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Photonic band structure of oxidized macroporous silicon

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We investigated theoretically the effect of surface silicon oxide layer on the photonic band structure of a macroporous silicon photonic crystal. Using the plain wave method we have shown that the bandgap in oxidized structure is shifted to the higher frequencies relative to non-oxidized case. We also demonstrate that comparatively wide absolute bandgap can be obtained for low air filling fractions by using thick SiO_2 layer. As an example of possible application of such three-component systems, we have shown the concept of a selector of electromagnetic modes based on our calculations.

Keywords: macroporous silicon, surface oxide layer, bandgap shift.

1. Introduction

Photonic bandgap materials excited a great interest during last decade due to their potential applications in all-optical logical elements, high-efficiency lasers fabrication, low-loss waveguides, and other fields. Photonic crystals of various configurations, symmetries, compositions were proposed since the beginning of the 1990'ies when the first theoretical and experimental methods for photonic crystals fabrication and investigations were established [1–7].

One of the widespread materials for fabrication of 2D photonic crystals is silicon [8]. Silicon wafer with periodic array of air holes, the so-called macroporous silicon (*ma*-Si), possess an absolute photonic bandgap for the waves that propagate in the plane of periodicity (Fig. 1) [8]. Although the oxidization of *ma*-Si during the fabrication process was used very frequently [8], we did not find a detailed consideration of the influence of the oxide layer on *ma*-Si optical properties. Thus, the aim of the present work is to investigate the photonic band structure of oxidized *ma*-Si photonic crystals and to compare it to non-oxidized case.

Silicon oxide is introduced as a ring-shaped intermediate layer between the pores and silicon background as it is depicted in Fig. 1. This model corresponds to the real oxidization process where SiO_2 layer grows up inside the silicon while the pore radius remains unchangeable. We used the following dielectric constants in our calculations, $\varepsilon_a = 1$ for air, $\varepsilon_b = 12$ for silicon, and $\varepsilon_i = 2$ for SiO_2.

We applied the plane wave method to calculate the electromagnetic wave propagation through the 2D lossless photonic crystals. This method was described in details previously [2,3,5–7] and we use the notations introduced by Maradudin and co-authors [3,7]. The accuracy of the results described below is ~2% for the plots in Figs. 2 and 3, and ~0.5% for the data in Table 1. The direction of propagation of the electromagnetic waves in all the cases is in the plane x_1x_2 (Fig. 1).

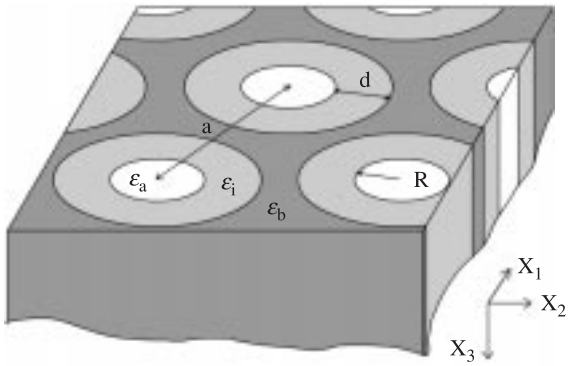

Fig. 1. Fragment of the considered system, $\varepsilon_a = 1$, $\varepsilon_b = 12$, and $\varepsilon_i = 2$ are the dielectric constants of the pore, background, and interlayer, respectively. R is the pores radius, d is the interlayer thickness, and a is the lattice constant.

Table 1. Positions of TE and TM gap edges for different values of interlayer thickness, $R = 210$ nm and $a = 500$ nm.

	TE_{lower} (μm)	TE_{upper} (μm)	TM_{lower} (μm)	TM_{upper} (μm)
$d = 0$	1.1	1.86	1.26	1.32
$d = 5$ nm ($0.01a$)	1.08	1.8	1.23	1.31
$d = 10$ nm ($0.02a$)	1.05	1.73	1.18	1.28

2. Photonic band structure of a macroporous silicon photonic crystal. Discussion of results

Figure 2 shows the dependencies of the TE (solid) and TM (dashed) bandgap edges positions in the triangular lattice photonic crystal with $R = 0.42a$ on the thickness of the silicon oxide layer. The shift of the bandgaps edges to the

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higher frequencies, in Fig. 2, is connected with decreasing effective dielectric constant of the system, since the medium with dielectric constant 12 is replaced by the medium of dielectric constant 2 (Fig. 1). This conclusion follows from the fact that the Fourier coefficients of the dielectric function are inversely proportional to the square of frequency in Maxwell equations in the reciprocal space. Thus, decrease in effective dielectric constant leads to increasing eigenfrequencies. Such scaling shift can be achieved by varying either dielectric constants or filling fractions of the components, since the Fourier coefficients contain both quantities [2,3,5–7].

