Single-waveguide-based microresonators for optical sensing

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Optical biosensors with a high sensitivity and a low detection limit play a highly significant role in extensive scenarios related to our daily life. Combined with a specific numerical simulation based on the transfer matrix and resonance condition, the idea of novel single-waveguide-based microresonators with a double-spiral-racetrack (DSR) shape is proposed and their geometry optimizations and sensing characteristics are also investigated based on the Vernier effect. The devices show good sensing performances, such as a high quality factor of $1.23 \times 10^5$, a wide wavelength range of over 120 nm, a high extinction ratio (ER) over 62.1 dB, a high sensitivity of 698.5 nm/RIU, and a low detection limit of $1.8 \times 10^{-5}$. Furthermore, single-waveguide-based resonators can also be built by cascading two DSR structures in series, called twin-DSRs, and the results show that the sensing properties are enhanced in terms of quasi free spectral range (FSR) and ER due to the double Vernier effect. Excellent features indicate that our novel single-waveguide-based resonators have the potential for future compact and highly integrated biosensors.


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Whispering-gallery-mode (WGM) microresonators\cite{1,2} are extremely useful for numerous applications in many areas such as disease diagnostics, environmental monitoring, food safety, and biomedicine. Specifically, intense efforts have been made on how to harness their potential for label-free biosensing fields\cite{4}. The devices basically rely on the overlap interaction between the evanescent wave and bioanalytes absorbed on device surfaces or in the surrounding medium\cite{4}. They are typically based on silicon-on-isolator (SOI) material systems offering extremely low absorption and bending losses, which allows many flexible geometry designs such as rings\cite{2}, disks\cite{2}, or toroids\cite{7}. Their attractive properties, such as high quality factor (Q factor) and small footprint, mean that the light would circle the resonators dozens of times before being lost, which makes high power enhancement easy to achieve and, accordingly, makes attractive high sensitivity possible. Single biomolecule detection has already been achieved\cite{8,9} in this way.

Except for the different shapes of microresonators, another smart strategy is to integrate more sensitivity-enhancing methods to further improve the sensing performances. The idea of slot waveguides is an excellent choice to replace the common solid ones to render a larger overlap between the optical mode and the bioanalyte\cite{10}. Another idea is to introduce the asymmetric Fano resonance effect\cite{11} to obtain a steeper spectrum slope or to introduce the Vernier effect\cite{12,13,14} with special sensor designs, which extremely increases the sensitivity and quasi free spectral range (FSR).

In this Letter, novel single-waveguide-based microresonators on an SOI substrate are proposed. The particular feature is that the whole device is made up of one single waveguide a certain way. Thanks to the Vernier effect, the devices show a high sensitivity, a high extinction ratio (ER), as well as a large measurement range. We provide the design considerations and the sensing performances in the following.

Our novel single-waveguide-based micro-resonators have the double-spiral-racetrack (DSR) shape, as shown in Fig. 1. The waveguide, fabricated on a SOI wafer with 220 nm Si on a 2 μm buried oxide layer, starts from a Bragg grating coupler as the input port, forms four straight sections connected by four semicircle sections. The injected light passes through all the sections and then outputs from the right end.

To easily analyze the principle of DSR resonators, the single waveguide is separated into two subsections, an equivalent Mach–Zehnder interferometer (MZI), and an equivalent microring resonator, which is illustrated in Fig. 2, respectively.

In Fig. 2, the MZI structure is highlighted in the gray area, and the semiring $R_2$ forms one arm of the equivalent MZI while semiring $R_4$ and two straight waveguides $L_{S2}$...
In the equivalent microring resonator, feedback path for electric fields related as transmission and coupling coefficients can be transmission coefficients. In the lossless coupling mechanism factor, respectively. 

\[ K \]

induced by coupler I and coupler II as mission factor, respectively, and 

\[ L \]

pling coefficients of the electric fields for coupler I and coupler II, respectively, and 

\[ R \]

form the other arm. Together with two directional couplers, the equivalent MZI forms. In terms of the equivalent microring resonator, marked by the black waveguide as shown in Fig. 2, it is made up of two semirings \( R_2, R_3 \) and three straight waveguides \( L_1, L_2, L_{S1} \). We employ the transfer matrix method (TMM) to analyze the electric transmission characteristics of the DSR device and the port numbers are marked in Fig. 2. Using a transfer matrix, the input and output electric fields in the equivalent MZI can be explained as

\[
\begin{bmatrix}
E'_4 \\
E_4
\end{bmatrix} = e^{-i(\phi_1 + \phi_2)} \cdot \begin{bmatrix}
\tau_2 - ik_2 \\
-i k_2 \tau_2
\end{bmatrix} \cdot \begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix} \cdot \begin{bmatrix}
\tau_1 - ik_1 \\
-i k_1 \tau_1
\end{bmatrix} \cdot \begin{bmatrix}
E'_1 \\
E_1
\end{bmatrix} \\
= e^{-i(\phi_1 + \phi_2)} \cdot M \cdot \begin{bmatrix}
E'_1 \\
E_1
\end{bmatrix},
\]

