# Modeling of subwavelength-diameter optical wire waveguides for optical sensing applications

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## ABSTRACT

Low-loss optical wave guiding along a subwavelength-diameter silica wire leaves a large amount of the guided field outside the solid core as evanescent wave and at the same time maintains the coherence of the light, making it possible to develop sensitive and miniaturized optical sensors for physical, chemical and biological applications. Here we introduce, for the first time to our knowledge, a scheme to develop optical sensors based on evanescent-wave-guiding properties of subwavelength-diameter wires. Optical wave guiding properties of these wires that are pertinent to a waveguide sensor, such as single-mode condition, evanescent field, Poynting vector and optical loss are investigated. By measuring the phase shift of the guided light, we propose a Mach-Zehnder-type sensor assembled with two silica wires. The sensitivity and size of the sensor are also estimated, which shows that, subwavelength-diameter silica wires are promising for developing optical sensors with high sensitivity and small size.

**Keywords:** Optical sensor, evanescent field, subwavelength-diameter, silica nanowire, wire waveguide, sensitivity, miniaturization.

## 1. INTRODUCTION

In the past years, extensive research and development activities have been devoted to evanescent-field-based optical waveguide sensors, which are now playing important roles in a variety of sensing applications[1-3]. By means of measuring small changes in optical phase or intensity of the guided light, these sensors present excellent properties such as high sensitivity, fast response, high reliability, immunity to electromagnetic fields, and safety in the detection of combustible and explosive materials. Along with increasing demands and rapid development of nanotechnology in various fields in recent years, the combination of nanotechnology, biology, chemistry and photonics opens the opportunity of developing optical sensors with subwavelength or nanometric structures, and many believe that one of the most effective methods in achieving better performances and wider applications of this kind of sensor lies in the miniaturization of the sensing structure, as those have been realized with fiber-optic nanotips or electrically conductive nanowires[4-7]. Recently, subwavelength-diameter silica wires have been reported for guiding light within the visible and near infrared spectral ranges[8]. Fabricated by a high-temperature taper-drawing process, these wires show excellent diameter uniformity and atomic-level sidewall smoothness, making them possible to guide light with low optical losses. Here we investigate the possibility of using subwavelength-diameter optical wires as guiding structures in an evanescent-field-based waveguide sensor. A prototype of a wire-guiding structure with a Mach-Zehnder interferometry detection system is modeled. Mostly concerned properties such as single-mode condition, evanescent fields, Poynting vector and optical loss of the guiding structure, as well as size and sensitivity of the sensor are investigated. By reducing the width of the waveguide to a

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Advanced Sensor Systems and Applications II, edited by Yun-Jiang Rao,
Osuk Y. Kwon, Gang-Ding Peng, Proceedings of SPIE Vol. 5634
(SPIE, Bellingham, WA, 2005) · 0277-786X/05/$15 · doi: 10.1117/12.575626

subwavelength scale, much more energy of the probing light can be made to propagate outside the waveguide, making it more sensitive to the changes of the environment. In addition, the reduced size of the waveguide allowing sensing in microenvironment of smaller size, and require fewer samples as well. Based on the results obtained here, we believe that the model presented in this work is promising to be developed into real systems for physical, chemical and biological sensing applications.

## 2. OPTICAL WAVE GUIDING PROPERTIES OF SUBWAVELENGTH-DIAMETER SILICA WIRE WAVEGUIDES

The details of optical wave guiding properties of subwavelength-diameter silica wire waveguides have been reported else where[9], here we make some further investigations on those properties that are concerned for optical sensing applications of these wire waveguides.

### 2.1 Propagation constant and single-mode condition

As in previous work[9], we assume that the wire has a circular cross-section, an infinite air clad, and a step-index profile. The wire diameter ($D$) is not very small (e.g. $D$>10 nm) so that the statistic parameters — permittivity ($\varepsilon$) and permeability ($\mu$) — can be used to describe the responses of a dielectric medium to an incident electromagnetic field. The length of the wire is large enough (e.g. longer than 10 μm) to establish the spatial steady state. We also assume that the wire is very uniform in diameter and smooth in sidewall, which has been proved possible in silica wires fabricated with taper-drawing method[8].

