger the d/λ is, the higher the relative sensitivity is, beside it is more sensitive to change of above two parameters than PCF in visible wave. In generally, PCF periodical structure confinement to mode field is weaker in long wavelengths, so for long operating wavelength, effective mode field area expand and evanescent wave strengthen. Furthermore, if d/λ is enough large, air-polyethylene surface volume increase, it is more convenient for evanescent field penetrating into the air holes. The relative sensitivity is up to 55.04% in 1.8mm operating wavelength when d/λ equal to 0.9.

Confinement loss (CL) is also a key factor in affecting sensitivity, CL is defined as:

$$CL(dB/m) = \frac{20}{\ln 10} * \frac{2\pi}{\lambda} * \text{Im}(n_{eff}) * 10^6 \quad (6)$$

Too much CL leads to the reduce of the relative sensitivity, any PCF exist CL since number of air holes in cladding can't be unlimited. By introducing the perfectly matched layers (PML) concept into FEM, we investigated CL of above THZ-PCF, as shown in Fig.3

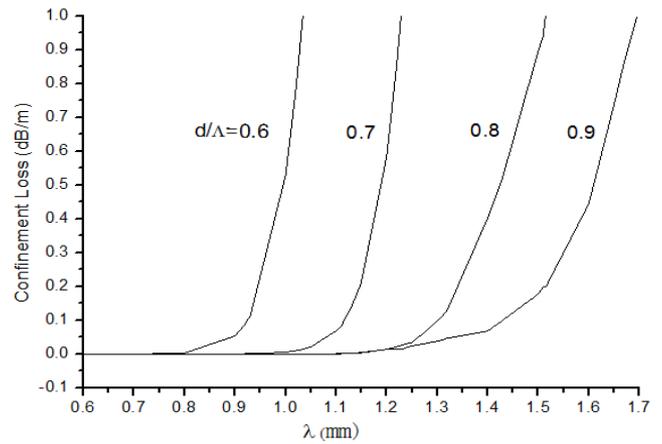


Fig.3 confinement loss of THZ-PCF versus wavelength for different d/λ .

As seen from Fig.3, The CL increases with the growth of wavelength. For a particular d/Λ value, there exists a critical wavelength λ , beyond which the CL begins to increase sharply, this critical value increases with d/Λ . For d/Λ is 0.9, if 1 dB/m level of CL is accepted, the wavelength should be limited to less than 1.6935 mm and the corresponding relative sensitivity will be 51.85% as show in Fig. 2. If the acceptable loss level is 0.1 dB/m, wavelength should be below 1.43 mm and the relative sensitivity will be limited to around 37.39%. The values of above two loss corresponding to wavelength for different d/Λ from 0.6 to 0.9 were calculated and are shown in Fig. 2 as dash lines. Operating on the left-hand side of the dash lines will ensure that the CL is lower than 1 dB/m and 0.1 dB/m respectively^[10], which are available in theory. Although relative sensitivity of THZ-PCF for d/Λ is 0.9 is high, it is difficult to manufacture, so we choice THZ-PCF for d/Λ is 0.8 for sensing application.

4. Modified evanescent wave THZ-PCF design for high sensitivity

The relative sensitivity is crucial factor which decide a sensor can do real time and fast speed detection. Traditional solid core PCF evanescent wave sensor can only use evanescent field in first-layer air holes surrounding fiber core and sensitivity is very lower evidently, so it is necessary to do some improvement to fiber core. According to inserting several small holes in solid fiber core, it can be greatly enhanced to the relative sensitivity in the premise of not changing guide light mechanism (the total internal reflection) for a large portion of mode field extending into small holes as evanescent wave. Mode field distribution with different fiber core structure design when wavelength are assumed to be $\lambda=1.2\text{mm}$ are shown in Fig. 4.

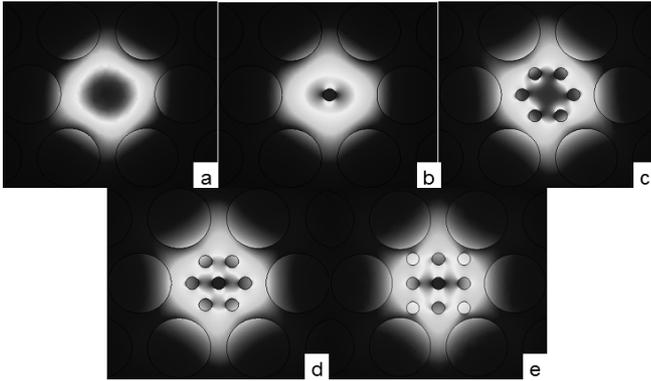


Fig. 4. Mode field distribution with different fiber core structure design when wavelength are assumed to be $\lambda=1.2\text{mm}$. (a) Traditional solid core (b) Center with a hole (c) Six holes arranged hexagonal lattice (d) Seven holes arranged hexagonal lattice (e) Nine holes arranged square lattice.

PCF that cladding $d=0.8$ is selected, among them the diameter of the fiber core hole is 0.1mm , the small hole spacing in the fiber core is 0.2mm . the cladding structure parameter as the same as above. It can be seen from figure that the fraction of power gathered in air holes arise. We have received the corresponding curve of relative sensitivity with varying wavelength for aforementioned different fiber core structure design. as shown in Fig. 5.