(1)

In the equivalent microring resonator, \( R_3 \) and \( L_{S1} \) form the feedback path for electric fields \( E'_1 \) and \( E_4 \), so a feedback relationship exists:

\[ E'_1 = E_4 \cdot a_3 \cdot e^{-i\theta_1}. \]

(3)

In the above equations, \( k_1 \) and \( k_2 \) are the amplitude coupling coefficients of the electric fields for coupler I and coupler II, respectively, and \( \tau_1 \) and \( \tau_2 \) are the corresponding transmission coefficients. In the lossless coupling mechanism, transmission and coupling coefficients can be related as

\[ \kappa^2 + \tau^2 = K + T = 1, \]

(4)

where \( K \) and \( T \) are the power coupling factor and transmission factor, respectively. \( \phi_1 \) and \( \phi_2 \) are the phase shifts induced by coupler I and coupler II as

\[ \phi_1 = \beta \cdot L_1 = \frac{2\pi n_{\text{eff}}}{\lambda} \cdot L_1, \quad \phi_2 = \beta \cdot L_2 = \frac{2\pi n_{\text{eff}}}{\lambda} \cdot L_2, \]

(5)

where \( \beta \) is the propagation constant, \( n_{\text{eff}} \) is the efficient index, and \( L_1 \) and \( L_2 \) are the coupling lengths. \( a_1, a_2, a_3 \) are the transmission coefficients of the two arms of the equivalent MZI and the feedback path, and \( \theta_1, \theta_2, \theta_3 \) are the corresponding phase shifts. They are related to the waveguide lengths, loss coefficients, and propagation constants as

\[ a_1 = e^{-a_0 \cdot \pi R_2}, \quad a_1 = e^{-a_0 \cdot \pi R_2}, \quad a_3 = e^{-a_0 \cdot (\pi R_3 + L_{S1})} \]

(6)

\[ \theta_1 = \pi R_2 \beta, \quad \theta_2 = (\pi R_4 + 2L_{S2})\beta, \quad \theta_3 = (\pi R_3 + L_{S1})\beta. \]

(7)

In Eq. (6), \( a_0 \) is the loss coefficient of light in the waveguide, which can be adjusted under different fabrication conditions.

Then the electric fields can be calculated as

\[
E'_4 = e^{-i(\phi_1 + \phi_2)} \left( A \cdot a_3 \cdot e^{-i\theta_1} \cdot \frac{D \cdot E_1}{e^{i(\phi_1 + \phi_2)} - a_3 \cdot e^{-i\theta_1} + B \cdot E_1} \right). \]

(8)

So the transmission of the DSR device can be written as

\[
T'_4 = \left| \frac{E'_4}{E_4} \right|^2 = \left| e^{-i(\phi_1 + \phi_2)} \left( A \cdot a_3 \cdot e^{-i\theta_1} \cdot \frac{D}{e^{i(\phi_1 + \phi_2)} - a_3 \cdot e^{-i\theta_1} + B} \right) \right|^2. \]

(9)

The resonance in the DSR device occurs when the resonance conditions of the equivalent microring resonator and the equivalent MZI are satisfied simultaneously, which leads to sharp and steep resonance peaks with a high Q factor and ER in the spectrum. The resonance conditions are described as

\[ n_{\text{eff}} \cdot C_R = (m_R - 1/4) \cdot \lambda_R, \]

(10)

\[ n_{\text{eff}} \cdot \Delta L = m_{\text{MZI}} \cdot \lambda_{\text{MZI}}, \]

(11)
where \( C_R \) is the circumference of the equivalent microring and \( \Delta L \) is the difference between the two arms of the equivalent MZI, both of which can be expressed as

\[
C_R = L_1 + L_2 + L_{S1} + \pi R_2 + \pi R_3, \tag{12}
\]
\[
\Delta L = 2L_{\alpha 2} + \pi R_4 - \pi R_2, \tag{13}
\]

where \( \lambda_R, \lambda_{MZI} \) are the resonance wavelengths and \( m_R, m_{MZI} \) are the corresponding resonance orders of the equivalent ring resonator and the equivalent MZI, respectively. The item \((-1/4)\) in Eq. (10) represents the phase change of \( \pi/2 \) caused by optical coupling from coupler I. When both resonance conditions are satisfied, we arrive at

\[
\frac{n_{\text{eff}} \cdot \Delta L}{m_{MZI}} = \frac{n_{\text{eff}} \cdot C_R}{(m_R - 1/4)}. \tag{14}
\]

Obviously, the resonance parameters such as resonance wavelengths and resonance orders are relevant to the structure parameters. When a specific wavelength is selected as the resonance wavelength, the device structure parameters can be mainly determined by resonance orders.