Based on the mathematic model described above, we solve Helmholtz equations and eigenvalue equations numerically to obtain the propagation constants ($\beta$) of the guided modes[9,10]. Calculated propagation constants (normalized as $\beta\cdot\lambda_0$, where $\lambda_0$ is the wavelength of the guided light in vacuum) of the first four modes ($HE_{11}$, $TE_{01}$, $TM_{01}$ and $HE_{21}$) are shown in Fig.1. The abscissa in Fig.1 is the $V$-number, which is directly related to the wire diameter ($D$) as $V= k_0\cdot D\ (n_1^2-n_2^2)^{1/2}/2$, where $k_0=2\pi/\lambda_0$, $n_1$ and $n_2$ are refractive indices of wire material and air respectively. Starting from the propagation constants, a variety of guiding properties of the wire waveguides can be obtained.

From the results in Fig.1, we can see that, when the wire diameter reduced to a certain value, only $HE_{11}$ mode exists, corresponding to the single mode operation. Single-mode condition of a cylindrical wire waveguide can be obtained as[10]:

$$V = 2\pi \cdot \frac{a}{\lambda_0} \cdot \left(n_1^{\ 2} - n_2^{\ 2}\right)^{\frac{1}{2}} \approx 2.405. \qquad (1)$$

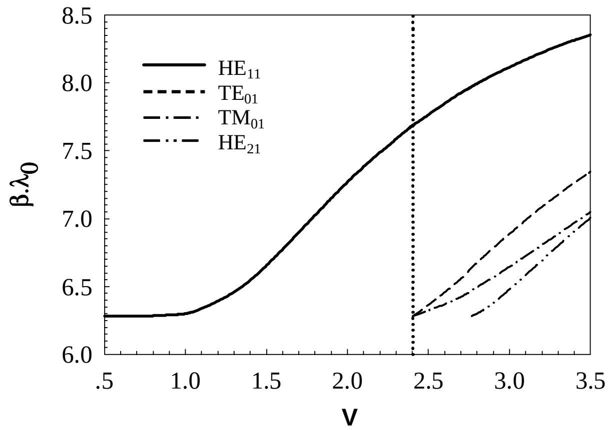


Fig.1. Numerical solutions of propagation constant ($\beta$, normalized as $\beta\cdot\lambda_0$) versus V number [$V= k_0\cdot D\ (n_1^2-n_2^2)^{1/2}/2$] of air-clad silica wire. Dotted lines, single-mode cutoff at V=2.405. The four mode indices presented in the figure are $HE_{11}$, $TE_{01}$, $TM_{01}$ and $HE_{21}$ respectively.

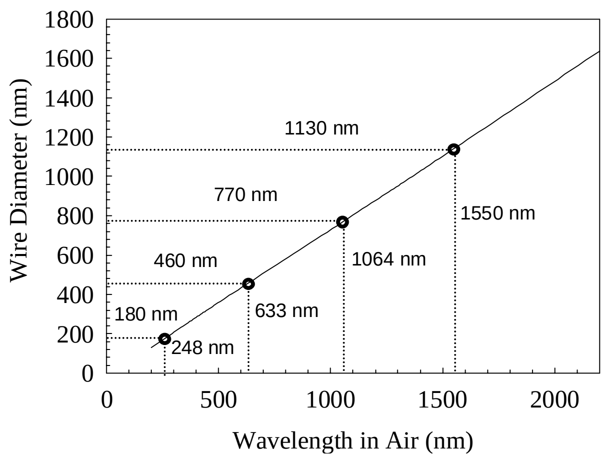


Fig.2. Calculated single-mode diameter of the silica wire waveguide. Critical diameters for single-mode operation of wires at typical wavelengths are labeled on the curve.

