CMOS compatible multichannel mid-infrared photonic crystal sensor

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Abstract: We propose a multichannel two-dimensional optical chemical sensor in a photonic crystal (PhC) slab. The device is composed of four cavities with a center wavelength at 3.3 μm, and the channels are spaced by 10 nm. The sensor is designed on an 800-nm-thick silicon-on-insulator platform for standard CMOS technology. The optical characteristics of the nanocavity structure are simulated by 3-D finite difference time-domain (FDTD) method. The transmittance of each channel is about 39%, with non-uniformity of transmittance across channels less than 0.25 dB. The capability of the sensor is demonstrated by detecting carbon tetrachloride and benzene solutions, and shows a sensitivity of 209.2 nm/RIU.

Key words: photonic crystal, sensor, multichannel, mid-infrared

PACS: 07.07. Df Sensors, 42.70. Qs Photonic bandgap materials, 42.82. Gw Other integrated optical elements and systems

CMOS兼容的中红外多通道光子晶体传感器

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摘要：提出了一种基于光子晶体的二维多通道光学化学传感器。该器件由波长为3.3 μm的四个腔组成。各通道工作波长间隔为10 nm。该传感器采用800 nm厚的绝缘体上硅材料，可利用标准CMOS技术加工。通过三维时差有限差分法对微腔结构的光学特性进行模拟。每个通道的传输效率为39%，通道之间的传输效率不一致性小于0.25 dB。该传感器的功能为检测四氯化碳和苯溶液浓度，其灵敏度为209.2 nm/RIU。

关 键 词：光子晶体；传感器；多通道；中红外

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Introduction

In recent years, chemical and biological sensor arrays using photonic crystals have been vigorously studied because of their potential for nanophotonic label-free environmental monitoring and biomedical detection [1-12]. The mid-infrared wavelength range (2-20 μm) represents the characteristic absorption fingerprints of most molecules. For instance, aromatic C-H stretch, which is stable in structure, difficult to decompose, and highly toxic, has a strong absorption at λ = 3.3 μm [9]. The silicon-on-insulator (SOI) structure with a 3-5 μm transmission window is an ideal material to design PhC sensor to detect aromatic compounds [4].

With photonic band gaps, PhC can afford us complete control over light propagation by preventing light from propagating in certain direction with specific frequencies. Nevertheless, the actual fabrication of a three-dimension periodic structure remains difficult. So PhC slabs using two-dimensional periodicity combined with vertical index-guiding are proposed. By introducing line and point defects in PhC slabs, one can create waveguides [3], cavities [5-7], bends [8-9], splitters [10] and filters [11-13] of compact size. Frequency-domain plane-wave expanded method is used for the solution of partial differential equations to find band structure ω(k) and the asso-
1 Design and Optimization of Sensor

The schematic of the designed multiport in-plane sensor is depicted in Fig. 1, which consists of a bus waveguide, drop waveguides, and cavities. Two 60° bend line defects are introduced into multichannel operation.

![Schematic structure of the designed multiport in-plane sensor](image)

**Fig. 1** Schematic structure of the designed multiport in-plane sensor

The band structure for a crystal consisting of air holes in silicon ($\varepsilon = 11.792$) with radius $r = 0.4a$ is plotted in Fig. 2. There is a gap between the first and second TE bands, from $\omega a/2\pi c = 0.248$ to $\omega a/2\pi c = 0.405$ with the bandwidth as 47.9%. There are light cones ($\omega \geq c|\mathbf{k}|$) for the extended modes propagating in the air or SiO$_2$ substrate, where $\mathbf{k}$ is the horizontal wave vector. As the light cone exists, we select our operating wavelength $\lambda = 2\pi c/\omega = 3.3\mu m$ to lie at frequency $\omega a/2\pi c = 0.291$. So we can calculate the lattice constant as $a = 960nm$, and the air hole radius $r = 0.4a = 384nm$. We set the thickness of slab as 800nm, which is thick enough for the fundamental mode to be well confined and thin enough to forbid higher-order modes to propagate within the slab.

A photonic crystal sensor is composed of a cavity and two waveguides, i.e., the bus waveguide and the drop waveguide. For multi-channel operation, two 60° bend line defects are introduced. We apply a simple optimization method, which makes the bend mode as symmetric as the straight waveguide mode'. The two air holes at the corner are of radius $R_c=300\ nm$, and they are shifted 50 nm away in opposite directions along the symmetric axis of the bend. The mechanism for improvement of transmission is to match both the symmetry of modes and their wave numbers in the straight waveguide and the bend”. Fig. 3(a) and 3(b) show the energy distribution in the bends at $\lambda = 3.3\ \mu m$. The scattering at the bend corner has been efficiently alleviated. The transmittance in bend waveguide at $\lambda = 3.3\ \mu m$ is 85% compared to normal straight waveguide.

