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Optimization of figure of merit in label-free biochemical sensors by designing a ring defect coupled resonator

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ABSTRACT

We propose a high figure of merit (*FOM*) biochemical sensor by designing a ring defect coupled resonator (RDCR) based on photonic crystal (PhC) slab. The design consists of ring resonant cavity which is coupled in and out with ring and line defect PhC structure. By a three dimensional finite-different time-domain (3D-FDTD) method, we demonstrate that the quality (*Q*) factor is greatly enhanced by altering the radius of air holes inner the ring resonant cavity and adjusting the width of line defect waveguide. In this paper, we obtain a highest *Q* up to 10^7 through numerical calculations. Even though water absorption at telecom wavelength range and random roughness of fabrication is considered, a *Q* of ~33,517 can be achieved. Simultaneously the proposed sensor possesses sensitivity (*S*) of 330 nm/RIU (refractive index unit), resulting in *FOM* of ~8000. Moreover, a minimal detection limit (DL) is obtained as good as 1.24×10^{-5}. Therefore, these suggest that this design is a promising candidate for label-free biochemical sensing in medical diagnosis, life science and environmental monitoring.

1. Introduction

In the past few decades, due to the robust characteristics such as ultracompact size, high sensitivity, accurate detection limit and easily integrated, optical refractive index (RI) sensors are widely researched for a large number of applications and dominant among the commercial landscapes of current sensing technologies. So far, optical RI sensors include surface plasmon resonance (SPR) sensors [1–3], long-period fiber grating (LPFG) sensors [4,5], ring resonators [6–13], micro-tube [14–16] and photonic crystal structure sensors [17–31]. A large number of sensors are used as biochemical sensors [3,6–17,19,21,24,27–29]. In these sensors, optical resonance peaks can be easily observed. That is, a change in RI around the region probed by resonant mode causes a relevant wavelength shift of optical sensor, and this change in resonant wavelength is converted to the sensing signal.

As shown in Table 1, micro-tube resonator sensors [14–16] and PhC-based sensors [17–26] have overall larger *Q* factor and sensitivity. The *Q*-factors of most PhC geometries are of 10^3–10^4 and the *S*'s are around 100–1500 nm/RIU at around 1550 nm wavelength, resulting in figure of merit ($FOM=S{\bullet}Q/\lambda_0$) are of 100–5000, where *S*, *Q* and λ_0 represent the sensitivity, quality factor and resonant wavelength, respectively. For example, Dorfner et al. [21] presented the design of L3 nanocavity coupled to photonic crystal waveguide for optical biosensor where *Q* factor of 6788 and *S* of 104 nm/RIU were obtained. Wang et al. [25] demonstrated *S* of 900 nm/RIU in slot double-beam cavities, whereas the *Q* factor was limited to 700. Yang et al. [26] demonstrated a nano-slotted parallel multibeam cavity which possesses *S* exceeding 800 nm/RIU and *Q* exceeding 10^7. Taking water absorption into consideration at telecom wavelength range, the *Q* of the sensor is limited to 10^4, resulting in *FOM* of ~5000. In order to enhance the *FOM*, we must increase the product of *S* and *Q*. However, the trade-off between *S* and *Q* limits *FOM*; we can make the optical mode more localized in the waveguide medium to achieve enough high quality factors, but simultaneously we must make the optical mode overlap strongly with the detecting target to obtain high sensitivity.

In this paper, we propose a novel paradigm employing photonic crystal ring defect coupled resonator (RDCR) for medical diagnosis and life science. We make optical mode more localized to obtain high *Q* by adjusting the radius of air hole and the width of waveguide. Simultaneously, we also make optical mode overlap strongly with the detecting target to enhance sensitivity.

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Table 1
Q factor, *S*, and *FOM* of Various Optical Index Sensors.

Sensing structure		Ref.	Q factor in water (At Telecom Range)	Sensitivity (nm/RIU)	*FOM*
SPR	Gold mushrooms	[3]	200	1015	108
Whispering-gallery mode(WGM) based	Microring	[6–13]	10^3–10^4	70–200	45–142
	Micro-tube	[14–16]	10^2–10^4	100–1100	55–8000
PhPhC based	1D nanobeam	[17]	$\sim 10^4$	~100	~645
	2D slab	[18–22]	10^3–10^4	100–300	200–645
	PhC slot	[23–26]	$\sim 10^4$	490–1500	300–5000