Calculated single-mode diameter ($D_{SM}$, the maximum allowable diameter for single-mode operation at a certain wavelength) of the wire waveguide calculated from Eq.(1) is shown in Fig.2. Where $D_{SM}$ at typical wavelengths (e.g. 248 nm of an excimer laser, 633 nm of a He-Ne laser, 1064 nm of a Nd:YAG laser, and 1550 nm of a laser diode for optical communication) are labeled on the curve. It shows that, $D_{SM}$ has a nearly linear dependence on the wavelength (it is exactly linear if there is no dispersion of the silica material). Since silica has a broad spectral range (e.g. from near infrared beyond 2 μm to ultraviolet below 200 nm in wavelength [11]) for low-loss optical wave guiding, the single-mode diameter for low-loss operation ranges from less than 150 nm to over 1500 nm. For example, for infrared light with wavelength of 1550 nm, the single-mode diameter of the wire can be larger than 1 micrometer; while for ultraviolet at 248-nm wavelength, the wire diameter must below 180 nm in order to make it single-mode. Since single-mode operation is usually required in waveguide-based optical sensing when coherent (rather than intensity) detection is used to achieve high sensitivity, we consider the guiding properties of the fundamental modes ($HE_{11}$ modes) and model sensors with single-mode wire waveguides in the following text.

**2.2 Evanescent fields and Poynting vector**

For evanescent-wave-based optical sensing, it is important to know the profile of the evanescent fields and power distribution around the waveguide. For reference, Fig.3 gives radial component of electric fields of $HE_{11}$ modes in cylindrical coordination for silica wires at 633-nm wavelength. It shows that, for wires with relatively large diameters, e.g. $D$=800 nm, most of the electric field are confined inside the silica core (the edge of the core is marked with a dotted line in the figure); when the wire diameter reduces below the single-mode diameter (about 460 nm at 633-nm wavelength), e.g. $D$=400 nm, more and more field moves out of the silica core and propagates as evanescent waves. The large amount of evanescent field makes the wire possible for optical sensing with high sensitivity.

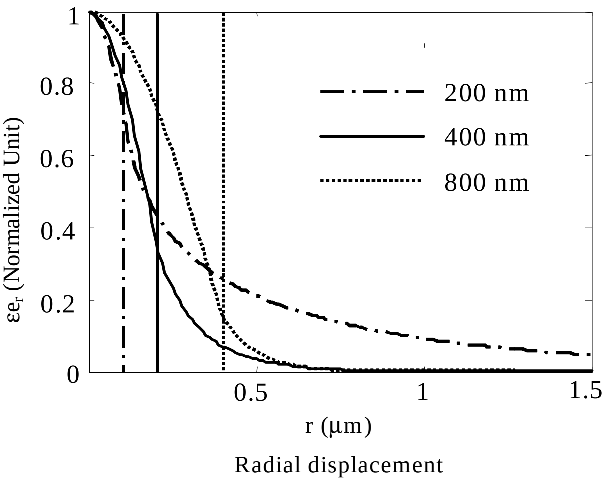


Fig.3. radial component of electric fields of $HE_{11}$ modes in cylindrical coordination for silica wires at 633-nm wavelength. Vertical lines stand for edges of the wire cores.

In order to obtain exact power distribution of the guided mode around the wire for quantitative modeling of optical sensing with silica wire waveguides, we calculate the z-components of Poynting vectors as [10]

inside the core ($0<r<a$):

$$S_{z1} = \frac{1}{2}\left(\frac{\varepsilon_0}{\mu_0}\right)^{\frac{1}{2}} \frac{kn_1^{\,2}}{\beta J_1^{\,2}(U)}\left[a_1a_3J_0^{\,2}(UR) + a_2a_4J_2^{\,2}(UR) + \frac{1-F_1F_2}{2}J_0(UR)J_2(UR)\cos(2\phi)\right] \quad (2)$$

outside the core ($a \le r < \infty$):