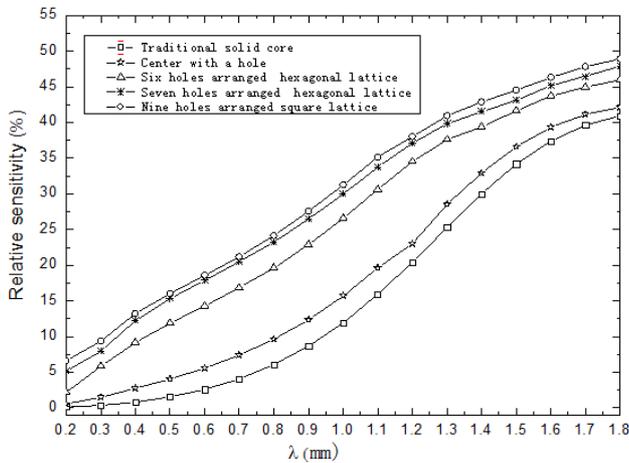


Fig.5 Relative sensitivity of THZ-PCF with varying wavelength for different fiber core structure design.

From Fig.5, we can see that the relative sensitivity will increase when the fiber holes number increase with same wavelength. In the rang of short-middle wavelength on which gas explosives resonance absorption peaks focus, with from 0.3mm to 1.3mm , the relative sensitivity vary obviously. The reason is that fiber core effective refractive index decreases along with the holes number increase, cladding effective refractive index is constant, so effective refractive index difference between fiber core and cladding reduce, the confinement to propagating light weakened,

and then light power extending into cladding first layer air holes enhance, the relative sensitivity increase. Beside decrease of fiber core effective refractive index results in the mode effective refractive index reduce, according to formula (4), the relative sensitivity further improve. Furthermore, propagating light energy mainly transport in fiber core, more holes in fiber core makes overlap with evanescent wave and gas explosives being measured easier^[11]. The structure parameter of THZ-PCF is in the magnitude of mm, and diameter of fiber core small holes is also dozens of micron, it is more easier for analyte filling than PCF in visible wave what cladding holes diameter is several micron or smaller. At last, such modified structure contribution on confinement loss increase is little, for nine holes arranged square lattice PCF, its relative sensitivity is 40.47% for 1dB/m loss, compared to traditional solid core PCF that of which is 34.77% , has improved by 16.4% .

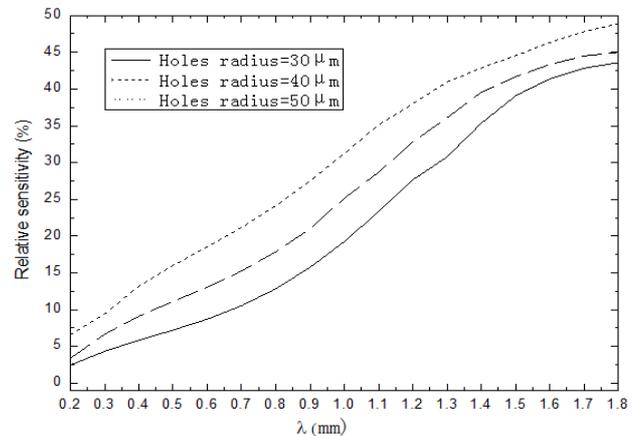


Fig. 6. Relative sensitivity of THZ-PCF with varying wavelength for different Fiber core holes radius.

Fiber core holes radius influence curve on the relative sensitivity is shown as in Fig.6. Choosing nine holes arranged square lattice shape PCF, taking holes radius= $30\mu\text{m}$, $40\mu\text{m}$ and $50\mu\text{m}$, the relationship between the relative sensitivity and wavelength is simulated by FEM. From the simulation results it can be seen that increase the holes radius with the same holes number and arrangement structure, evanescent wave energy as the sensing will be significantly increased, so as a PCF sensor, large diameter structure should be used. However, the fiber core holes number and holes radius can't increase indefinitely, due to much the two parameters can change guide light principle from total internal reflection to band gap type which have a complex guide light mechanism and confinement on transmission wavelength range, not the light of all wavelengths can guide in fiber core. By simulating, we discover that fiber core nine holes arranged square lattice PCF what holes radius is $50\mu\text{m}$ is the best choice.

All above discussion refers to the THZ-PCF with a symmetric fiber core holes distribution. To acquire a more comprehensive conclusion, the holes which are

asymmetric distribution is also simulated and calculated. Compared to the symmetric distribution counterparts, its mode field distribution is accordingly asymmetry and irregular, the relative sensitivity is lower than that of symmetric holes PCF what structure parameters is exactly the same as the former. Meanwhile, it probably produces birefringence phenomenon which is disadvantageous for sensing detection, here it isn't analysed detailedly.

5. Conclusion

This paper make a simulation and calculation for the relative sensitivity of evanescent wave solid core HDPE-PCF for gas explosives sensing detection in terahertz wave by finite element method (FEM), The relative sensitivity of PCF increases rapidly with the growth of operating wavelength, for the same operating wavelength, the larger the cladding d/Λ is, the higher the relative sensitivity is, the relative sensitivity is up to 55.04% in 1.8mm operating wavelength when d/Λ equal to 0.9. However, it is difficult to manufacture PCF for d/Λ is 0.9, so we choice THZ-PCF for d/Λ is 0.8 for sensing application. Relative sensitivity of several different fiber core structure PCF is also compared when d/Λ is set be 0.8, the relative sensitivity will increase with both the fiber core holes number and holes radius increase in the premise of not changing guide light principle. The symmetric fiber core nine holes arranged square lattice PCF what holes radius is 50 μ m, with relative sensitivity is 40.47% for 1dB/m loss, compared to traditional solid core PCF that of which is 34.77%, has improved by 16.4%, so it is suitable for evanescent wave THZ-PCF gas explosives sensing detection device.

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