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Conference Paper

Modeling and Optimization of the Porous Silicon Photonic Structures

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Abstract

Photonic crystals and optical devices based on them are of great interest nowadays and are widely used in photonics, optoelectronics, and biosensing. One of the most practically using materials to fabricate one-dimensional photonic crystal is porous silicon due to the simple fabrication process, high porosity and ability to select precisely the refractive index by controlling the porosity. It has already been shown as the suitable material to be used as an element of many photonic devices including gas sensors and biosensors. However, because of the complicated porous structure, and silicon oxidation, occurring at the atmosphere conditions, optical properties of porous silicon photonic structures need to be stabilized by preventive oxidation. In order to predict eventual optical properties of fabricated photonic structures an adequate modeling should be performed. In our study we have developed a calculation model based on the combination of effective media approximations and transfer matrix method, which could precisely predict the reflection, transmission of the porous silicon photonic structures taking into account the dispersion of the refractive index of silicon and silicon oxide, and the oxidation degree. We also used numerical finite-difference time-domain calculations in order to investigate the luminescent properties of the lumiphores embedded into the porous photonic structure.

Keywords: Porous silicon, microcavity, transfer matrix, effective media, FDTD

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1. Introduction

Porous silicon (pSi) is a widely used material for fabrication of porous structures, which could be used in different devices including gas sensors and biosensors [1]–[3]. Ability to precisely control the porosity and hence the refractive index during the formation makes porous silicon suitable to obtain various multilayer porous structures including one-dimensional photonic crystals [4], [5]. Among them one of the most interesting for practical application are distributed Bragg reflectors and microcavities [6], [7]. In order to estimate the physical features of the structures with definite optical characteristics, appropriate mathematical models should be developed. In our study we have performed theoretical modeling of the optical properties of porous silicon one-dimensional photonic crystals using different approaches.

We have developed the model for calculating the refractive index of the layers with different porosities using three-component effective media approximation [8], [9], taking into account the oxidation and refractive index dispersion of the silicon. Using these data, we have performed the calculations for the optical properties of one-dimensional multilayer structures with different porosities applying transfer matrix [10] and numerical finite-difference time-domain methods [11]. In order to estimate the accuracy of the methods we compared the calculated results with the experiment. Photonic crystals have been fabricated using electro-chemical etching of monocrystalline silicon wafers in hydrofluoric acid solutions [12]. Semiconductor quantum dots [13], [14] have been used as luminophores for embedding in order to obtain luminescent structures. The influence of photonic crystals structure on the photoluminescence has been investigated as well.

2. Materials and methods

Refractive index dependence on the porosity and oxidation for different wavelengths has been calculated using effective media approximation. Bruggeman model was shown to be more accurate for highly porous structures. The refractive index of silicon and silicon oxide dependence on the wavelength in the visible range could be well approximated by the following polyexponential and Sellmeier equations [15], [16]:

$$n_{Si}(\lambda) = 36036 \cdot e^{\left(\frac{-\lambda}{37.8}\right)} + 11.96 \cdot e^{\left(\frac{-\lambda}{152}\right)} + 0.892 \cdot e^{\left(\frac{-\lambda}{499}\right)} + 3.435 \tag{1}$$

$$n^2_{SiO_2}(\lambda) = 1 + \frac{0.6961663\lambda^2}{\lambda^2 - 0.0684043^2} + \frac{0.4079426\lambda^2}{\lambda^2 - 0.1162414^2} + \frac{0.8974794\lambda^2}{\lambda^2 - 9.896161^2} \tag{2}$$

