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## Highly Sensitive Biomolecular Sensing.

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### ABSTRACT

Sensing of biomolecule needs highly sensitive sensing technique Present work shows that using single mode silica nanowire, a single bimolecular layer adsorbed on a silica nanowire surface over a length of few tens of micrometers can be detected. This reduces requirement of amount of the sample, which is the inherent need of medical field application.

**Keywords:** biomolecular sensing, silica nanowire.

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INTRODUCTION

Sensing of biomolecule such as protein molecule has gained much attention for analysis of a bio-sample. Various techniques based on electrical and optical measurement have been exploited so far. The optical techniques show the advantage of higher sensitivity over electrical measurement techniques. Due to high sensitivity, sensing regions can be small. Thus, requirement of amount of sample reduces. This is an advantage for sensing a biomolecule. Optical sensing with high sensitivity can be carried out using single mode silica nanowire.

Recently, single mode silica nanowires have gained much attention for sensing application due to huge evanescent field, which leads to high sensitivity of the sensor device. Silica nanowire can be fabricated by simple and low cost, high temperature fiber drawing technique. The fabricated nanowire shows excellent diameter uniformity, surface smoothness and good mechanical strength [1]. The reported scattering loss is as low as 0.0014dB/mm [2]. Silica nanowire is also identified as the potential candidate for building integrated devices.

In the present work, it is shown that, using single mode silica nanowire, biomolecular detection can be carried out with high sensitivity. This reduces sample requirement and also leads to miniaturisation, which is very much required in medical application. In this work, an optical sensor using single mode silica nanowire is modeled and simulated for detection of a biomolecular layer. The model for the sensor device is constructed by using Mach-Zehnder interferometer (MZI). In the subsequent sections, construction of the sensor and numerical simulations are presented. Sensitivity and detection limit are calculated.

WAVEGUIDANCE IN SILICA NANOWIRE

The power profile for an air-clad single mode silica nanowire at a wavelength of 1.55µm obtained. The refractive index of silica core 1.55µm wavelength is 1.4468. The nanowire exhibits tight light confinement. In order to plot power profile, using dispersion equation (1), the propagation constant (β) is first calculated and using the expressions given in [3], the z-component of the Poynting vector (Sz) is calculated.

$$\left(\frac{J'_n(u)}{u J_n(u)} + \frac{K'_n(w)}{w K_n(w)}\right) \left(\frac{J'_n(u)}{u J_n(u)} + \left(\frac{n_0}{n_1}\right)^2 \frac{K'_n(w)}{w K_n(w)}\right) = n^2 \left(\frac{1}{u^2} + \frac{1}{w^2}\right) \left(\frac{1}{u^2} + \left(\frac{n_0}{n_1}\right)^2 \frac{1}{w^2}\right) \dots(1)$$

In equation (1), u and w are the transverse wave numbers in core and cladding regions, which are given by  $u = \sqrt{k^2 n_1^2 - \beta^2}$  and  $w = \sqrt{\beta^2 - k^2 n_2^2}$ , respectively.  $n_1$  and  $n_2$  represent the refractive indices of core and cladding, respectively. k is the wave vector and β being the propagation constant. n represents mode number. Single mode silica fiber exhibits only fundamental HE<sub>11</sub> mode, for which n is equal to 1. J and K represent the Bessel function and the modified Bessel function, respectively. The single mode cut-off diameter for the air-clad silica nanowire is calculated as 1135nm. Power profile for the air-clad single mode silica nanowire of 400nm diameter is obtained by calculating the Poynting vector (Sz) and is plotted as shown in Fig. 1.

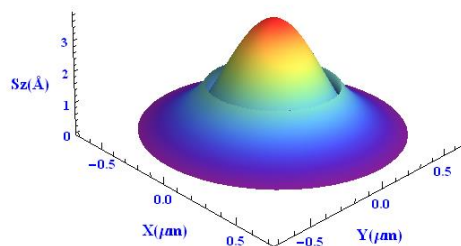


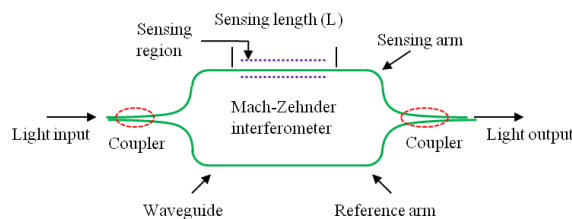
Figure 1: Power profile for the air-clad single mode silica nanowire of 400nm diameter at 1.55µm wavelength.

From Fig. 1, it is observed that the nanowire shows large discontinuity and increased field amplitude at the core-clad boundary, which indicates that the single mode silica nanowire is suitable for surface sensing.

**THE MODEL**

After exposure, a biomolecular layer of 12nm thickness is formed on the nanowire surface. This changes the external refractive index to 1.41, which corresponds to the refractive index of the biomolecular layer, over the layer thickness. Due to this, the instantaneous phase of propagating wave in the silica nanowire changes. In the present model, the phase change is measured by employing Mach-Zehnder interferometer (MZI).

The schematic of MZI is shown in Fig. 2. It has two arms, the reference arm and the sensing arm [4]. The sensing arm has a small sensing region of length L, which is functionalized for binding the analyte molecule. Light is launched in one of the two arms from one end and is bifurcated by a coupler. Before exposure, light waves having same phases travel through the two arms. After exposure, in the model, a finite biomolecular layer changes the refractive index to 1.41 over the layer thickness of 12nm. Due to this, the instantaneous phases in the two arms now differ, leading to a phase difference in the two arms. The waves are coupled back in the unsealed region.