For practice applications, the high Q factor and ER of the DSR sensor are required. For a ring resonator based on the same SOI substrate, the bend loss can be neglected once the bending radius is more than 5 \( \mu m \)\(^\text{[18]} \), so the Q factor of the DSR mainly depends on the propagation loss and coupling loss\(^\text{[19]} \) if all the radii of the semirings that are over 5 \( \mu m \). The ER depends strongly on the coupling loss, so it will reach a maximal value at a critical coupling point where the coupling loss equals the intrinsic loss. The propagation loss is decided by the propagation loss factor and the transmission distance \( L \), so in order to achieve a high ER and Q factor the geometry size and coupling parameters have to be carefully optimized. Several optimal parameters, such as the resonance order, propagation loss, and coupling coefficients are considered.

Based on our simulation, the most efficient choice is to fix \( m_{MZI} \) and scan \( m_R \) as \( m_R \) has a greater influence on the structure parameters. So the dependence of the device properties, Q factor and ER, on \( m_R \) and \( \alpha_0 \) are first investigated.

The overall Q factor and ER in this case are plotted in Fig. 3. The highest contrast ratio requires moderate values of \( m_R \) and \( \alpha_0 \), and a larger Q factor occurs at larger \( m_R \) values and smaller \( \alpha_0 \) values. However, the optimal parameter regions for the best Q factor and ER do not overlap. In our design, high ER values should be the primary focus to suppress the side mode in terms of the Vernier effect induced by the equivalent MZI and ring resonator of the DSR. Meanwhile, considering that the detection limit is primarily determined by the Q factor, it is also important to maintain the Q factor at a high level to lower the detection limit. Therefore, the optimal \( m_R \) and \( \alpha_0 \) are chosen at 121 and 2.3 dB/cm, respectively.

The dependence of the device performances, i.e., the ER and Q factor, on \( K_1 \) and \( K_2 \) are then investigated and shown in Fig. 4. Similar to the scenario before, there is a tradeoff between a high ER and high Q factor. It needs a \( K_2 \) than the latter to achieve s better ER, and it requires larger \( K_1 \) values than the former to get a better Q factor. Therefore \( K_1 \) and \( K_2 \) are set to 0.5 and 0.43, respectively, where a Q factor of \( 1.23 \times 10^5 \) and an ER value of 62.1 dB can be obtained. The selected \( K_1 \) and \( K_2 \) can only be realized by varying the coupling gaps of corresponding couplers.

Fig. 3. (a) Variation of ER and (b) the variation of the Q factor by changing \( m_R \) and \( \alpha_0 \).

Fig. 4. Schematic of (a) the variation of ER and (b) the variation of the Q factor by changing \( K_1 \) and \( K_2 \).
Based on all the optimizations above, the device parameters are calculated and listed in Table 1. And the optimal transmission spectrum is plotted in Fig. 5 in which a quasi-FSR of about 120 nm is realized.

To investigate homogeneous sensing properties, the device is supposed to be immersed in a solution containing bioanalytes, so the variations of transmission spectra can be calculated and presented in Fig. 6(a) as the effective index changes due to the change of the surrounding medium. It is obvious that a higher bioanalyte concentration induces a larger effective refractive index change and then leads to a larger resonant wavelength shift, as shown in Fig. 6(b), which shows an excellent linear relationship between the resonant wavelength shift and the variation of the effective refractive index. Then the sensitivity is calculated as

\[ S = \frac{\Delta \lambda}{\Delta n_{\text{eff}}} = 698.5 \, \text{(nm/RIU)}. \]  

Another important performance of biosensors is the limit of detection (LOD), defined as the minimum detectable change of the refractive index in our case. The LOD is limited by the accuracy of the detection system and the sensitivity of the biosensor. Considering the detection capability only, the LOD of the biosensor can be calculated according to the definition of the Q factor and the sensitivity (S) of the sensor as

\[ \text{LOD} = \Delta n_{\text{min}} = \frac{\Delta \lambda_{\text{min}}}{S} = \frac{\lambda_R}{Q \cdot S}. \]  

Based on all the simulation results, the detection limit is calculated to be $1.8 \times 10^{-5}$ RIU in terms of the change of effective refractive index.