$$S_{z2} = \frac{1}{2}\left(\frac{\varepsilon_0}{\mu_0}\right)^{\frac{1}{2}} \frac{kn_1^{2}}{\beta K_1^{\,2}(W)}\frac{U^2}{W^2}\left[a_1a_5K_0^{\,2}(WR) + a_2a_6K_2^{\,2}(WR) - \frac{1-2\Delta - F_1F_2}{2}K_0(WR)K_2(WR)\cos(2\phi)\right] \quad (3)$$

where $J_v$ is the Bessel function of the first kind, and $K_v$ is the modified Bessel function of the second kind, $U=D(k_0^2n_1^2-\beta^2)^{1/2}/2$, $W=D(\beta^2-k_0^2n_2^2)^{1/2}/2$, $V=k_0 \cdot a\,(n_1^2-n_2^2)^{1/2}$, $R=2r/D$,
and

$$a_1 = \frac{F_2 - 1}{2};\ a_3 = \frac{F_1 - 1}{2},\ a_5 = \frac{F_1 - 1 + 2\Delta}{2},\ a_2 = \frac{F_2 + 1}{2},\ a_4 = \frac{F_1 + 1}{2},\ a_6 = \frac{F_1 + 1 - 2\Delta}{2},$$

$$F_1 = \left(\frac{UW}{V}\right)^2 [b_1 + (1 - 2\Delta)b_2],\quad F_2 = \left(\frac{V}{UW}\right)^2 \frac{1}{b_1 + b_2},$$

$$b_1 = \frac{1}{2U}\left\{\frac{J_0(U)}{J_1(U)} - \frac{J_2(U)}{J_1(U)}\right\},\ b_2 = -\frac{1}{2W}\left\{\frac{K_0(W)}{K_1(W)} + \frac{K_2(W)}{K_1(W)}\right\}.$$

Profiles of Poynting vectors for 800-, 400- and 200-nm-diameter silica wires at 633-nm wavelength are shown in Fig.4, in which the mesh profile stands for propagating fields inside the wire, and the gradient stands for evanescent fields in air. As we can see, when the wire diameter reduced from 800 nm to 200 nm, more and more power moves out of the silica wire. For a 200-nm diameter wire, the majority of the light is guided outside the silica core.

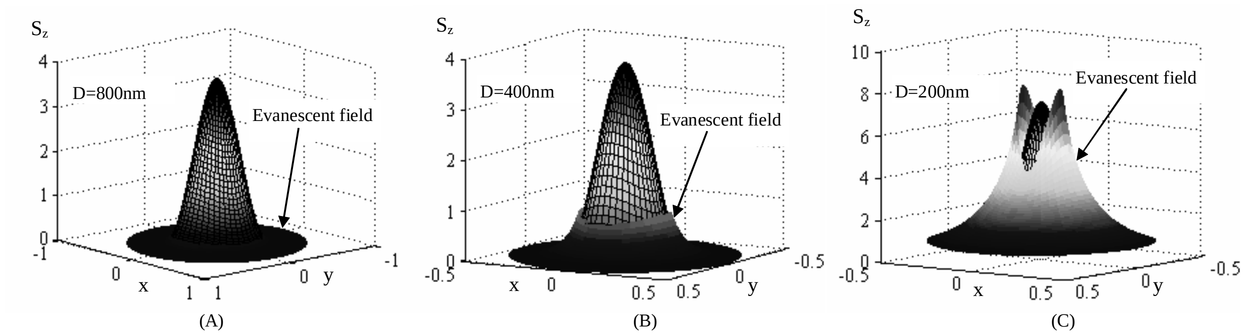


Fig.4. Z-direction Poynting vectors of silica wires at 633-nm wavelength with diameters of (A) 800 nm, (B) 400 nm, and (C) 200 nm. Mesh area stands for field inside the core, and gradient area stands for field outside the core.

