Photonics and Nanostructures – Fundamentals and Applications 25 (2017) 46–51

Contents lists available at ScienceDirect

Photonics and Nanostructures – Fundamentals and Applications

journal homepage: www.elsevier.com/locate/photonics

Invited Paper

Enhanced geometries of macroporous silicon photonic crystals for optical gas sensing applications

D. Cardador[a,*], D. Vega[a], D. Segura[a], T. Trifonov[b], A. Rodríguez[a]

[a] Micro i Nanotecnologies, Departament d'Enginyeria Electrònica, Universitat Politècnica de Catalunya, C/Jordi Girona, 31, 08031, Barcelona, Spain
[b] Center for Research in NanoEngineering, CrNE—Universitat Politècnica de Catalunya, UPC, Barcelona 08028, Spain

ARTICLE INFO

Article history:
Received 14 November 2016
Received in revised form 21 March 2017
Accepted 18 April 2017
Available online 10 May 2017

Keywords:
Macroporous silicon
Photonic crystals
Photonic bandgap
Resonant cavity
Gas detection

ABSTRACT

A macroporous silicon photonic crystal is designed and optimized theoretically for its use in gas sensing applications and IR optical filters. Light impinges perpendicularly onto the sample surface (vertical propagation) so a three-dimensional (3d) structure is used. For gas sensing, a sharp resonance is desired in order to isolate an absorption line of the gas of interest. The high Q-factors needed mandate the use of a plane defect inside the PhC to give rise to a resonant mode inside the bandgap tuned to the gas absorption line. Furthermore to allow gas passage through the device, an open membrane is required. This can affect the mechanical resilience. To improve the strength of the photonic crystal the pores are extended after the "active" 3d part. The number of modulations, and the extension length have been optimized to obtain the largest Q-factor with reasonable transmitted power. These proposed structures have been experimentally performed, probing an enhancement of almost an order of magnitude in the Q-factor in respect with the basic case. Simulations considering CO_2 have been performed showing that the proposed structures are promising as precise optical gas sensors.

1. Introduction

Photonic crystals (PhCs) exhibit photonic bandgaps (PBGs) in their optical spectra [1,2], because of the periodical modulation of their refractive index. This feature allows creating resonating cavities, and thus PhCs can be used to create IR filters and devices for the optical detection of gases [3,4]. These cavities are created by placing defects in the periodical structure of the PhC [5]. The detection can be then performed by directly monitoring the absorption of light, or by measuring a frequency shift of the peak. The direct measure method is based on the Beer-Lambert law, which states that the intensity absorption is an exponential function of substance concentration and optical length [6]. Gases, in particular, have strong optical absorption bands at specific wavelengths unique for each gas; its *fingerprint* [6]. Therefore to sense a certain gas, it is necessary to measure the absorption at some of its specific wavelengths. That imposes isolating the absorption line, which can be accomplished with a high Q-factor PhC filter. The main drawback of such method is that to have good sensitivities, long interaction lengths must be attained.

An alternative to the previous methods was reported in other studies [7–9]. In them, it is proposed the use of the slow group velocities that the band structure of carefully crafted macroporous silicon (MPS) PhCs have at the band edges of the PBG. Theoretically this method was shown to work well, but light coupling was shown to be a major problem. Furthermore, losses due to scattering and absorption were also very high as the signal had to traverse a very long silicon structure.

In this paper we study a 3d MPS structure as proposed elsewhere [4,10] for gas sensing, using out-of-plane (vertical) propagation. Although these PhCs are more complex, they can be fabricated using cheap methods, such as electrochemical etching (EE), and are very versatile structures. Furthermore, light coupling into and out of the sample is simpler than for in-plane devices. Additionally, MPS can be made to be inert to ambient conditions and aggressive gases, and are mechanically very stable.

The MPS PhC device analyzed in this paper has a modulated profile, and would be fabricated by EE. The proposed structure has a cavity to induce a resonance state which has been engineered to correspond with the absorption band of CO_2 at $\lambda = 4.25\ \mu m$. This device works as a filter to be placed in the optical path with an embedded resonator that introduces a narrow passband in the transmission spectrum to select the CO_2 absorption band and to discard other wavelengths. In order to optimize the optical response, the number of periods used in the modulated part of the PhC is

* Corresponding author.
E-mail address: david.cardador@upc.edu (D. Cardador).