![Band diagram for the PhC slab](image)

**Fig. 2** Band diagram for the PhC slab.

![The energy distribution of (a) the normal bend and (b) the optimized bend](image)

**Fig. 3** The energy distribution of (a) the normal bend and (b) the optimized bend.

We can design a cavity by removing or adjusting some holes around a single point. Resonant phenomena in cavities are dependent on the precise geometric properties, such as size and shape. To excite the whispering gallery mode (WGM)’, we remove the central air hole and reduce the radius of the border holes in the cavity which is denoted as $R_b$. Such bound modes are guided by means of repeated reflections. After infinite repetitions, absorption, scattering, and material dispersion could be neglected. The structure schemes diagram and energy distribution of the hexapole mode are shown in Fig. 4(a). Due to the hexagonally symmetric WGM field distribution, the phases of adjacent lobes are opposite to each other, so destructive interference occurs and decreases the horizontal radiation. Near the resonant frequency, light from the input waveguide can couple into the cavity, and the cavity in turn can couple into the output waveguide efficiently when $Q_0 = Q_i$ is obtained’,” where $Q$ is vertical quality factor representing the emission phenomena occurring between the
The desired resonant frequency could be $m \lambda = \lambda_{res}$ with $\lambda$ being the wavelength in the cavity and $R$ being the radius of the cavity. The resonant wavelength is sensitive to the refractive index and can be obtained when $\lambda_{res}$ is in the range of $3.30$ to $3.32$ μm in air, changes of resonant wavelength and changes of concentration are shown in Fig. 6 (b). The sensitivity of a sensor is defined as the rate of resonant wavelength shifts with respect to the change in the refractive index, with the corresponding unit of nm/RIU. The sensitivity is calculated as 209.2 nm/RIU. This linear red-shift could be explained as the perturbation theory for linear Hermitian eigenproblem. The kernel of the Maxwell equations for a harmonic mode in a mixed dielectric medium is a differential equation for electric field $E(r)$, given by:

$$\nabla \times \nabla \times E(r) = \left( \frac{\omega}{c} \right)^2 \varepsilon(r) E(r),$$  (1)

By applying the perturbation procedure to equation (1), we obtain a formula for the frequency shift $\Delta \omega$ that results from a small perturbation $\Delta \varepsilon$ of the dielectric function $\varepsilon$:

$$\Delta \omega = -(\omega/2) \cdot \left( \int d^3 \Delta \varepsilon(r) |E(r)|^2 \right)/\left( \int d^3 \varepsilon(r) |E(r)|^2 \right) + o(\Delta \varepsilon^2),$$  (2)

In this equation, $\omega$ and $E(r)$ are the frequency and the mode profile for the perfectly linear and unperturbed dielectric function $\varepsilon$. Consider the case of the holes with a refractive index $n = \varepsilon^{1/2}$, in which the index is perturbed in some regions by an amount $\Delta n$. The volume integral in the numerator of equation (2) has nonzero contributions only from the perturbed regions. The fractional change in frequency is equal to the fractional change in index multiplied by fraction of the electric-field energy inside the perturbed regions:

$$\Delta \omega \omega = -F \cdot \Delta n/n,$$  (3)

$F$ is a sensitivity function related to the mode profile for the dielectric function $\varepsilon$, and it is constant since the
cavities and free space, and $Q_h$ is horizontal quality factor representing the trapping phenomena occurring between the waveguides and the cavities. The total quality factor $Q$ for a coupled cavity can be written as $Q^T = Q_a + Q_b$. The expected high quality factor is deduced by the decaying signal in the simulation, because the electromagnetic fields cannot completely decay in the simulation in a reasonably time. The largest $Q \sim 1.2 \times 10^6$ is obtained when $R_i$ is 200nm. The cavity works as a WGM cavity, and the resonant peak is dependent on the cavity diameter $D = m \lambda/2n_{eff}$, where $m$ is the order of peaks. The desirable resonant frequency could be reached by shifting the border holes to change the diameter of the cavity.
change of the mode profile is negligible in this case shown in Fig. 4 (b). The change is proportional to the analyte concentration and represents quantitative information about the concentration of the chemical.

![Image](image.png)

Fig. 6 (a) The shifts in the resonant wavelength of the sensor in pure CCl₄ solutions, pure benzene solutions and mixture of these solutions with different concentrations. (b) The linear fits of four channels of the sensor (with center wavelength \( \lambda = 3.29, 3.30, 3.31 \) and 3.32 \( \mu \text{m} \) in air) between changes of resonant wavelength and changes of concentration.

