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Designing of convenient PCF structure for SERS applications

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ABSTRACT

We investigated that the performance of side-channel photonic crystal fiber (SC-PCF) is controlled by the subtended angle of the liquid channel to the center point of the core (channel angle). This investigation is used for designing the SC-PCF to enhance the Surface Enhanced Raman Spectroscopy (SERS) signal. The deviation of the maximum normalized field intensity from the solid core center, and the mode field diameter change with the channel angle. We used finite element method (FEM) to obtain the normalized field intensity distributions, and a Gaussian approximation with position parameter is utilized to analyze them. The normalized field intensity on core liquid interface and the evanescent field ratio are considered to measure the performance. It is found that the performance is maximized when the channel angle is 90^o at 632.8 *nm* of excitation wavelength. These results are very important for the sensing application in chemical, biomedical engineering and research fields.

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1. Introduction

Surface-enhanced Raman scattering (SERS) is used to study and quantify of molecules with high accuracy and sensitivity in chemical and biomedical engineering and research fields [1]. The substantial enhancement of the electromagnetic field around metallic nanostructures by localized surface plasmon resonance and surface chemical enhancement is used to carry Raman signals of the molecule with its structural information that signal can be amplified by orders of magnitude [1–3]. The enrichment of differential scattering cross-section of multiple molecules causing by the adsorption on the metal surface is the phenomenon of Raman enhancement [4]. Photonic crystal fibers (PCFs) are convenient to apply in SERS sensing as a promising optofluidic platform for biological and chemical sensing since the sample can be pumped to air holes and the structures are of flexible design [5]. The features of solid-core PCF fiber (SCPCF) and hollow-core PCF fiber (HCPCF) [6,7] are widely reported. And these type of PCFs have used very intensely for the application of SERS [1]. The use of hollow-core PCF is very convenient because of its easy infiltration of samples [8], but the transmitted light may not be well confined due to the low evanescent field ratio in the air channels (holes) [1]. Therefore side-channel PCF has been introduced to obtained the properties such as high infiltration [2], low transmission loss, high evanescent field ratio and single mode propagation at the wavelength 632.8 *nm* [5]. The SC-PCF is designed by removing a portion (one third [2]) of cladding from the solid core hexagonal PCF. The side-channel is required to enable the liquid infiltration of the sample and to enlarge the effective interaction area between samples and fiber core guided light wave [2]. The fraction of evanescent field ratio of the side-channel can be increased if the pitch (distance between two adjacent air holes) is decreased or the ratio of the air hole diameter to pitch increases [2]. The core diameter is reduced with the ratio of air hole diameter to pitch, and therefore

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smallest core diameter gives the highest evanescent field ratio [9]. Moreover, the evanescent field ratio in the side-channel is linearly increased with increasing the refractive index of liquid [2]. A nano-scaled metal coating on the surface of the liquid channel is essential to create SERS signal. In addition to that, the evanescent field penetration to the liquid channel, and the interactive surface area of the core liquid interface are also essential to strengthen the SERS signal. The most common way to increase the evanescent field and enlarge the interactive area is to modify the PCF structure [1]. The evanescent penetration to the side channel directly corresponds to the normalized field intensity on core liquid interface.

In this research work, we studied the performance of side-channel PCF with different channel angles. The normalized field intensity of core liquid interface and evanescent field ratio are considered as the performance parameters. The finite element method (FEM) offers the versatility and flexibility to solve modes among the many methods that are able to model the guidance property of TIR PCF [10,11]. We used FEM simulation using COMSOL to study the electric field intensity distribution of the fundamental mode in the core for the SC-PCF designs to obtain best suitable structure for future SERS configurations. It is observed that the maximum value of normalized field intensity distribution moves towards the opposite side on the subtended angle of the side-channel with increasing channel angle, as shown in Fig. 3. Thus, the normalized field of fundamental mode is tightly fitted with Gaussian distribution when the diameter of hole to pitch ratio (d/Λ) is large [12]. We analyzed the values of the normalized field intensity, evanescent field ratio and average normalized field intensity for different channel angle using the normalized field intensity distribution in fundamental mode (shown in Fig. 5). According to the literature, the excitation wavelength of simulation is selected as 632.8 nm and the optimum value for core diameter in the hexagonal array is 2.8 μm when pitch and air hole diameter is selected as 3 μm and 2.1 μm respectively [5]. The intention of this research work is to find suitable channel angle which has the properties of low transmission loss, high evanescent field ratio, and single mode propagation.

2. Principle and method

The cross-section of the SC-PCF structure is symmetric with the horizontal axis on the center of the solid core. Therefore, the normalized field intensity distributions with that horizontal axis (shown in Fig. 2) are obtained for every FEM simulation (shown in Fig. 5). The normalized field distribution of PCF structure in the fundamental mode can be assumed as Gaussian distribution [12], and hence that can be expressed as a function of distance x [13]. The normalized field intensity distribution of PCF in the fundamental mode can be recorded for Gaussian function [14]:

$$E(x) = Ae^{-\left(\frac{x}{w}\right)^2} \tag{1}$$

where A is the maximum field intensity and w is the mode field radius. When $A = 1$ the distribution is normalized. Therefore the field normalized intensity distribution is characterized with the parameter called mode field diameter ($MFD = 2w$), and it is defined in [14,15], as shown in Eq. (2). The mode field diameter with different channel angle is shown in the Fig. 6(a).

$$MFD = 2w = 2\left(\frac{2\int_0^{+\infty} r^3E^2(r)\,dr}{\int_0^{+\infty} rE^2(r)\,dr}\right)^{1/2} \tag{2}$$

On the other hand, the mode field diameter is the roots of the inverse function of distribution when the intensity is ($1/e$) or the field power is ($1/e^2$) [16]. These routes are the boundaries of the effective area.

$$w_0 = E^{-1}\left(\frac{1}{\mathrm{e}}\right) \tag{3}$$

The normalized field intensity distribution is very effective when the value of distance x is within the range of $[-w, w]$. The area surrounded by that range is called effective area A_{eff} of the normalized field intensity distribution and that can be derived to express in terms of mode field diameter [17] as shown in Eq. (4).

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

where k_n is the correction factor (theoretically it is taken as 1). The idea of Eq. (4) is that the effective area is increased with the mode field diameter. For the most of circular symmetric microstructured fibers, the normalized field intensity distribution is balanced on vertical and horizontal axis and hence the normalized field intensity and evanescent field ratios are depending on mode field diameter. Therefore, the boundary level of the normalized field intensity pattern can be expressed as the roots of Eq. (3).

$$x_1 = -x_2 = w \tag{5}$$

We observed that the maximum value of normalized field intensity distribution deviates from the center point to negative x direction with the channel angle Fig. 5. Therefore, the Gaussian distribution as describe in Eq. (1) is to be modified with the new term called position parameter α as shown in the Eq. (6).

$$E(x) = E_{max} \cdot e^{-\frac{(x+\alpha)^2}{w^2}} \tag{6}$$

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