http://dx.doi.org/10.1016/j.photonics.2017.04.005

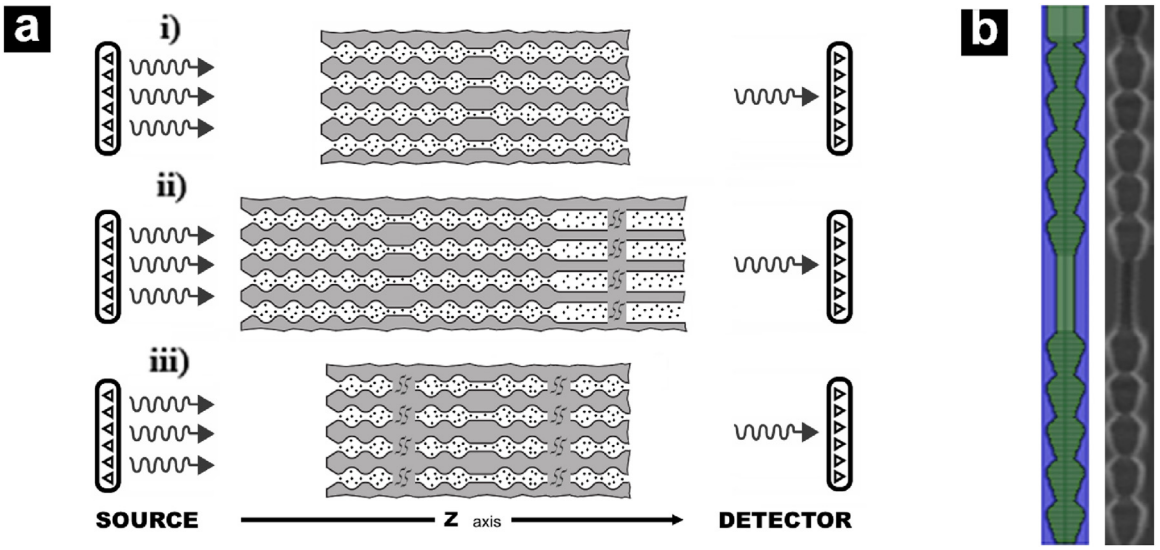

Fig. 1. (a) Schematic representation of the different structure variations. A broadband light impinges the sample and travels through the photonic crystal (i) the basic structure consists of two modulated areas separated by a cavity in the middle. (ii) The modulated pores have been extended with a length of constant diameter pores. (iii) The number of periods before and after the defect is changed. As shown, light propagates along the Z axis, i.e. aligned to the pores' axis. (b) Comparison of simulated and etched basic profiles.

changed from a few periods to a large number of them. Besides, as the PhC structure is a membrane to allow the passage of gas through its pores, the mechanical resilience has to be considered. As these membranes are very thin, porosification is continued after the 3d part of PhC is finished, consisting of straight pores. This section forms the *tail* of the pores. This is done in the same fabrication step and results in a thicker and robust device. This tail may result in unwanted optical features, and therefore the effect of its length is studied. The tail length is changed from non-existent to about the double of the PhC depth, to determine its impact or possible benefits to the optical transmittance of the proposed device. These proposed photonic crystals have been experimentally fabricated, showing a good accordance with the theoretical study. Although the experimental Q-factors are lower than the theoretical ones (due to non-idealities in the fabricated design), we report an enhancement of almost an order of magnitude in the quality factor of the peak. This achievement shows that the new structures are a promising option to be used in spectroscopic gas sensing. Finally, an improvement of the sensitivity due to the increase in the peak's quality factor is theoretically predicted.

2. Numerical study

The simulations of the 3d photonic crystals were done in Optiwave's OptiFDTD software, which uses the finite-difference time-domain method (FDTD). For the simulations, a single pore was designed with its axis aligned to the Z axis, and with light propagating along the Z axis. Periodic boundary conditions were applied on the *XZ* and *YZ* walls while perfect absorbing layers were used for the top and bottom of the simulation space in order to model an ideal PhC. The base shape of this pore consisted in two main parts: the modulated areas and the defect. Modulations were done by an number of periods composed, each one of them, by an ellipsoid and a cylinder—whose radius were optimized in our previous works [10]. —Simulations dimensions were normalized to the lattice XY periodicity and each modulation period was defined in a normalized cell box of size $1 \times 1 \times 1$ units. The defect, embedded halfway the pore depth, was introduced by removing a period, keeping a constant radius and extending as needed its length. For a real device, the lattice period would be $p_{\text{lattice}} = 0.7\ \mu\text{m}$ in order to make the bandgap and defect state correspond with the carbon dioxide absorption line at $\lambda = 4.25\ \mu\text{m}$. It should be taken into account that the profile obtained experimentally shows certain variability compared to the designed one. As it can be seen in Fig. 1(b), these variations are small and have little impact on the bandgap, as reported in [11]. However, small variations in the length of the defect can lead to a mismatch with respect to the working frequency for which it was designed. However, the position of the peak within the bandgap can be easily adjusted in few iterations in fabrication [11].

The quality factor of the cavity is calculated using the usual definition as $Q = f_{\text{peak}}/\text{FWHM}$ from the spectral data, where f_{peak} is the central frequency of the resonant state, and FWHM is the width of the peak at half of its maximum value. In order to achieve the strongest resonance and the highest Q-factor in transmission, and enhance the optical features of the photonic crystal, two modifications of the initial structure were performed. The first one was to introduce a region of porous silicon with a straight profile—i.e. with a constant radius—as a continuation of the modulated pores, that is a *tail* of the pores. The second was to increase the number of periods. All the simulated structures are permeable membranes, both pore ends open allowing the passage of gas. The studied morphologies are schematically depicted in Fig. 1.

The illumination was done with a plane wave coming from the top of the pore and impinging on the front face of the PhC. The light wave was a Gaussian pulse with a linewidth of $\Delta = 4\ m\text{m}$ and a central wavelength about 5 μm, so to make it correspond to the CO_2 absorption line. The transmission spectrum was obtained by placing a plane detector 5 μm after the pore end. The spectrum was calculated by integrating the power flux through the detector plane and normalizing to the incident wave.

To perform the simulations, the refractive index of the bulk material was set to $n \approx 3.43$, which corresponds with the value of silicon in the range of 4 μm–4.4 μm at room temperature [12]. As reported in previous works [13], the absorption in low doped silicon has almost no effect in the propagation of light through the PhC. So, in consequence, no losses were introduced in the bulk material (imaginary part of its refractive index, $\kappa = 0$). The pores were filled initially with air. The structure optimization was performed under these conditions. After optimization, the air was changed with car-