The previously reported PhC sensors have achieved sensitivities of 363.8 nm/RIU \(^{(9)}\), 396 nm/RIU \(^{(20)}\), 460 nm/RIU \(^{(19-22)}\), 500 nm/RIU \(^{(1)}\), higher than the sensitivity of our sensors. However, these sensors have only one channel. A reported multichannel PhC sensor \(^{(12)}\) is able to detect four different analytes (with refractive index \( n = 2.5, 2.175 \) and 1.5) in four channels, respectively. But this sensor is unable to detect the change of the concentration of analytes (with minor change of refractive index) thus no sensitivity data is shown in this work, which limits the practical application. Besides, the non-uniformity of transmission across the four-channel device in this work is rather large, with the transmittance of four channels ranging from 35% to 95%. In our work, we have achieved a four-channel sensor, which is able to detect the concentration change of mixture of carbon tetrachloride and benzene solutions with a sensitivity of 209 nm/RIU. And the nonuniformity of transmittance across the four channels in our work is very small, less than 0.022 (i.e., 0.25 dB).

### 2 Potential Fabrication and Application

The fabrication of the proposed silicon PhC sensor can be realized on an SOI platform using electron beam lithography (EBL) and inductively-coupled plasma (ICP) dry etching which includes the following steps. First, SOI wafer with appropriate top-silicon-thickness should be chosen. Then, electron-beam resist (e.g., ZEP520) is spin coated on top of an SOI wafer. Then after exposure to electron beam, the developing and fixing steps are carried out. After that, ICP etching in a gas environment of SF₆ and C₄F₈ is used to form the air holes in PhC sensor. Finally, by removing the resist, the fabrication of PhC sensors is completed. As for the mass production in the future, EBL is replaced by ultra-violet (UV) lithography. First, a mask is fabricated according to the design parameters. Then, using UV lithography technique and the following ICP etching technique, thousands of PhC sensors are fabricated on an SOI wafer. Finally, slicing, encapsulation and testing of PhC sensors are carried out.

Standard CMOS process can introduce variations to hole size because of optical proximity effects. The variations in hole size can be considered as deviations from the designed lattice, affecting out-of-plane loss and the photon lifetime of the cavity. Different hole radius, ranging from 374 nm to 394 nm, are simulated to evaluate the tolerance of the sensor, and the results are listed in Table 2. These simulations verify that the sensitivity function is stable with a level about 200 nm/RIU though resonant wavelength has shifted as expected. The stability of the sensitivity function can be explained by the unchanged energy distribution of the hexapole whispering gallery mode and quality factor of the sensor. The tolerance of the sensor is large enough to be fabricated by deep UV lithography for the batch production nowadays.

<table>
<thead>
<tr>
<th>Table 2 Resonant wavelengths and sensitivity function versus R</th>
<th>μm</th>
<th>nm/RIU</th>
<th>Q</th>
<th>P(nm/RIU)</th>
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<tbody>
<tr>
<td>357</td>
<td>3343.14</td>
<td>1.044.81</td>
<td>203.7</td>
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<tr>
<td>379</td>
<td>3323.79</td>
<td>1.204.23</td>
<td>209.9</td>
<td></td>
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<tr>
<td>384</td>
<td>3300.02</td>
<td>1.335.04</td>
<td>209.2</td>
<td></td>
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<tr>
<td>398</td>
<td>3280.28</td>
<td>1.120.02</td>
<td>209.9</td>
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<tr>
<td>394</td>
<td>3257.9</td>
<td>1.059.84</td>
<td>209.9</td>
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</tbody>
</table>

Before the successful application to label-free environmental monitoring and biomedical detection, further work should be done. In this work, we use mixture of carbon tetrachloride and benzene solutions as an example. We need to broaden the working waveband in order to detect more kinds of chemical compounds and molecules. Furthermore, sensitivity should be raised to detect minor change of concentration. In addition, integration of sensors with sources and analyzers are necessary, which includes broadband mid-IR source, polarizer, input fiber, PhC sensor, output fiber, optical spectrum an-
alyzer. Finally, reliability and portability should be considered in future applications.

3 Conclusion

We have proposed a four-channel SOI based 2-D photonic crystal optical sensor suitable for label-free sensing. First, our simulation shows a transmission of 60% for the linear defect waveguide (i.e., the bus waveguide) at $\lambda = 3.3 \, \mu m$. Second, we have designed cavities with hexagonally symmetric WGM field distribution reaching a quality factor of about $1.2 \times 10^6$. And then, the output bend waveguide is optimized to obtain 85% transmission compared to normal straight waveguide. Finally, the nonuniformity of transmittance across the four-channel device is less than 0.25 dB, and a sensitivity of 209.2 nm/RIU is presented. The sensitivity function remains stable when the hole diameter varies ±10 nm. This sensor has potential applications in nanophotonic label-free environmental monitoring and biomedical detection.

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References