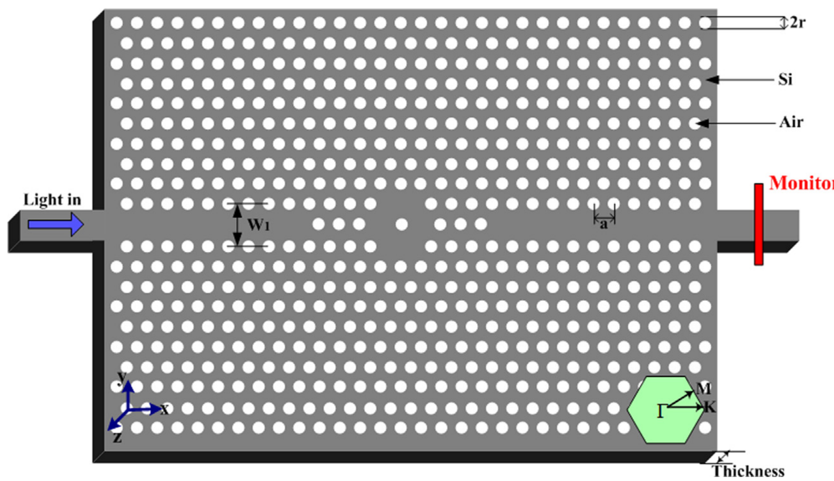

Fig. 1. 3D illustration of the initial ring defect coupled resonator, where $a=348$ nm, $r=0.34a$, $T=0.55a$, $W_1=\sqrt{3}a$.

The extensive simulation results demonstrate that the RDCR can possess high *Q* up to 10^7 in air medium when r_c and *W* equal to 0.40*a* and 0.985W_1, respectively. Even if we consider the absorption of water and random roughness of fabrication at telecom wavelength range in simulation, a *Q* factor up to 33,517 can be obtained. We alter refractive index with $n=1.315$, 1.330 and 1.345, corresponding to deuterium water ($n_{1.330}$) and glycerol solutions ($n_{1.345}$), and the sensitivity *S* of 330 nm/RIU is calculated, resulting in *FOM* of ~8000. This is, to the best of our knowledge, the first geometry photonic crystal sensor structure that can lead to high *FOM*.

2. Ring defect coupled resonator design

The schematic diagram of the initial RDCR based on ring and line defect PhC slab structure is shown in Fig. 1. Compared with the pillar-array based PhC [22], the structure employs triangular lattice, hole-array PhC slab with large enough photonic band-gap (PBG) and small vertical loss (Fig. 1). In this paper, triangular lattice air holes are arranged in a silicon slab ($n_{si}=3.48$), where part of air holes is removed in order to form a ring and line defect waveguide. We simulate the RDCR structure by using the open source 3D-FDTD software Meep. In the simulation process, light source is placed at the head of the input line defect waveguide and monitor is placed at the end of the output line waveguide. We obtain the transmittance spectra through dividing the output power detected with the monitor by the input power of the source. We set resolution to 20 (that is, with a grid spacing of *a*/20, where *a* represents the lattice constant). The TE Gaussian-pulse source is used and run for several iterations. One-spatial unit thick perfectly matched layer (PML) which surrounds the simulation area absorbs the fields leaving the simulation region to implement reflections.

As shown in Fig. 1, the lattice constant *a* equals to 348 nm and the holes radius *r* is 0.34*a* (118 nm). The slab thickness, denoted as *T* and realized on silicon slab waveguide, equals to 0.55*a* (191 nm). Fig. 1 shows detailed design about the structure parameters including lattice constant, radius of holes, and thickness of PhC slab. The simulation results of the light propagation through the initial RDCR are showed in Fig. 2, in which we can find that the leakage of light is suppressed in out-plane direction (vertically) and the TE-like polarized light is coupled into the ring waveguide in-plane direction (horizontally). Fig. 3 shows the transmission spectra of initial RDCR and perfect PhC. As can be seen in Fig. 3, the effective working frequency of guided mode with the PBG is between $0.213(2\pi c/a)$ and $0.313\ (2\pi c/a)$, which is sufficiently wide for the sensor design. In initial RDCR design, the results show several different resonant modes at normalized frequency of $0.2261(2\pi c/a)$, $0.2311(2\pi c/a)$, $0.2646(2\pi c/a)$, $0.3043(2\pi c/a)$, and $0.3075(2\pi c/a)$, which correspond to resonant wavelengths of 1816.67 nm, 1777.36 nm, 1552.34 nm, 1349.82 nm, 1335.75nm, respectively. We choose the resonant frequency of $0.2646(2\pi c/a)$ to observe the shift of resonant wavelength when the structure and the refractive index are altered, respectively. By numerical calculations, the *Q* factor of resonant frequency 0.2646 $(2\pi c/a)$ surrounded by red dashed equals to 6.02×10^6.

The *Q* factor of a cavity is determined by the energy loss per cycle versus the energy stored. The energy loss includes mainly reflection loss and the absorption loss of cavity material. Therefore, to improve the *Q* factor of the RDCR design, we should minimize the energy loss. With the RDCR structure, the corresponding *Q* factor can be given by [18,32]:

$$\frac{1}{Q}=\frac{1}{Q_{couple}}+\frac{1}{Q_{loss}} \quad (1)$$

where Q_{couple} represents the lifetime, that is, light can decay from the cavity into the waveguide, and Q_{loss} refers to materials