Optik 127 (2016) 3480–3483

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.de/ijleo

Lab-on-chip based optical biosensors for the application of dental fluorosis

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ARTICLE INFO

Article history:
Received 24 August 2015
Accepted 11 December 2015

Keywords:
PBG fluorosis

ABSTRACT

Optical biosensors are powerful detection and analysis tool that has vast applications in biomedical research, healthcare, pharmaceuticals, environmental monitoring, and the battlefield. Biosensors consist of a biological entity that can be an enzyme, antibody, or nucleic acid that interacts with an analyte and produces the signal that is measured electronically. A variety of substances including nucleic acids, proteins (particularly antibodies and enzymes), lectins (plant proteins that bind sugar moieties) and complex materials (organelles, tissue slices, microorganism), can be used as the biological components. Fluoride content in drinkable groundwater directly affects the quality of drinking water. In this paper we have demonstrated a 2-dimensional photonic crystal based biosensor with line defect which can detect different fluorides in water. Simulation and analysis has been done for calcium fluoride, cesium fluoride, potassium fluoride, lithium fluoride and strontium fluoride and peak has been observed. One such major detection is to detect dental fluorosis caused by the fluorides present in water. Finite Difference Time Domain (FDTD) method has been used for the analysis. MEEP is Maxwell's Electromagnetic Equation Propagation simulation tool. The application of FDTD method is computation of transmission spectrum. MEEP is simulation package for the computation of transmission/reflection spectra, field patterns, resonant modes & frequencies in dielectric structures.

1. Introduction

Dental fluorosis is a alteration in the advent of the tooth's enamel. These variations can vary from hardlyperceptible white spots in mild forms to staining and pitting in the more severe forms. Dental fluorosis only occurs when younger children devour too much fluoride, from any source, over long periods when teeth are evolving under the gums. The advantageous effects of fluoride on dental caries are due predominantly to the topical effect of fluoride after the teeth have vented in the oral cavity. Biosensors function by coupling a biological sensing element with a detector system using a transducer [1] and biosensor for living cell [2]. Optical biosensors are powerful detection and analysis tool that has vast applications in biomedical research, healthcare, pharmaceuticals, environmental monitoring, and the battlefield [3]. Fluoride is a naturally occurring compound derived from fluorine, the 13th most abundant element on Earth. The basics of knowledge of Fluoride and Causes of fluoride in drinking water [4].

The organic bio molecules get excited from lower energy state to higher energy state, when optical beam is incident and lose their energy in the form of photons and relax to the ground state [5]. Maxwell's Curl equations are expanded in rectangular Coordinate system which results in six coupled Partial Differential Equations. The design of the sensor consists of the two dimensional square lattice waveguide photonic crystal structure in rods (silicon) in air configuration [7].

MEEP (MIT Electromagnetic Equation Propagation). The computational technique used is MEEP, a freely available finite-difference time-domain implementation. MEEP allows 3-D photonic crystal slab (PCS) structures to be simulated with the use of periodic boundary conditions (PBCs) and perfectly matched layers (PMLs) applied to the unit cell. MEEP was used to calculate the instantaneous field energies and distributions, which are used to evaluate the sensing metrics presented [9].

The optical properties of porous silicon PBGs [10] are sensitive to small changes of refractive index in the porous layers, which makes them a good sensing platform capable of detecting binding

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http://dx.doi.org/10.1016/j.ijleo.2015.12.113

Table 1
Transmission spectrum for frequency shift.

Name of the Fluoride	Frequency spectrum (normalized)	
	Peak frequency	Shift in frequency
Water without fluoride	0.2955	–
Calcium fluoride	0.2919	0.0036
Cesium fluoride	0.2733	0.0222
Lithium fluoride	0.2923	0.0032
Potassium fluoride	0.2727	0.0228
Strontium fluoride	0.2913	0.0042

Table 3
Transmission spectrum for wavelength shift.

Name of the fluoride	Wavelength spectrum (normalized)	
	Peak wavelength	Shift in wavelength
Water without fluoride	3.384	–
Calcium fluoride	3.426	0.042
Cesium fluoride	3.66	0.276
Lithium fluoride	3.421	0.037
Potassium fluoride	3.668	0.284
Strontium fluoride	3.433	0.049

of the target molecules to the bioreceptors. The material nanostructure and device configuration that lead to optimum performance of the devices are investigated in detail by modeling the optical response. It is shown that porous silicon based PBG sensors are useful for detecting biological matter, from small molecules to larger proteins.