## 2.3 Optical loss and coherence

Another important property of silica wire for optical sensing is the guiding loss, which directly affect the intensity and coherence of the signal. In addition, because silica is non-dissipative in the spectral range we concerned, the optical loss (if there exists) is mostly contributed by scattering, which may deteriorate signal-to-noise ratio (SNR) of the detection system.

Fortunately, one of the merits of subwavelength-diameter silica wires fabricated with the taper-drawing technique is its low optical loss. As shown in Fig.5, optical loss of a single-mode wire is lower than 0.1dB/mm in the first report[8], and recently it has been further reduced[12]. Such a low loss is very favorable for achieving high SNR, as well as for maintaining the coherence of the guided light, which is critically required by coherent detection for achieving high sensitivity.

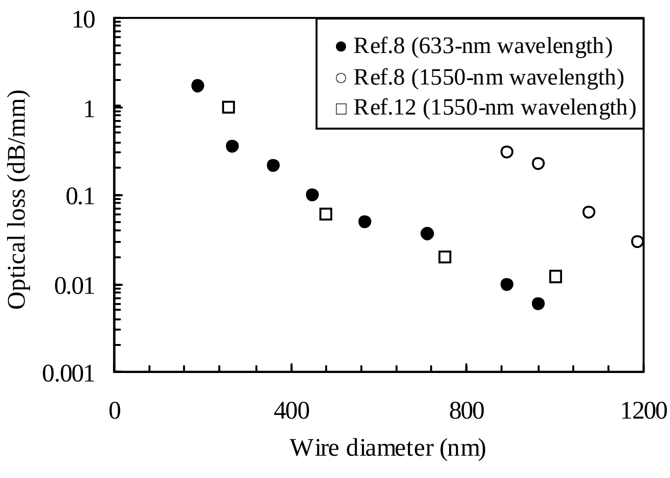


Fig.5. Optical loss of subwavelength-diameter silica wires in recent reports

## 3. SENSOR MODELING WITH SUBWAVELENGTH-DIAMETER SILICA WIRE WAVEGUIDES

### 3.1 Construction of sensor system with subwavelength-diameter silica wires

From the optical wave guiding properties investigated above, we know that subwavelength cross-sectional size of a silica nanowire leads to a significant portion of the light to be guided outside the core as evanescent wave. Based on this evanescent field, as well as coherence-maintained and low-loss guiding properties, we propose to functionalize the wire waveguide as sensing elements for detecting a variety of species that present index difference from the environment.

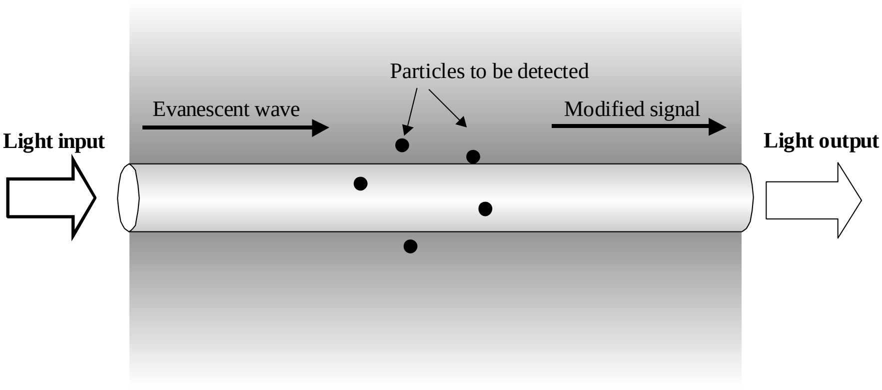


Fig.6. Schematic diagram of the wire-waveguide sensing element.

