Sensitivity optimization in whispering gallery mode optical cylindrical biosensors

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Abstract. Whispering-gallery-mode resonances propagated in cylindrical resonators have two angular and radial orders of \( l \) and \( i \). In this work, the higher radial order whispering-gallery-mode resonances, \((i = 1 - 4)\), at a fixed \( l \) are examined. The sensitivity of these resonances is analysed as a function of the structural parameters of the cylindrical resonator like different radii and refractive index of composed material of the resonator. A practical application where cylindrical resonators are used for the measurement of glucose concentration in water is presented as a biosensor demonstrator. We calculate the wavelength shifts of the WG1-4, in several glucose/water solutions, with concentrations spanning from 0.0% to 9.0% (weight/weight). Improved sensitivity can be achieved using multi-WGM cylindrical resonators with radius of \( R = 100 \, \mu m \) and resonator composed material of MgF\(_2\) with refractive index of \( n_c = 1.38 \). Also the effect of polarization on sensitivity is considered for all four WGMs. The best sensitivity of 83.07 nm/RIU for the fourth WGM with transverse magnetic polarization, is reported. These results propose optimized parameters aimed to fast designing of cylindrical resonators as optical biosensors, where both the sensitivity and the geometries can be optimized.

1. Introduction

An outstanding group of dielectric optical resonators are circular resonators which can support Whispering-gallery-mode (WGM) resonances. WGM resonators can have different geometries such as cylinder [1, 2, 3], microsphere [4, 5, 6], microfiber coils and microdisk [7]. In these geometries, due to light recycling nature, light-matter interaction is greatly enhanced. This allows fabricating of high-quality factor optical resonators, which enables confining significant optical powers in small regions for extended time periods [6]. Cylindrical micro-resonators have especially attracted a significant level of interest in biosensing [1, 2, 3]. In this work, we propose the use of cylindrical micro-resonators with optimized structural parameters for optical biosensing. This kind of optical biosensor detects changes in the surrounding refractive index through the electromagnetic (EM) field evanescent depth of WGMs, travelling outside the cylindrical resonator boundary, providing label-free sensing ability [8, 9, 10]. WGM resonances in these structures can have two degrees or orders of freedom \( i \) and \( l \) or \( \nu \), where \( i \) is radial order and \( l \) or \( \nu \) is the angular order of a WGM. In this work, we analyse the high angular WGMs with radial orders \( i = 1 - 4 \), or just WG1-4, in two different polarizations transverse electric (TE), and transverse magnetic (TM). The full theoretical examination of WGMs in cylindrical resonators within the framework of classical electrodynamics requires the application of Mie theory [11]. In this paper we use an analytical model of Airy approximations to the full Mie/Debye solutions, for
extracting closed form of WGM resonance wavelengths. Resonance wavelength shifts of WGMs are simulated in different concentrations of glucose-water solutions in surrounding medium of the cylindrical resonator. The sensitivity of these resonances is analysed as a function of the structural parameters of the cylindrical resonator, like different radii and different refractive indexes of composed material.

2. Theory
As mentioned, the full theoretical examination of WGMs in cylindrical resonators within the framework of classical electrodynamics requires the application of Mie theory [11, 12]. This also involves complicated computational effort due to the need for numerical calculation of the sums of series of Bessel functions [12]. This can be avoided with simpler models based on elementary optics [6] or on analytical approximations to the exact Mie/Debye solutions [13]. In the following, we will use an analytical model based on the formulation of Airy approximations to the full Mie/Debye solutions. With this formulation the calculation of WGM resonance wavelengths with different radial and angular orders is possible.

2.1. Formulation
The analytical closed form of WGM resonance wavelengths for two different polarizations of TE and TM, are expressed as follow:

\[
\lambda_{TE}^{i}(\nu, l, R, m) = 2\pi n_c R (A \nu + B_i \nu_1^{1/3} - \frac{m}{\sqrt{m^2 - 1}} + C_i \nu_1^{2/3} - \frac{D_{TE} m^3}{(m^2 - 1)^{1/3}} \nu_2^{1/3} + o(\nu^{-1}))^{-1}
\]

\[
\lambda_{TM}^{i}(\nu, l, R, m) = 2\pi n_c R (A \nu + B_i \nu_1^{1/3} - \frac{1}{m \sqrt{m^2 - 1}} + C_i \nu_1^{2/3} - \frac{D_{TM} (m^4 - \frac{2}{3})}{m^3 (m^2 - 1)^{2/3}} \nu_2^{1/3} + o(\nu^{-1}))^{-1}
\]

Where \( \nu = l + \frac{1}{2} \), \( \nu \) and \( l \) are angular orders in spherical and cylindrical resonators respectively, \( m = \frac{n_c}{n_s} \) is the relative refractive index between the cylinder \( n_c \), and the surrounding medium \( n_s \), and \( i \) is the \( i^{th} \) zero of the Airy function and represent radial order of WGMs. With exact calculation of the numerical coefficients of \( A_i \), \( B_i \), \( C_i \) and \( D_i \), WGM resonance wavelengths can be easily calculated. The superiority of using these formulations with only an error order of \( \nu^{-1} \) from the exact solutions, is that these equations, provide analytical functions that can be simply implemented into a fitting routine for simultaneous determination of the parameters \( \nu \), \( m \), and \( R \), while the exact solution involves a difficult numerical procedure.

