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Infiltrated photonic crystal cavity as a highly sensitive platform for glucose concentration detection

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A B S T R A C T

A Bio-sensing platform based on an infiltrated photonic crystal ring shaped holes cavity-coupled waveguide system is proposed for glucose concentration detection. Considering silicon-on-insulator (SOI) technology, it has been demonstrated that the ring shaped holes configuration provides an excellent optical confinement within the cavity region, which further enhances the light-matter interactions at the precise location of the analyte medium. Thus, the sensitivity and the quality factor (Q) can be significantly improved. The transmission characteristics of light in the biosensor under different refractive indices that correspond to the change in the analyte glucose concentration are analyzed by performing finite-difference time-domain (FDTD) simulations. Accordingly, an improved sensitivity of 462 nm/RIU and a Q factor as high as 1.11×10^5 have been achieved, resulting in a detection limit of 3.03×10^{-6} RIU. Such combination of attributes makes the designed structure a promising element for performing label-free biosensing in medical diagnosis and environmental monitoring.

1. Introduction

Optical sensors that provide instantaneous detection and quantification of biological analytes have emerged as a field of great interest due to their promising characteristics such as safety in an inflammable and explosive environment, immunity to electromagnetic interference, rapid response speed and the remote on-line sensing capability. The most well exploited techniques for optical sensing are based on the principle of surface plasmon resonance (SPR) [1,2], colorimetric resonances, and interferometry methods [3]. Among those optical resonance technologies, responsive photonic crystal (PhC) based sensors have attracted substantial attention because of their miniaturized size, their high spectral sensitivity, minimal sample preparation without fluorescence labeling and the possibility of integrating MEMS (Micro-Electro-Mechanical Systems) [4]. These highly ordered devices can be fabricated using microelectronic fabrication techniques, and can be easily integrated with microelectronics, microfluidics [5,6] and other kinds of photonic devices. A typical planar photonic crystal (PhC) consists of cylindrical air holes with defined lattice constant in a thin silicon membrane. PhC sensors provide strong light confinement within the analyte itself due to the photonic band-gap effect [7]. Light can be concentrated in a very small volume, leading to a large light-matter interaction [8]. This phenomenon makes the sensor highly sensitive to small refractive index (RI) variations that are produced by biological species immobilization on the PhC pore walls.

The ideal sensing technology should be highly selective and appropriately sensitive to the biological analyte concentrations. Hence, different techniques and setup configurations are constantly being developed and optimized to increase the detection performances. Therefore, a proper PhC design for biosensing is an essential task which should be carefully handled to obtain the required sensing properties. Various designs and configurations of biosensing devices have been proposed and performed using different types of PhC structures such as microcavities [9–14], ring resonators [15] waveguides [16–19], slot waveguides [20,21], heterostructures [22]. They all exploit extremely sensitive resonant conditions for guided modes in the PhC with respect to RI changes in the ambient medium. In practical applications, due to the difficulties in coupling light into the PhC resonator-only system, the waveguide-resonator system is usually preferred. Incorporating with PhC waveguide, coupled microcavities [23–26] provide several advantages in terms of compactness, high sensitivity and quality (Q) factor, easy extension to sensor arrays and

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the capability of parallel measurement [27–29]. Examples of such designs include that of Dorfner et al. [30], who experimentally demonstrated a PhC channel drop filter for fluid sensing applications with a Q-factor of 3000 and a sensitivity of 155 nm/RIU, as well as that of Zhou et al. [31] who have proposed the integration of high transmittance H2 nanocavity and broadband waveguide, the obtained results revealed a RI sensitivity of 131.70 nm/RIU with a Q factor of about 3000. Further, Liu et al. [32] proposed an experimental model of an optical PhC sensor based on a channel-drop configuration, where simulation and experimental results showed a good agreement with RI sensitivity of 153 nm/RIU. It is argued that higher Q factors will contribute to detect a very small shift in the resonance wavelengths. Therefore, maximizing the Q factor of the resonator, will reduce the impact of noise on the determination of the resonance wavelength [33], this would further enhance the sensitivity and accurate the detection limit. However, for sensing applications, the quality factor is not the only crucial parameter to gain higher sensitivities. The detection performances can also be enhanced by conducting improvements in the sensor setup such as temperature stabilization, coupling enhancement and the topology optimization of device geometry (the shape, the size of the holes and the thickness of the Si layer) which further enhance the intensity within the detection area. The alteration of the cavity geometric parameters offers a great structural freedom to tune the sensor optical properties [34,35]. Some critical issues such as achieving high refractive index sensitivity or enhancing light coupling into PhC structures must still be overcome.

