Optical biosensors utilizing polymer-based athermal microring resonators

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ABSTRACT

Optical waveguide biosensors are attracting more and more attentions and presenting great potential applications. Polymer-based optical biosensors are promising for their unique advantages: low cost, easy fabrication, possibility of functionalization with chemicals for the detection of biological molecules, and flexible operating wavelength in both the infrared communication wavelength band (1310-1550nm) and the visible wavelength region (500-800nm). Operating in the visible wavelength, the optical biosensing can avoid the high optical absorption loss of water solution, which can hardly be done for Si-based optical sensors. In this paper, an optical biosensor utilizing polymer-based athermal optical waveguide microring resonator is presented. The athermal design of the microring resonator can make the resonant wavelength drift with temperature be greatly reduced, and an optical biosensing platform with high thermal stability can be achieved. The simulation results show that the maximal resonant wavelength drift is -0.0085nm when the temperature varies from 20°C to 65°C and the maximal wavelength drift slope is -0.0009nm/K. With the microring resonators fabricated by using a simple UV based soft imprint technique with self-developed UV-curable polymer PSQ-L materials, experimental investigations on the specific surface detection of target molecules have been preliminarily performed. The results show that the optical biosensors based on the polymer optical microring resonators would have potential applications for label-free surface sensing.

Keywords: Biosensor, microring resonator, polymer waveguide, photonics, optical waveguide

1. INTRODUCTION

Recently, planar integrated photonic devices are receiving more and more attentions and presenting great potential applications, label-free optical biosensing is among one of them[1, 2]. With optical biosensors, people don't need to resort to labor and time-consuming immunoassay method such as enzyme-linked immunosorbent assay (ELISA), greatly saving the analyzing cost. These optical biosensors can be designed in different structures. Among them, microring resonator becomes the main choice of many research groups and institutes due to its distinct advantages, which include small footprint, high sensitivity and so on[3~6].

So far, microring resonators fabricated with different kinds of materials have been reported, where silicon and polymer are two typically important ones. Unfortunately, both of these two materials have high thermal optical coefficient (TOC)[7]. For example, the TOC of silicon is as high as $1.8 \times 10^{-4}/^{\circ}\text{C}$, while that of polymer normally in the same scale with silicon but with negative value. The high material TOC makes these microring resonators very sensitive to their surrounding environmental temperature change. These temperature induced noises will be

superimposed onto the useful signals when performing biosensing, which lowers the signal to noise ratio (SNR) of the measuring system. This will be even more harmful when the useful signals are small.

There are several approaches to circumvent this problem. The straightforward one is to incorporate a temperature stabilization subsystem to mitigate the temperature influence on the microring resonators. But this method would require extra space and energy. The other usual approach is introducing another reference microring placed close to the one performing the sensing function[8, 9]. With this method, the reference microring should be isolated well from the sensing analytes with a cladding layer and it must be guaranteed that both the reference and sensing microring have the same feeling towards the temperature change. All of these require extra fabrication step and good dimensional control.

In this paper, we propose an athermal microring resonator based on polymer, which will be used for optical label-free biosensor. Compared with those built on other material platforms, polymer-based optical biosensors are attractive because of some unique advantages: low cost, easy fabrication, easy surface functionalization with chemicals for the detection of biological molecules, flexible operating wavelength in both the infrared communication wavelength band (1310-1550nm) and the visible wavelength region (500-800nm) and so on. The athermalization is achieved with an all-polymer structure. By this design, the temperature dependant resonant wavelength shift of the microring resonator can be greatly reduced, and an optical biosensing platform with high thermal stability is promising. The simulation results show that the maximal resonant wavelength drift is less than 10pm when the temperature varies from 10°C to 60°C by choosing proper substrate. In the vicinity of the room temperature, 20°C for example, this wavelength variation can even be neglected. A model is built to estimate the wavelength shift caused by the binding events happening on the functionalized surface of the microring resonator. By comparison, the noise level of temperature is found to be several tens of times less than that of the sensing signal. The results indicate that the proposed all-polymer microring resonators would have good potential in label-free biosensing.