A schematic diagram of the basic element of the proposed sensor is shown in Fig.6. When exotic particles move approach the wire surface, they change the phase and intensity of the guided light in the evanescent field. By measuring these changes in the output of the wire waveguide, the information of the particles can be retrieved. To detect the small change in the optical phase, we propose to use a Mach-Zehnder interferometer. As shown in Fig.7, two silica wires with same diameters are assembled to a Mach-Zender structure. Part of silica wire 1 (the upper one in the figure) is used as a sensing arm, which is exposed to the environment to be detected. Part of silica wire 2 (the lower one) is used as a reference arm, which is kept in a constant medium and is isolated from the measurand. When we send the probing light into the left end of wire 1, it propagates along wire 1 and is bifurcated by the first 3-dB coupler. After traveling through the active area where exotic particles have access to evanescent fields of the wire, the signal guided along the sensing arm meets with the reference (traveled along the reference arm) by the second 3-dB connection, where highly sensitive interferometry

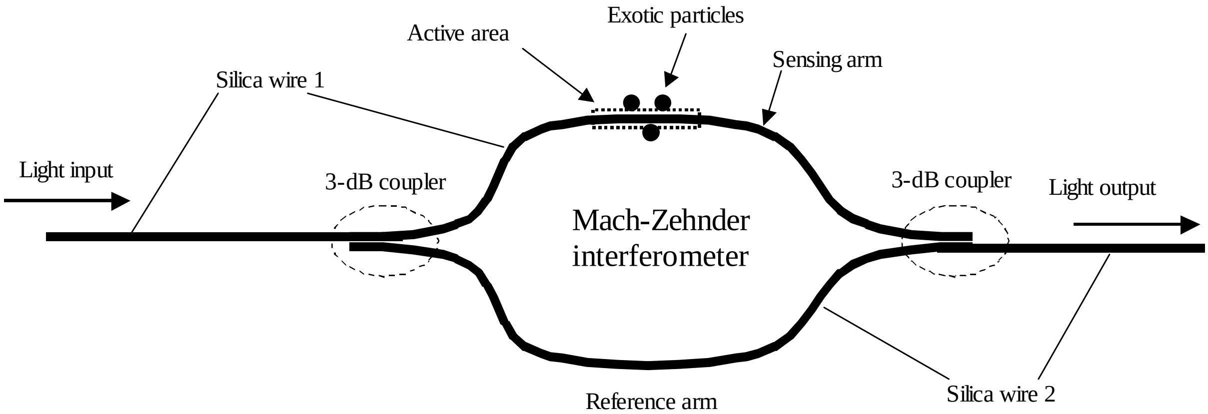


Fig.7 Schematic of the Mach-Zehnder interferometry detection of the phase change in a silica-wire-based optical sensor

technique is used to measure the phase shift of the probing light. Because of the enormous evanescent field of a subwavelength-diameter wire, the 3-dB coupler can be directly formed by pulling the two wires in touch.

### 3.2 Investigation of the sensitivity of the proposed sensor

To investigate the sensitivity of the proposed sensor, we assume that the light propagates along the axis of the nanowire (the $z$ direction as we assumed in the forementioned model). With z components of Poynting vector obtained from Eqs.(2) and (3), we can estimate the sensitivity of the sensor for detecting micro- or nano- particles with known optical properties. As a typical case, we use He-Ne laser (633-nm wavelength) as probing light; at 633-nm wavelength, the maximum single-mode diameter for a silica wire is about 460 nm, thus we assume the wire we used is 400 nm in diameter, with about 30% of the light energy propagated outside the wire.

For simplicity, we assume the nanoparticle to be a cylinder with a radius $B$, a height of $B$ and a homogeneous refractive index $n_m$. We also assume that the particle is bound on the sidewall of the wire at the position where the Poynting vector is at its maximum, then the optical phase shift ($\Delta\Phi$) caused by a single particle can be estimated as:

$$\Delta\Phi = \frac{2\pi B \cdot \int_{r=0}^{B} r dr \int_{\phi=0}^{2\pi} d\phi \int_{z=0}^{2B} dz \cdot (n_m - n_0) \cdot S_z(\frac{r}{a},\phi)}{\lambda \cdot \int_{r=0}^{\infty} r dr \int_{\phi=0}^{2\pi} d\phi \int_{z=0}^{2B} dz \cdot S_z(\frac{r}{a},\phi)} \qquad (4)$$

For particles of several typical sizes and refractive indices, calculated phase shifts are listed in Table.1.