It follows from Fig. 2 that even interlayer of the thickness $d = 0.01a$ influences the bandgaps position. We have estimated quantitatively the shift of the gap edges position for some "real" structures. The lattice constant $a = 0.5$ μm was taken from Ref. 9. For this case, Fig. 2 corresponds to the photonic crystal with the radius $R = 0.21$ μm and the SiO_2 layer thickness d changing from 0 to 40 nm. The values of the TE and TM gaps edges, without and with a thin SiO_2 interlayer in the structure with $a = 0.5$ μm and $R = 0.21$ μm, are presented in Table 1. Relative shifts of the bandgap edges, in comparison with the case of no interlayer, have the magnitudes near 1.5–3% for the interlayer thickness $d = 5$ nm and 4–7% for $d = 10$ nm. As it can be seen from Table 1, the absolute values of the shifts are over several tens of nanometers.

The silicon surface usually contains the native oxide layer with the thickness of the order of a few nanometers and dielectric constant that does not differ from the bulk silica [10]. Thus, in some cases, especially for the structures with small lattice pitch ($a < 1$ μm), a correction for existence of the native oxide layer should be taken into consideration.

It is well-known [3,6] that maximal bandgap width in triangular lattice ma-Si photonic crystals is achieved at high air filling fractions of more than $f_a = 0.8$. Such a big

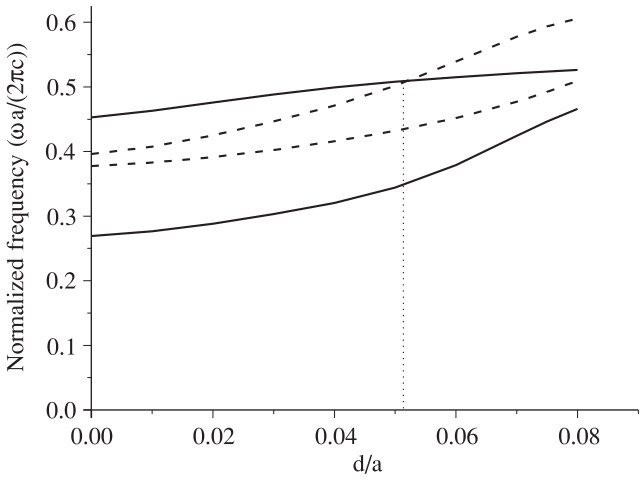

Fig. 2. TM (dashed) and TE (solid) gap edges position *vs*. thickness of oxide layer. Vertical dotted line shows the case of maximal absolute bandgap width.

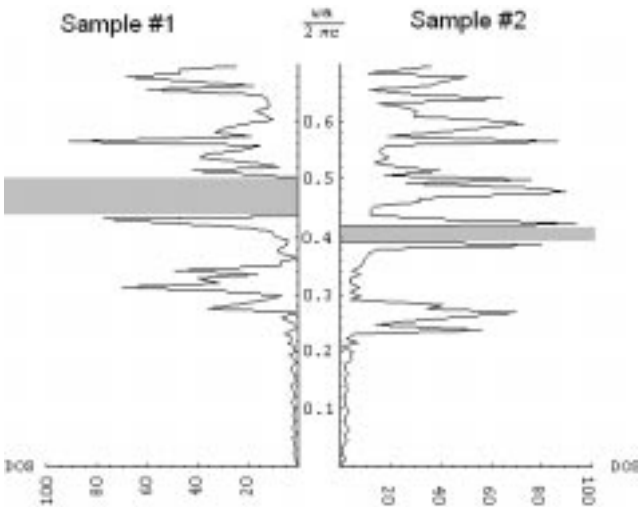

Fig. 3. Densities of photonic states for two structures: sample 1 – $R = 0.42a$, $d = 0.05a$, sample 2 – $R = 0.42a$, $d = 0.02a$. Shaded regions are the absolute photonic band gaps.

porosity may be obtained by subsequent thermal oxidation of the pore walls and chemical etching of the oxide layer [8]. But in this case, the shortest distance between the air regions is less than $l = 0.06a$ that in turn may influence mechanical strength of the pattern. The maximal absolute bandgap width in the oxidized *ma*-Si (Fig. 2) achieved at $R = 0.42a$ ($f_a = 0.64$) and $d = 0.052a$ equals 15.6% of the midgap frequency. Our calculations show that the absolute bandgap appears even for the initial pore radius $R = 0.35a$ ($f_a = 0.44$) and subsequent oxidization up to the oxide thicknesses $d > 0.06a$ and reaches the maximum value of 12% near $d = 0.117a$. For comparison, the absolute bandgap in two-component photonic crystal (without SiO_2 layer) does not exist for the values $R < 0.4a$ ($f_a < 0.58$). Thus, insertion of surface SiO_2 layer into the *ma*-Si photonic crystal allow us to obtain comparatively wide bandgaps under low air filling factors that is impossible in two-component structure.