**Figure 2: Schematic of sensor model employing MZI**

If  $\beta$  and  $\beta_0$  are the propagation constants of the fields in the two arms after exposure to the analyte gas, then the phase difference between the two arms is given by  $\Delta\beta = (\beta - \beta_0) \times L = \Delta\beta \times L$  [4]. Phase difference is measured by the Mach-Zehnder interferometer, in terms of intensity.

**SIMULATIONS**

In simulating the model, propagation constants before and after are calculated and compared for various nanowire diameters. The nanowire diameters are identified, which show higher difference in the propagation constants. Sensitivity and detection limit are also calculated. Minimum measurable refractive index over a small sensing length such as 1mm is calculated.

The nanowire before exposure exhibits the waveguide structure given in the previous section. After exposure, the nanowire exhibits three layer waveguide structure having silica core, 12nm thick biomolecular layer thickness having refractive index of 1.41 and air as the external medium. The field equations for the tightly guiding nanowire structure, having successively decreasing refractive index profile, having Bessel function 'J' in the core region, a combination of 'I' and 'K', which are the modified Bessel function of first kind and modified Bessel function of second kind, respectively, in the layer region and Bessel function 'K' as given above in cladding region. The transverse numbers are written. Considering the  $E_z$ ,  $H_z$  and  $E_\theta$ ,  $H_\theta$  field continuities at each boundary, eight simultaneous equations are written, which are solved by writing the resulting 8 x 8 matrix. The determinant of the matrix equals to zero is solved for finding the propagation constant  $\beta$  for this case.

**RESULTS AND DISCUSSION**

The phase difference in the two arms of MZI is calculated for various sensing lengths of 1mm, 3mm and 5mm and plotted in Fig. 3. From Fig.3, it is observed that even with small sensing lengths, appreciable phase difference is obtained for 700nm-1000nm nanowire diameters. The phase difference varies from  $0.37\pi$  to  $0.425\pi$  for the range of 700nm-1000nm diameter, for 1mm sensing length as shown in Fig.3. In comparison, the detection limit of MZI is very small, i.e. is  $2 \times 10^{-3}\pi$  [5]. This result indicates that surface sensing of an

adsorbed biomolecule on the silica nanowire surface is possible. The middle diameters show better results as compared to other diameters and 800nm diameter is the best candidate.

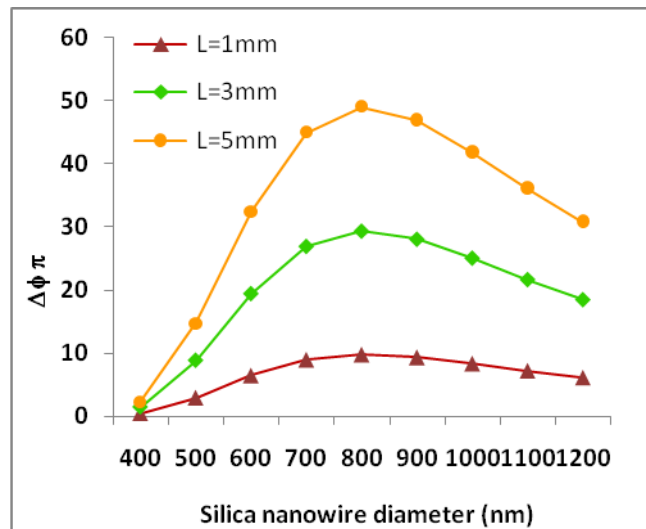


Figure 3: Phase difference in the two arms of Mach-Zehnder interferometer

Phase sensitivity and detection limit of this gas sensor model are also calculated by using following expression (2).

$$S_{\text{phase}} = \frac{1}{L} \frac{d(\Delta\phi)}{dn_c} \dots (2)$$

In expression (3), L is the sensing length and d(Δφ) is small variation in phase difference due to a small variation in refractive index, which is considered to be from 1.41 to 1.411, i.e. 0.001. It is observed that the sensitivity values vary from about 0.0204 μm<sup>-1</sup> to 0.0665 μm<sup>-1</sup>. The sensitivity is found high for middle range of diameters. It is highest for 800nm diameter. It is thus possible to measure the refractive index variation, as small as 0.001 in the value of 1.41 in this model. This is due to the use of silica nanowire in this model. This is useful in identifying the presence of some other species.

For the variation in refractive index of 0.001 as mentioned above, d(Δφ) for 1mm sensing length for 800nm diameter is 0.0235 π. If this phase difference is considered for instance, then with the detection limit of MZI considered to be 2×10<sup>-3</sup> π, the sensing length of 89μm is sufficient to produce this much phase difference. Also, the measurable refractive index over a sensing length of 1mm is found to be of the order of 10<sup>-4</sup> in the value of 1.41 which is quite low. Thus, the sensing length, as small as a fraction of one millimeter, is sufficient for building this sensor. In comparison, biosensors built with conventional integrated waveguides require a sensing length of 15mm to achieve a detection limit of 6×10<sup>-4</sup> of a monolayer [5]. Thus, the sensitivity obtained in these models is much higher than the other waveguiding devices. High sensitivity obtained in this model leads to miniaturization.

Since the optical loss of a taper-drawn silica nanowire for single-mode waveguiding is reported as below 0.0014dB/mm, the losses are small in the model.

### CONCLUSION

The field amplitude at core-cladding boundary of silica nanowire is high. It facilitates surface sensing of a biomolecular monolayer with high sensitivity. Because of this, small sensing lengths are required, which leads to the miniaturization of the sensor device. Refractive index variation of the order of 10<sup>-4</sup> can be measured using this model, which can be helpful in identifying the type of biomolecule. Due to miniaturization, small amount of sample is required for the analysis, which is the inherent need of medical field. The sensor based on the present model is a potential candidate for biomolecular detection.



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