In this paper, we report the design and the simulation of an integrated PhC biosensor that is potentially used for glucose concentration detection. Considering silicon-on-insulator (SOI) technology, the designed structure is formed by two waveguides and one cavity system. The device sensitivity is determined by the magnitude of light-matter interaction. Therefore, to achieve higher sensitivities, the optical resonant field needs to be strongly localized and overlapping with the analyte. In this context and in order to enhance the electric field intensity and hence the light-matter interactions within the cavity sensing area, the ring shaped holes cavity configuration is adopted. Results obtained by performing FDTD simulations indicate that by adjusting the ring's width as well as the number of functionalized holes around the cavity sensing area, the sensitivity and the quality factor can be greatly improved. Moreover, we demonstrated that the resonant wavelength mode shifts its spectral position following a linear behaviour when a glucose concentration ranging between 0% and 60% is applied. For the glucose detection, a sensitivity of 462.61 nm/ RIU and a detection limit of $3.03\text{x}10^{-6}$ RIU are observed.

2. Modeling and theory

Mathematically, light propagation in photonic crystals is evaluated by solving Maxwell's equations in a mixed dielectric medium, expressed in Eqs. (1) and (2) E and H are the electric and magnetic field intensities.

$$\nabla \times \mathrm{E}(\mathrm{r},\, \mathrm{t}) = -\frac{\partial}{\partial \mathrm{t}}[\mu_0 \mathrm{H}(\mathrm{r},\, \mathrm{t})] \tag{1}$$

$$\nabla \times \mathrm{H}(\mathrm{r},\, \mathrm{t}) = -\frac{\partial}{\partial \mathrm{t}}[\varepsilon\varepsilon_0(\mathrm{r})\mathrm{E}(\mathrm{r},\, \mathrm{t})] \tag{2}$$

μ is the permeability which is equals to μ_0 as the considered material is non-magnetic and ε represents the permittivity which is usually written as $\varepsilon=\varepsilon_0\varepsilon(\mathrm{r})$, where ε_0 is the permittivity of vacuum and $\varepsilon(\mathrm{r})$ is the relative permittivity of the material.

Eq. (3) is obtained by solving Eq. (1) and inserting it into the time derivative of Eq. (2)

$$\nabla \times \left(\frac{1}{\varepsilon(\mathrm{r})}\nabla \times \mathrm{H}(\mathrm{r},\, \mathrm{t})\right) = -\frac{\partial^2}{\partial \mathrm{t}^2}[\mu_0 \mathrm{H}(\mathrm{r},\, \mathrm{t})] \tag{3}$$

Assuming harmonic time dependence for the magnetic field with (angular) frequency ω.
$\mathrm{H}(\mathrm{r},\, \mathrm{t}) = \mathrm{H}(\mathrm{r})e^{-i\omega t}$, we obtain the master equation for the magnetic field:

$$\nabla \times \left(\frac{1}{\varepsilon(\vec{\mathrm{r}})}\nabla \times \mathrm{H}(\vec{\mathrm{r}})\right) = \left(\frac{\omega}{\mathrm{c}}\right)^2 \mathrm{H}(\vec{r}) \tag{4}$$

where $\mathrm{c} = 1/\sqrt{\mu_0\varepsilon_0}$ is the speed of light in vacuum.