2. TEMPERATURE CHARACTERISTICS OF MICRORING RESONATOR

The resonant condition of microring resonator (MRR) can be expressed as[10]:

$$n_{eff}L = m\lambda_R \quad (1)$$

where n_{eff} is the effective refractive index of the guided mode, L is the perimeter of the MRR, λ_R is the resonant wavelength and $m(=1, 2, 3, \dots)$ is the resonant series. By differentiating the equation (1) with respect to temperature T , the temperature dependent wavelength shift slope of the MRR can be derived as:

$$\frac{d\lambda_R}{dT} = \frac{\lambda_R}{n_{eff}} \left(\frac{dn_{eff}}{dT} + n_{eff}\alpha_{sub} \right) \quad (2)$$

where $\frac{dn_{eff}}{dT}$ is the TOC of waveguide, and $\alpha_{sub} = \frac{1}{L} \frac{dL}{dT}$ is the thermal expansion coefficient (TEC) not of the waveguide, but of the substrate, because the thickness of the waveguide layer is much less than that of the substrate[11]. This equation indicates that athermal MRR which shows no temperature dependent resonant wavelength can be realized by properly selecting the substrate and waveguide material to satisfy the following condition:

$$\frac{dn_{eff}}{dT} + n_{eff}\alpha_{sub} = 0 \quad (3)$$

The effective TOC of polymer waveguide mode is negative and in the same level with its material TOC ($\sim 10^{-4}/^{\circ}\text{C}$). By selecting the substrate TEC with positive and the same magnitude as the effective TOC of polymer waveguide mode, the athermal condition can be satisfied. The TEC of polymer materials is about $0.5\sim 3.9\times 10^{-4}/^{\circ}\text{C}$ [12, 13], so it is possible to realize the athermalization of microring resonator with all-polymer structure.

Through transforming the equation (2), and integrating with respect to dT from T_0 to T , the resonant wavelength shift is obtained as:

$$\Delta\lambda_R = \lambda_R - \lambda_{R0} = \frac{\lambda_{R0}}{n_{eff0}} \{n_{eff} \exp[\alpha_{sub}(T - T_0)] - n_{eff0}\} \quad (4)$$

where λ_{R0} and n_{eff0} are the resonant wavelength and the effective refractive index at T_0 , respectively.

3. TEMPERATURE DEPENDENCE OF MRR WITH SILICON AND POLYMER SUBSTRATE

By taking into account the polymer material refractive index, water absorption loss, the polymer material optical loss, the waveguide bend loss, the scattering loss and the single mode transmission, the racetrack microring resonator is designed as Fig. 1. The parameters are as follows: the refractive index of polymer waveguide core is $n_{core}=1.52$ with TOC of $-2.4\times 10^{-4}/^{\circ}\text{C}$. The refractive index of under cladding is $n_{cladding}=1.45$ with TOC of $-2.2\times 10^{-4}/^{\circ}\text{C}$ [14]. Because this work is designed for biosensing, water acts as upper-cladding with the index $n_{water}=1.3105$. The TOC of water is $-1.0\times 10^{-4}/^{\circ}\text{C}$. The waveguide width is $W=2.3\mu\text{m}$. The waveguide height is $H=2.1\mu\text{m}$ with a slab layer which has thickness of $S=0.2\mu\text{m}$; the radius of bend waveguide is $R=350\mu\text{m}$; the straight waveguide length of the coupling region is $L=150\mu\text{m}$ and the distance between the two straight waveguides is $\text{Gap}=1.0\mu\text{m}$. It is noted that currently we still use the telecommunication wavelength 1550nm , at which water has high absorption. This needs to be taken into consideration when designing the microring resonator. It can be improved in the future by switching the working wavelength to visible wavelength region.

Fig.1 Schematic structure of racetrack waveguide microring resonator

3.1 Temperature dependence of MRR with silicon substrate

The polymer waveguide devices are usually fabricated on the silicon substrate, which has $\text{TEC} = 2.63\times 10^{-6}/^{\circ}\text{C}$. For $T=20^{\circ}\text{C}$ as the reference temperature, the transmission spectrum from the drop port of the racetrack microring resonator at different temperature are plotted in Fig. 2. It can be seen that the resonant wavelength shifts to shorter wavelength. This is because the effective refractive index of the waveguide will

decrease when the temperature increases due to the negative TOC of the polymer. According to equation (1), the resonant wavelength with the same resonant series becomes shorter. From Fig. 2 the resonant wavelength shifts at $T=40^{\circ}\text{C}$ and $T=60^{\circ}\text{C}$ are -5.008nm and -10.015nm compared with the one at reference temperature $T=20^{\circ}\text{C}$. The resonant wavelength dependence on the temperature is as high as $0.21\text{nm}/^{\circ}\text{C}$, which would induce high temperature noise into the resonant wavelength measurement results.

Fig.2 Transmission spectra from drop port of microring resonator with silicon substrate and water up-cladding at different temperatures

3.2 Athermalization of all-polymer MRR

The basic reason for the high temperature dependence of polymer microring resonator with a silicon substrate is that the TEC of silicon substrate is two times of magnitude less than the effective TOC of polymer waveguide. It can hardly have influence on the total thermal effect. However, if we adjust the equation (3) to (5), it can be seen that athermalization of polymer MMR can be realized with proper substrate TEC to counteract the resonant wavelength shift induced by the negative effective TOC.

$$\alpha_{sub} = -\frac{1}{n_{eff}} \frac{dn_{eff}}{dT} \quad (5)$$

Figure 3 gives the TEC of substrate for athermalization of the PSQ polymer based MMR with temperature change from 10°C to 60°C . It can be seen that the TEC of substrate should be $1.614\sim 1.624\times 10^{-4}/^{\circ}\text{C}$ for the athermal condition.