Table 1. Geometry Parameters for DSR Devices

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value (μm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_1$</td>
<td>5</td>
</tr>
<tr>
<td>$R_2$</td>
<td>6.8</td>
</tr>
<tr>
<td>$R_3$</td>
<td>6.9</td>
</tr>
<tr>
<td>$R_4$</td>
<td>7.0</td>
</tr>
<tr>
<td>$L_1$</td>
<td>15</td>
</tr>
<tr>
<td>$L_2$</td>
<td>20</td>
</tr>
<tr>
<td>$L_{S1}$</td>
<td>5</td>
</tr>
<tr>
<td>$L_{S2}$</td>
<td>4.6</td>
</tr>
</tbody>
</table>

![Fig. 5. Optimal transmission spectrum of the DSR device (Solid line) and the dash line represents the transmission spectrum of the MZI structure. The inset shows the enlarged resonance peak at 1.55 μm.](image)

![Fig. 6. Schematic of (a) the variations of the transmission spectra with change of effective refractive index and (b) the relationship between the resonant wavelength drift and the change of effective refractive index.](image)

Table 2. Sensing Performance Comparisons of Microring, Microdisk Resonator and DSR Device

<table>
<thead>
<tr>
<th>Performance Parameter</th>
<th>Microring Resonator</th>
<th>Microdisk Resonator</th>
<th>DSR</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q$</td>
<td>$2.22 \times 10^4$</td>
<td>$1.52 \times 10^4$</td>
<td>$1.23 \times 10^5$</td>
</tr>
<tr>
<td>FSR (nm)</td>
<td>22.3</td>
<td>18.8</td>
<td>120</td>
</tr>
<tr>
<td>ER (dB)</td>
<td>18.9</td>
<td>6.9</td>
<td>62.1</td>
</tr>
<tr>
<td>$S$ (nm/RIU)</td>
<td>38.7</td>
<td>63.4</td>
<td>698.5</td>
</tr>
</tbody>
</table>
resonator are listed in Table 2. Compared with the conventional microresonator, the DSR shows a higher Q, and a larger FSR, ER and S, showing the greatest sensing performance.

More interestingly, this DSR device can be extended to a more complex structure, but still realized by a single waveguide. Figure 7 illustrates this cascaded scheme, called the twin-DSR (T-DSR) device. The light launches into the T-DSR from the left side and outputs from the right side through two Bragg grating couplers. This scheme would upgrade the quasi-FSR and ER due to the double Vernier effect.

The first DSR in the T-DSR structure is the same as the aforementioned optimized one, and the second DSR differs from the first one slightly by inducing a small size difference, which leads to a tiny mismatch of their quasi-FSRs. With reference to the double Vernier effect, the quasi-FSR of the T-DSR will be efficiently broadened to more than 600 nm and the ER is also enhanced to more than 100 dB.

Following the same routine, the resonant wavelength shift scheme is also performed and the result shows that the sensitivity of the T-DSR has not been improved compared with the DSR device. It probably means that the sensing performances of our simulated and optimized DSR device are too excellent to be improved further. However, if imperfection issues such as the surface scattering loss and fabrication errors are introduced in practical situations, their sensing properties would be degraded and cannot remain as good as the simulation results. In these cases, the T-DSR devices introducing the second Vernier effect would be definitely helpful to enhance the Q factor and sensitivity to the expected levels.

In conclusion, novel single-waveguide-based DSR and T-DSR biosensors are studied for homogeneous sensing numerically. The former device with a Q factor of $1.23 \times 10^5$, an ER of 62.1 dB, and a quasi-FSR of 120 nm shows a high sensitivity over 698.5 nm/RIU and a low LOD of $1.8 \times 10^{-5}$ RIU. While the latter enhances the quasi-FSR to more than 600 nm and the ER to 70 dB. The theoretical analysis and optimization routine to achieve good sensing performances are included. A high ER combined with a large FSR makes covering the large refractive index change of different bioanalytes convenient. Meanwhile, a larger quasi-FSR would be convenient to multiplex the resonant sensor array to realize multitarget parallel sensing. Our novel single-waveguide-based biosensors meet the demand of biomolecular detection at low concentration with the benefits of a wide measurement range and high sensitivity. Their excellent features would aid in the development of miniature and highly sensitive sensors with potential applications.

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References