Table 1. Maximum phase shift ($\Delta\Phi$) of a 633-nm-wavelength light caused by a single particle placed on the sidewall of a 400-nm-diameter silica wire

| Particle size (2B) (nm) | Refractive index | Phase shift $\Delta\Phi$ (rad) |
|---|---|---|
| 10 | 1.35 | $1.2\times10^{-5}\pi$ |
| | 1.50 | $1.3\times10^{-5}\pi$ |
| 50 | 1.35 | $1.1\times10^{-4}\pi$ |
| | 1.50 | $1.1\times10^{-4}\pi$ |
| 100 | 1.35 | $5.2\times10^{-4}\pi$ |
| | 1.50 | $6.6\times10^{-4}\pi$ |

Generally, the sensitivity of detecting optical phase shift in an integrated waveguide Mach-Zehnder interferometer can go down to $2\times10^{-3}\pi$ [Ref.13]. Hence, from $\Delta\Phi$ listed in Table 1, the expected detection limit on the number of nanoparticles for the proposed sensor is about 200 for a 10-nm diameter nanoparticle with a refractive index of 1.35, or 4 for a 100-nm diameter nanoparticle with a refractive index of 1.50. If the sensitive/active length of the wire used for sensing is 50 $\mu$m and is used in a biosensor, the corresponding sensitivity will be $10^{-4}$ of a monolayer or 10 pg/cm$^2$ (assuming a detection limit of 50 proteins with molecular mass of 50 kDa), which is a much higher sensitivity than Mach-Zehnder inteferometry based biosensors reported else where (generally a $10^{-3}$ of a monolayer or 100pg/cm$^2$) [13-16].

### 3.3 Size estimation

Another concerned parameter of the sensor in this work is its size. The reduction in sensor size will allow sensing in microenvironment of smaller volume and require fewer samples. Also, miniaturization in size will be helpful for high-density integration of sensor arrays.

In a sensor system described above, the sensitivity of the sensor is determined by the phase shift ($\Delta\Phi$) of the signal. In most practical applications, the whole length of the active area is exposed to the environment/medium to be detected, therefore, $\Delta\Phi$ is proportional to the length of the active area. For conventional sensors based on integrated optical Mach-Zehnder interferometer, the length of the sensing area is on the order of millimeters; for comparison, the length of the sensing area of the sensor modeled with subwavelength-diameter wire waveguides can go down to less than 100μm (e.g. 50 μm mentioned above) while still provides a sensitivity higher than the large ones. In addition, the auxiliary structures of the sensor modeled here can also be made very small. For example, the low-loss bend of a 400-nm-diameter silica wire can be achieved with bending radius less than 6 μm [Ref.17], and a 3-dB coupler/splitter with size smaller than 5 μm has been built with two 400-nm-diameter silica wires[18]. Therefore, the overall size of the sensor modeled here can be made much smaller than the conventional devices.

## 4. CONCLUSIONS

In conclusion, based on recent developments in subwavelength-diameter low-loss silica wire waveguides, we proposed to develop optical sensors based on evanescent-wave-guiding properties of these wires. Optical wave guiding properties that are closely related to a waveguide sensor, such as single-mode condition, evanescent fields, Poynting vector and optical loss are reviewed. By using a Mach-Zehnder interferometer assembled with two silica wires for detection of optical phase shift, prototype of an evanescent-wave-based optical waveguide sensor is modeled. Sensitivity and size of the sensor are estimated. Our results show that, subwavelength-diameter silica wire waveguides are promising for developing optical sensors with higher sensitivities and smaller sizes.

## ACKNOWLEDGEMENT

This work is supported by the National Natural Science Foundation of China (No. 60378036 and 60408001) and the US National Science Foundation (PHY-9988123). Limin Tong acknowledges support from the Centre for Imaging and Mesoscale Structures at Harvard University.

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