In this work we considered lossless medium because of relatively high porosities used. Relative increase of silicon oxide volume during the oxidation were considered as well. The corresponding equation for 3-component (silicon, silicon oxide and air) Bruggeman model has the following form:

$$\delta_{Air} \cdot \left(\frac{1-\varepsilon_{\text{eff}}}{1+2\varepsilon_{\text{eff}}}\right) + \delta_{Si} \cdot \left(\frac{\varepsilon_{Si}-\varepsilon_{\text{eff}}}{\varepsilon_{Si}+2\varepsilon_{\text{eff}}}\right) + \delta_{SiO_2} \cdot \left(\frac{\varepsilon_{SiO_2}-\varepsilon_{\text{eff}}}{\varepsilon_{SiO_2}+2\varepsilon_{\text{eff}}}\right) = 0 \tag{3}$$

$$\delta_{Air} + \delta_{Si} + \delta_{SiO_2} = 1, \tag{4}$$

where δ_i – volume fraction of the air, silicon, and silicon oxide of the porous layer, ϵ_i – corresponding dielectric constant, ϵ_{eff} – effective dielectric constant of the porous layer. In order to simplify the solution of the equation for 3-component system we have split the calculations into two steps. Firstly, we solved 2-component equation to estimate the refractive index of the solid part of porous structure consisted of both silicon and silicon oxide. Secondly, we solved 2-component equation for the final porous material. Characteristic dependencies of the refractive index on the porosity and oxidation are shown in Figure 1.

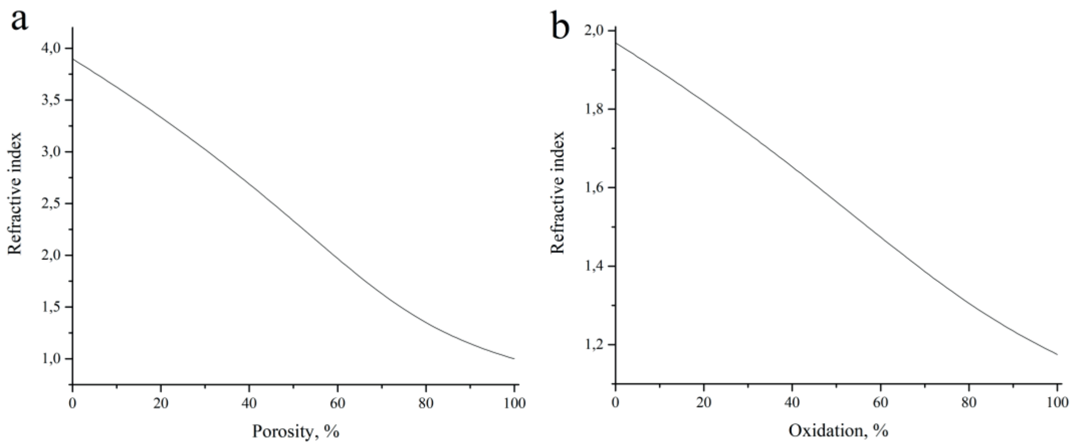

Figure 1: Refractive index of the porous silicon layer dependence on (a) porosity and (b) oxidation degree (for initial porosity 60%).

Transfer-matrix method [10] has been used to calculate the reflection and transmission of multilayer structures with different porosities. Porous silicon photonic structures were fabricated by an electrochemical etching method and their optical properties were measured using OceanOptics USB2000+ spectrometer. Numerical finite-difference time-domain calculations for the porous silicon photonic crystals containing luminophores were performed using free software MEEP from MIT. On the experiment we used the semiconductor quantum dots (QDs) for embedding.

3. Results and discussion

The comparison between the transfer matrix calculated spectrum and experimentally measured reflection spectrum of the pSi microcavity is shown in Figure 2. It could be seen that the microcavity has a very high reflection in the range of 600-700 nm corresponding to the photonic bandgap and a gap in it marking the position of the eigenmode. The calculated spectrum is in a good coincidence with the experimental one: the position and width of the eigenmode are the same as well as the parameters of the bandgap. The full width at half maximum (FWHM) of the calculated eigenmode is slightly less due to the non-ideality of the real structure morphology and the presence of scattering and absorption losses. Positions of the secondary peaks coincidence quite good as well.