2.2. Equation coefficients
The exact amounts and variations of different coefficients in the above relations have been plotted in Fig. 1a-1d. It must be noted that coefficient \( A_i \) is equal 1. The numerical amount of \( B_i \) and \( C_i \) coefficients, is the same for two different polarization of TE and TM. But the \( D_i \) coefficient is different for different polarizations. These are just some mathematical results because of the airy approximation applying to the Mie/Debye solutions. With known amounts of these coefficients, sensitivity of different WGM resonance wavelengths as sensing signals can be calculated.
3. Sensitivity simulations

The operational sensing principle in WGM biosensors is to monitor changes in the WGM resonance wavelength prompted by surrounding medium refractive index changes. This phenomenon can be realized as bulk refractive index sensitivity or only sensitivity (S), of an optical biosensor. The S parameter can be expressed as below:

\[ S = \frac{\Delta \lambda_{WGM}}{\Delta n_s} \]  (3)

where \( \Delta \lambda_{WGM} \) is WGM resonance wavelength shift, over the refractive index changes of the surrounding medium, \( \Delta n_s \). Indeed, interaction of the EM field evanescent depth of a WGM resonance wavelength with biological solution (flowing in the surrounding medium), causes changes in refractive index of the surrounding medium.

The silica cylindrical resonators, with refractive index of \( n_c = 1.45 \) and different radii of 50 – 100 μm are considered as optical biosensors. These parameters not only are complementary with real cylindrical device[14], but also support the propagation of multi WGM resonance. According to size parameter \( x = \frac{2\pi R}{\lambda} = \frac{l}{n} \) [6], WGMs with \( l > 360 \), will be investigated. In the following sections of this paper, we simulate the sensitivity of the proposed cylindrical sensor in several glucose/water solutions in surrounding medium, with concentrations spanning from 0.0% to 9.0%. The change in refractive index of the solution \( \Delta n_s \), is proportional to the glucose concentration \( C \) through the relation \( \Delta n_s = C \times 1.375 \times 10^{-3} \text{RIU}/\% \) as reported in

![Figure 1](image-url)

**Figure 1.** Variations of coefficients of a) \( B_i \) and b) \( C_i \) for both polarization TE and TM and c) \( D_i \) for TE and d) \( D_i \) for TM polarization, in terms of radial order \( i = 1 – 4 \)
Figure 2. WGM resonance wavelength shift in different refractive index of glucose-water for TE and TM a) WG1 at $R = 50 \mu m$, b) WG4 at $R = 50 \mu m$ and c) sensitivity of WG1-4 at fixed $R = 50 \mu m$.

[15]. WG1-4, in a fixed angular order $l = 442$ and their effective role in sensing performance, are studied. We have especially examined WGMs with $l = 442$, because the WGMs with this angular momentum have experimentally demonstrated in [14] as sensing signals in optical cylindrical biosensors. Also, we considered different composed material of cylindrical resonators to optimize the structural parameters for better sensing performance. It has a great significance for providing a theoretical guide for the fabrication of the device and its practical sensing applications.

3.1. Radial order and polarization
Each WGM has its unique $S$. Fig. 2a-2c shows the effect of both radial order and polarization on sensitivity. Higher radial order WGMs, have a longer evanescent depth of electromagnetic field into surrounding medium. This is why they have higher sensitivity. Also polarization change, has an effective role on $S$ of WGM resonance wavelengths.

3.2. Resonator radius
Then we investigate the effect of different radii $R = 50 - 100 \mu m$ on sensitivity. Fig. 3a-3c shows the calculated sensitivity versus $R$ under different radial orders $i = 1 - 4$ and polarizations TE and TM, while $n_c = 1.45$ remains unchanged. Higher radial order WGMs show more sensitivity. As they have more EM evanescent depth in surrounding medium. Also resonator radius increasing has a positive effect on sensitivity improvement. As we can see Fig. 3b, with
increasing resonator radius from $R = 50 \ \mu m$ to $R = 100 \ \mu m$, $S$ has increased from $35 \ \text{nm/RIU}$ to $71 \ \text{nm/RIU}$.

3.3. Composed materials of the resonator
Calculated sensitivity of our device with different WGMs versus the resonator refractive index $n_c$ has been plotted in Fig. 4a-4b. It can be seen that lower resonator refractive index possesses significantly higher sensitivity.

4. Conclusions
We proposed optimized structures of optical biosensors based on multi-WGM cylindrical resonators formed in silica glass with refractive index of $n_c = 1.45$. Analytical closed form of WGM resonance wavelengths with radial orders $i = 1 - 4$ have been calculated. Exact amounts of equation coefficients in these relations, have been extracted. Results showed a bulk refractive index sensitivity of $\sim 71 \ \text{nm/RIU}$ for TE WG4 and $\sim 83 \ \text{nm/RIU}$ for TM WG4 at resonator radius of $R=100 \ \mu m$. We indicated that higher radial orders of WGMs at bigger radii of resonator, and lower refractive index of the resonator material like MgF$_2$ material, lead to higher sensitivity. These results will be the theoretical guides for fast designing and fabrication of the optical biosensor device, where both the sensitivity and the geometries can be optimized.

**Figure 3.** a) and b) resonance wavelength shifts of WG1 and WG4 in different surrounding medium refractive index for TE polarization in different radii, $R = 50 - 100 \ \mu m$ of resonator; c) and d) biosensor sensitivity in different radii of cylindrical resonator for TE WG1-4 and TM WG1-4, respectively.
Figure 4. Sensitivity of WG1-4 as a function of resonator refractive index in resonator radius of a) $R = 50 \, \mu m$ and b) $R = 100 \, \mu m$.

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