To obtain numerical solutions for these equations, the finite difference time domain (FDTD) method is the best suitable [36]. This method has been one of the most commonly used for simulating pulse propagation through photonic crystal devices [37,38]. After introducing a known initial field and sources into the computational domain, time development of the electric and magnetic field in the structure can be calculated in discrete time steps [39]. The FDTD simulations in this work have been carried out using RSoft software.

In order to study the dispersion diagram and the modal distribution of the field through PhC structure, the plane-wave expansion method (PWE) is applied [40,41]. Using this method the solutions of Eq. (4) are expanded in a truncated basis of plane waves. These plane waves are expressed as a Fourier expansion series in k-space (reciprocal space), which facilitates the computation.

$$H(\vec{r}) = \sum_{\vec{\mathrm{G_i}},\mathrm{N}} \mathrm{h}(\vec{\mathrm{G}}_\mathrm{i}).\hat{\mathrm{e}}_\mathrm{N}.\exp.((\mathrm{i}\vec{\mathrm{k}}+\vec{\mathrm{G}}_\mathrm{i}).\ \vec{\mathrm{r}}) \tag{5}$$

where $\vec{\mathrm{G}}$ is the reciprocal lattice vector and $\vec{\mathrm{k}}$ is a wave vector in the first brillouin zone. N=1 or 2 and $\hat{\mathrm{e}}_1$, $\hat{\mathrm{e}}_2$ are orthogonal unit vectors perpendicular to $(\vec{\mathrm{k}}+\vec{\mathrm{G}}_\mathrm{i})$.

Because of the periodicity of the dielectric constant for PhC $\varepsilon(\vec{r})=\varepsilon(\vec{r}+\vec{R})$ with respect to the real space lattice vector $\vec{R}$, Bloch's theorem can also be applied to expand it in terms of plane waves:

$$\frac{1}{\varepsilon(\vec{r})} = \sum_{\vec{G}} \eta(\vec{G}).\exp\ (i\vec{G}.\ \vec{r}) \tag{6}$$

where and $\eta(\vec{G})$ represents the Fourier transform of the inverse of $\varepsilon(\vec{r})$. It is defined by:

$$\eta(\vec{G}) = \frac{1}{\Omega}\int_{cell}\frac{1}{\varepsilon(\vec{r})}.\exp(-i\vec{G}.\ \vec{r})d\vec{r} \tag{7}$$

Ω designates the unit surface cell.

For 2D-PhC structure and for the TE polarization the eigen value equation is given by:

$$\sum_{\vec{G'}} |\vec{k}+\vec{G}|\left|\vec{k}+\vec{G'}\right|\eta\left(\vec{G}-\vec{G'}\right)h_1\left(\vec{G'}\right) = \frac{\omega^2}{c^2}h_1(\vec{G}) \tag{8}$$

The Fourier coefficients of the inverse of $\varepsilon(\vec{r})$ for ring-shaped holes are given by [42,43]:

$$\eta(\vec{G}) = \begin{cases} \frac{1}{\varepsilon_b} + \frac{\pi}{\Omega}\left(\frac{1}{\varepsilon_a} - \frac{1}{\varepsilon_b}\right)(R_{out}{}^2 - R_{in}{}^2), & \vec{G}=0 \\ \frac{2\pi}{\Omega G}\left(\frac{1}{\varepsilon_a} - \frac{1}{\varepsilon_b}\right)[R_{out}J_1(G(R_{out})) - R_{in}J_1(G(R_{in}))], & \vec{G}\neq 0 \end{cases} \tag{9}$$

where J_1 is the Bessel function of the first kind, R_{in} and R_{out} are the inner and the outer radius of air rings, respectively. $\varepsilon_a=1$ is the dielectric constant of air rings and ε_b is the silicon permittivity. For PhC air holes case $R_{in}=0$ and $R_{out}=r$, where r is the air holes radius.

In this study, the dispersion diagram is computed numerically using BandSOLVE software [44,45]. Fully integrated into the RSoft Component Design Suite, BandSOLVE is ideal for producing band structures for PhC bandgap structures. The simulation engine is based on an advanced optimized implementation of the PWE technique for periodic structures.