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Sensing of toxic chemicals using polarized photonic crystal fiber in the terahertz regime



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Keywords:	Cyanide (CN) is a highly toxic chemical agent that is considered extremely harmful to humans. Considering the
Terahertz sensor	level of toxicity and harmfulness to human it is important to have an efficient and flexible detection method
Photonic crystal fiber	of CN. Based on this requirement, we propose a photonic crystal fiber (PCF) based terahertz sensor for the detection of CN. In a Zeonex substrate we use symmetrical and asymmetrical core structures inside a suspension
Birefringence	
Waveguide Cyanide	type cladding. The possible sensor architecture and methodology of sensing is also addressed. The fabrication of
	the proposed sensors is feasible employing existing fabrication technology.

1. Introduction

Cyanide is a chemical compound that consists of a triple bonded carbon atom to a nitrogen atom ($C \equiv N$). It is colorless, volatile, poisonous and fast acting chemical that depending on the level of exposure it can result in mortality within a minute [1]. Cyanide is used as an essential reagent for different industries such as mining and petroleum, electroplating, plastics and steel manufacturing, tanning, silver and gold extraction, automobile manufacture, synthetic fiber production and metallurgy [2]. However, the exposure of cyanide to humans is harmful and the above mentioned industries are mainly responsible for it because the possibility of CN exposure increases during heavy use and transportation. Biological sources such as fungi, bacteria and algae produce CN as part of their nitrogen (N) metabolic pathways. Dietary foodstuffs including cassava, lima beans, linseed, sweet potatoes, kernels of fruits, sorghum and bamboo shoots contain moderate to high levels of cyanogenic glycosides and these vegetables are considered to be main sources of cyanide ingestion to humans and animals. Moreover, tobacco smoke is also a common source of cyanide ingestion that transfers to blood cells [3]. Cyanide inhibits the normal respiratory function of tissue and cells because it irreversibly binds the iron atom to the hemoglobin that inhibits the hemoglobin from transporting oxygen (O_2) to the respiratory organs. Therefore, it is of utmost importance to discover a suitable method for cyanide detection.

Thus far, several cyanide detection modes such as chromatographic [4], electrometric [5], titrimetric [6], potentiometric [7] and voltammetric [8] techniques have been developed earlier but have drawbacks

due to a long analysis time, complex methodology and the need for a skilled user. Therefore, to eliminate the problems faced by the mentioned methods colorimetric strategies have been proposed [9]. The advantage of a colorimetric method is that it is cost effective and possible to detect CN with the naked-eye. However, such a method requires the use of sophisticated instruments with high detection limit. Later, in order to detect low concentration levels a fluorescence technique proved to be a more-powerful optical technique due to its simplicity in operation and rapid implementation.

Photonic crystal fiber is a promising technology nowadays for sensing due to its powerful light-matter interaction property. In a PCF the light guiding property such as material absorption loss, amount of core power, birefringence, confinement loss and dispersion can be modified by tuning its geometrical parameters such as core diameter, pitch distance, shape of air holes, air hole size that is not possible by using conventional optical fiber. Moreover in a PCF, instead of using air inside the air holes we can use different analytes (gas/chemicals/biological molecules) to use it in a sensing application [10]. In 2006, Cordeiro et al. [11] investigated a PCF based sensor using different analytes in the core air holes. In recent years, for chemical sensing a number of PCF designs [12-15] are reported in the optical wavelength. Moreover, considering the impact of employing terahertz we proposed a PCF based chemical sensor using a kagome structure in the cladding and a rectangular air hole structure in the core. We obtained a high chemical sensitivity with low loss [16] however the kagome structure is difficult

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Fig. 1. Schematic of the proposed sensor type-I.



Fig. 2. Schematic of the proposed sensor type-II.

to fabricate. Thus, considering the complexity of fabrication we provided a solution and designed a suspension type cladding that reduces the fabrication complexity than the kagome structure [17] as it does not contain any over-lapped rectangular parallel struts in the cladding region. Another advantage of the proposed PCFs over the conventional kagome PCF is that it is cost effective as it requires less material in the cladding during fabrication.

In this manuscript, utilizing the benefits of PCF we propose two PCF based sensors for toxic cyanide detection in the terahertz band. Instead of using a kagome structure we propose a more fabrication-ready suspension type cladding that consists of few rectangular struts. In the core of the PCF we use one symmetrical and one asymmetrical structure and characterize their sensing performances. Moreover, considering the fabrication tolerance we vary the core air hole size to determine how sensing performance varies with that. Besides sensitivity we also characterize other important optical properties such as effective material loss, confinement loss, bending loss and birefringence of both the proposed sensors.

2. Modeling of the proposed terahertz sensor

In PCF type-I, inside a suspension type cladding we use a hexagonal structure having circular shaped air holes. This is the extension of our previously published research work [17]. Note that, considering the fabrication tolerance we choose the values of core air hole diameter (d_c) and pitch distance (p_{c1}) and ensures sufficient distance between the air holes. See Figs. 1 and 2.

In PCF type-II, we used array of elliptical shaped air holes in a suspension type cladding. The reason for elliptical air holes is to introduce birefringence that is necessary for improving the sensing performance of a terahertz sensor [16]. In PCF type-II, the major axis and minor axis length of elliptical air holes are defined as L, L_1 , L_2 and w respectively.

In both PCFs, the strut thickness (*d*) is kept fixed at 6 μ m. Considering the fabrication tolerance, we could reduce the thickness down to 2 μ m but we kept it at 6 μ m so that the scattering effect due of a suspension type cladding can be reduced. The commonly used polymer material Zeonex (COP) is used as the background material for both PCFs as Zeonex has a number of superior characteristics suitable for terahertz compared to other polymer materials [18].

Note that, the practical realization of proposed PCFs are straightforward as there are existing technologies to fabricate these. Note that, the circular shaped air holes can easily be achieved using the capillary stacking technique whereas the elliptical and rectangular shaped air holes are obtainable by the extrusion and 3D printing techniques [19,20].

3. Analysis of numerical results and discussion

The electric field distribution of both the PCFs is shown through Figs. 3 and 4. For PCF type-I only one polarization mode is considered because of the circular shaped air hole in the core that will experience negligible birefringence. However, analyzing the direction of E-field in Fig. 3 it can be seen that fields are propagating only in one direction and thus it is considerable that PCF-I will operate in the single mode condition.

However, in PCF type-II the E-field distribution of both polarization modes is considered as the core is asymmetrical. At 1.8 THz the obtained effective refractive index of HCN for the *x* and *y* polarization modes are 1.248 and 1.254 respectively. Thus the simulation result indicate that there can be other modes present in the waveguide however for those modes the E-field will propagate through the cladding and not from the core. Thus when a fundamental Gaussian beam is launched at the center of the PCF only the fundamental modes will be excited and propagate through the core [16,21]. The modified total internal reflection (MTIR) light guiding mechanism works for both the proposed PCF as the core refractive index is larger than the refractive index of cladding.

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