Fig.3 Required TEC of substrate for athermallization at different temperatures

Fig. 4 Resonant wavelength shift versus temperature with different substrate TECs

Figure 4 shows the resonant wavelength shift versus temperature with TEC of substrate near $1.617 \times 10^{-4}/^\circ\text{C}$. It can be seen that the temperature dependence of MRR with all-polymer structure (polymer substrate) is substantially suppressed compared with that using silicon substrate. For example, as the TEC of substrate is $1.6191 \times 10^{-4}/^\circ\text{C}$, the resonant wavelength shift is suppressed within the scope of 4pm--8pm with temperature ranging from 10°C to 60°C. In the vicinity of the normal temperature for us to perform biosensing, 20°C for example, it is even smaller. The temperature independent condition is satisfied basically. Moreover, it also shows that near this temperature, we have relatively large freedom on choosing the substrate with proper TEC. Besides, we have estimated the influence of fabrication error on this temperature dependent value, which is shown in Figure 5. Near 20°C, $\pm 0.1\mu\text{m}$ width variation of the waveguide almost has no influence on the temperature dependent wavelength shift, thus it means that our proposed structure has large tolerance on the fabrication error.

Fig. 5 Resonant wavelength shift versus temperature for different waveguide widths

4. ESTIMATION OF THE RESONANT WAVELENGTH SHIFT CAUSED BY SURFACE SENSING

The temperature noise level can be compared with the desired signal induced by the surface sensing. In order to calculate this SNR value, an optical waveguide model with a uniform biomolecular layer is built with FIMMWAVE (Photon Design Ltd), in which the refractive index of this layer is chosen to be 1.45. The schematic picture is shown in Fig. 6. With this model, we are able to estimate the resonant wavelength shift due to the affinity of the targeted analytes to the bioreceptors immobilized on the waveguide surface of the MRR. The simulation result is shown in Fig. 7. It can be seen that both TE and TM mode have similar responsivity during surface sensing. For a monolayer of biomolecules attached to the MRR's surface, which typically is a number of nanometers, the resonant wavelength shift of MRR will be around hundreds of pm. If this is compared with the temperature noise level in Fig. 5, the later can almost be neglected. The above results indicate that we can perform biosensing with the fabricated device itself without other temperature stability subsystem or reference ring.

Water

Fig. 6 The optical model for the surface sensing

Fig. 7 The resonant wavelength shift of the MRR with the thickness of biomolecular layer.

5. PRELIMINARY FABRICATION AND MEASUREMENT RESULTS

Currently, we are developing a simple UV based soft imprint technique, with which the polymer waveguide patterns can be fabricated fast and efficiently with one step imprint process. As the first step of our investigation on polymer microring resonator-based label-free biosensors, polymer microring resonators with a silicon substrate have been fabricated, as shown in Fig. 8. The obtained microring resonator exhibits a very good optical characteristic, which is shown in Fig. 9. The Q value is as high as 5×10^4 . With these polymer microring resonators, surface biosensing is demonstrated preliminarily with protein A's affinity pair, human-IgG. The polymer microring resonators are functionalized efficiently with protein A molecules through physical immobilization method after careful investigation of the physicochemical and chemical properties of their surface. As shown in Fig. 10, the polymer microring resonator-based biosensors exhibit good responsivity to the antibody-antigen combinations. As for the athermal polymer microring resonators, there are still some challenges to their fabrication. The difficulty lies in the TEC matching between the waveguide layer and polymer substrate, and the proper polymer substrate material availability. These fabrication problems are currently under investigation.

Fig. 8 The fabrication process of UV based soft imprint technique.

Fig. 9 The transmission of the microring resonator at the drop port for TE mode.

Fig. 10 Real-time monitoring of the resonance peak of the microring resonator-based sensor with the flowing human-IgG solution.

6. CONCLUSION

In this paper, we present the design for a microring resonator with all-polymer structure. We found that by replacing the waveguide substrate with proper TEC, the device's sensitivity towards temperature can be greatly reduced. This temperature induced noise is much less than the desired optical signal of the surface sensing and thus can be neglected. Microring resonator with Q value as high as 5×10^4 is obtained through a simple UV based soft imprint technique. With the polymer microring resonators, experimental investigations on the specific surface detection of target molecules have been preliminarily performed. The results shows that the optical biosensors based on the polymer optical microring resonators would have potential applications for label-free surface sensing.

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