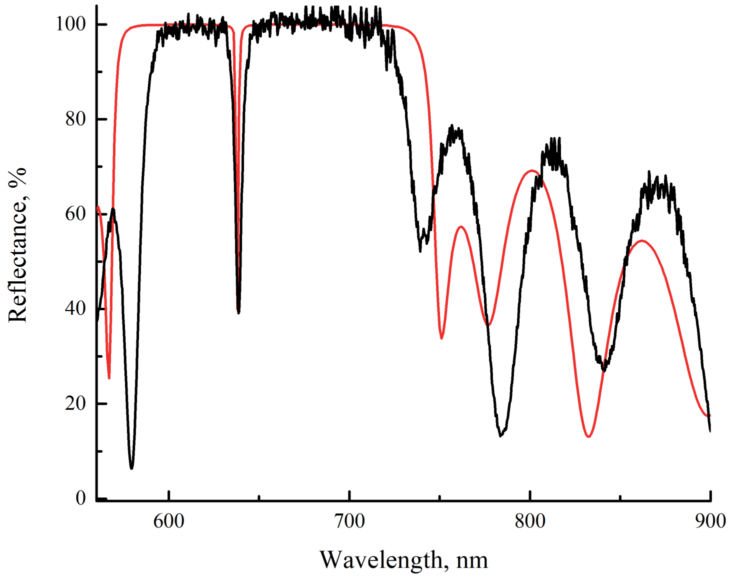

Figure 2: Measured (black line) and calculated (red line) reflection spectrum of the porous silicon microcavity.

In order to simulate the photoluminescence of the pSi structures with the embedded QDs we have used FDTD simulations of multilayer structure consisted of the layers with alterating refractive index and containing the light source at different positions. Emission spectrum was Gaussian shaped and corresponded to the photoluminescence spectrum of the QDs. The most important result is the dependence of the spectrum shape modification on the position of the light source, Figure 3. In case of light source covering the surface of the structure, which is equivalent to the film of QDs on the surface of pSi microcavity, the luminescence was modulated by the reflection spectrum of the microcavity and the gap appeared at the eigenmode position. When integrating the light source into the structure by filling the front Bragg mirror of the microcavity the luminescence spectrum significantly narrowed down to the value equaled the FWHM of the microcavity eigenmode. Further filling didn't influence the spectrum shape.

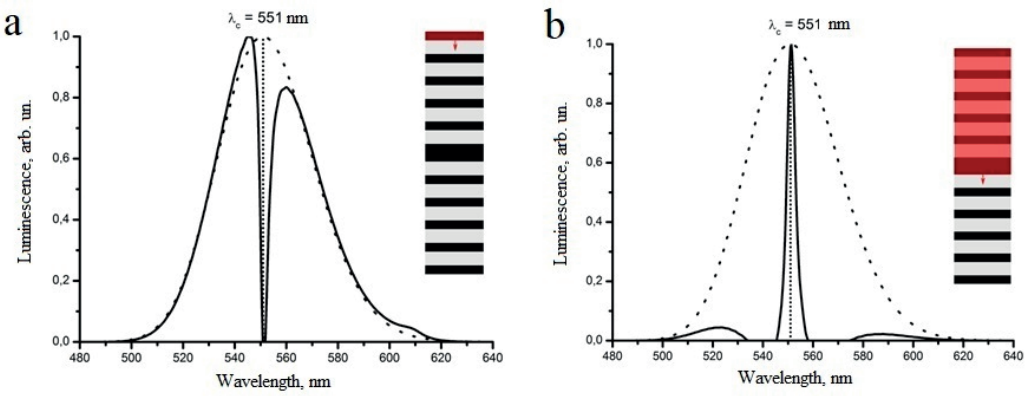

Figure 3: Luminescence spectrum (black solid) depending on the luminophore penetration depth inside the microcavity compared to the original (black doted) spectrum: (a) luminophore placed on the surface of the microcavity, (b) luminophore fills the front Bragg mirror.

4. Conclusions

In this study we have made the calculations of the optical properties of porous silicon photonic crystals in the visible range taking into account the refractive index dispersion and oxidation of pSi structures and compared the results to the experimentally measured spectra. Developed model have shown to be in a good agreement with the experiment. Using FDTD simulations we have shown the dependence of the QD photoluminescence inside the pSi microcavity on the depth of their penetration. It has been demonstrated that filling of the back Bragg mirror by the luminophore does not change the shape of luminescent spectrum.

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