2. Theory

Photonics has recently become an attractive alternative to electronics for communications and information processing. Devices that use photons rather than electrons as information carriers can benefit from higher speeds and reduced cross talk between optical channels.

Optical nanodevices can now be constructed in standard electronic semiconductor materials, such as silicon on insulator (SOI), GaAs and InP. By combining the need for integrated photonics with the capabilities offered by high-resolution micro fabrication, the field of nanophotonics has emerged. Thus, optical devices that have traditionally been constructed in glass and lithium niobate can now be scaled down using the higher refractive index contrast available in silicon, GaAs, or InP. Ultra-small optical systems can also be integrated, thus realizing for the first time the dream of large-scale multifunctional all-optical chips for information processing. Moreover, since nanophotonics devices are constructed from standard electronic materials, these can be integrated side by side with electronic components, enabling the construction of hybrid systems of higher complexity. On the other hand, nanoscale photonic structures also offer great promise for the investigation of fundamental physical laws that govern the behavior of photons. Strong coupling between light and matter, efficient control of spontaneous emission and enhanced nonlinear optics behavior are only a few examples of the many interesting phenomena that can be explored when light and matter interact at nanoscale dimensions (Tables 1–4).

The periodic variations of dielectric constant in photonic crystals have natural analogy with crystal structure of solid state material such as semiconductors. In the electronic crystals the moving electron encounter periodic variation in electric potential which forces them to occupy closely spaced discrete energy level forming energy bands called valence band, conduction band and forbidden band. If the crystal has perfect structure no electron can exists within the forbidden gap of the crystal.

Likewise photons propagating in photonic crystals encounter periodic variation in dielectric constant which forces them to organize them into different bands called dielectric band, air band and photonic band gap. Photonic crystals without any defect don't permit photons to propagate within the band gap. In order to tailor the conduction properties of semiconductors we add certain impurities materials which give rise p-type and n-type semiconductors. In similar fashion, the optical properties of photonic crystal can be tailored by adding or removing certain amount of dielectric. This analogy justifies the ability of photonic crystals to control the flow of photons the way semiconductors control the flow of electron through them. Thus by appropriate doping, the transmission properties of photonic crystals can be modified which would lead to the development of several new class of optical components.

3. Algorithm

MEEP is Maxwell's Electromagnetic Equation Propagation simulation tool. MEEP has been programmed by D. Roundy, M. Ibanescu, P. Bermel & S.G. Johson at the Massachusetts Institute of Technology (MIT). MEEP is a time domain tool. MEEP tool implements the finite difference time domain method. Simulation in 1D, 2D, 3D & spectral coordinates can be done by using MEEP. The application of FDTD method is computation of transmission spectrum. MEEP is simulation package for the computation of transmission/reflection spectra, field patterns, resonant modes & frequencies in dielectric structures. The transmitted flux can be computed at each frequency ω. For fields at a given frequency ω, this is the integral of the Poynting vector, over a plane on the far side of the photonic crystal structure:

$$P(\omega) = Re\hat{n} \times \int E_{\omega}(x)^{*} \times H_{\omega}(x) \mathrm{d}^{2}x \quad (1)$$

MEEP computes the integral $P(t)$ of the Poynting vector at each time, and then Fourier-transform this to find $P(\omega)$. MEEP computes the flux at the specified regions, and the frequencies that you want to compute. MEEP uses "dimensionless" units, where all εo, μo and c constants are unity. The transmitted amplitude values for corresponding frequency can be extracted from the MEEP output file using the UNIX command 'Grep'. These transmitted amplitude values are plotted against frequency values using MATLAB to obtain the transmission spectrum.

Table 2
Reflection spectrum for frequency shift.

Name of the fluoride	Frequency spectrum (normalized)	
	Peak frequency	Shift in frequency
Water without fluoride	0.2905	–
Calcium fluoride	0.2761	0.0144
Cesium fluoride	0.2721	0.0184
Lithium fluoride	0.2871	0.0034
Potassium fluoride	0.2759	0.0146
Strontium fluoride	0.2861	0.0044

Table 4
Reflection spectrum for wavelength shift.

Name of the fluoride	Wavelength spectrum (normalized)	
	Peak wavelength	Shift in wavelength
Water without fluoride	3.442	–
Calcium fluoride	3.622	0.18
Cesium fluoride	3.676	0.234
Lithium fluoride	3.483	0.041
Potassium fluoride	3.625	0.183
Strontium fluoride	3.495	0.053