One of the possible applications of the discussed bandgap shift effect, arising due to the interlayer insertion, is the fabrication of various electromagnetic splitters or selectors. Figure 3 shows the calculated densities of states for two structures $R = 0.42a$, $d = 0.05a$ (sample 1) and $R = 0.42a$, $d = 0.02a$ (sample 2). The former structure has the absolute gap between 0.4339 and 0.5070 and in the latter structure the gap is between 0.3925 and 0.4271 (shaded regions). Thus, there is a narrow region of the spectral width 0.4339 – 0.3925 = 0.0414 between two gaps where the propagation is allowed. Table 2 shows the positions and widths of the absolute bandgaps recalculated for the lattice constant $a = 700$ nm. We suppose that multimode signal with the mode wavelengths in the region of 1380–1772 nm, propagating successively through the samples, will be reflected by the first or second sample with the exception of the modes that lie between two gaps, namely in the region of 1613–1638 nm. The working range of such a selector

can be altered by suitable fitting of three parameters a, R, and d. It is necessary to note that the waves must propagate strictly in the plane x_1x_2 since departure from this plane leads to the gaps shift to the higher frequencies [7].

Table 2. Positions of the absolute bandgap edges for two DOSs, depicted in Fig. 5, recalculated for the lattice pitch a = 700 nm.

	Gap width (nm)	Lower edge (nm)	Upper edge (nm)
Sample 1	233	1380	1613
Sample 2	134	1638	1772

3. Conclusions

We have estimated the influence of SiO_2 interlayer on the optical properties of a *ma*-Si photonic crystal. It was shown that even thin oxide interlayer (d ~0.01a) shifts the edges of the lowest gap on 1.5–3% that may be essential for tunable photonic crystals with small lattice pitch (a < 1 μm). We propose to use the oxidized macroporous silicon with thick oxide interlayer as a photonic crystal instead of high-porous air-silicon structures. It is necessary to note that we have used the simplest approach of a real, positive, frequency-independent dielectric function. Though, the main effects are included, the surface of semiconductors possesses more complicated properties which require taking into consideration the imaginary part of the dielectric constants and their dependency on frequency.

References

1. E. Yablonovich, "Inhibited spontaneous emission in solid-state physics and electronics", *Phys Rev. Lett*. **58**, 2059–2062 (1987).
2. K.M. Ho, C.T. Chan, and C.M. Soukoulis, "Existence of a photonic bandgap in periodic dielectric structure", *Phys Rev. Lett*. **65**, 3152–3156 (1990).
3. M. Plihal and A.A. Maradudin, "Photonic band structure of two-dimensional systems: The triangular lattice", *Phys. Rev*. **B44**, 8565–8571 (1991).
4. V. Lehmann and H. Foll, "Formation mechanism and properties of electrochemically etched trenches in n-type silicon", *J. Electrochem. Soc*. **137**, 653–659 (1990).
5. R.D. Meade, K.D. Brommer, A.M. Rappe, and J.D. Joannopoulos, "Existence of a photonic bandgap in two dimensions", *Appl. Phys. Lett*. **61**, 495–499 (1992).
6. P.R. Villeneuve and M. Piche, "Photonic bandgaps in two-dimensional square and hexagonal lattices", *Phys. Rev*. **B46**, 4969–4972 (1992).
7. A.A. Maradudin and A.R. McGurn, "Out-of-plane propagation of electromagnetic waves in a two-dimensional periodic dielectric medium", *J. Mod. Opt*. **41**, 275–284 (1994).
8. A. Birner, R.B. Wehrspohn, U. Gösele, and K. Busch, "Silicon-based photonic crystals", *Adv. Matter* **13**, 377–388 (2001).
9. S.W. Leonard, H.M. van Driel, J. Schilling, and R.B. Wehrspohn, "Ultrafast band-edge tuning of a two-dimensional silicon photonic crystal via free-carrier injection", *Phys. Rev*. **B66**, R161102 (2002).
10. K. Hirose, H. Kitahara, and T. Hattori, "Dielectric constant of ultrathin SiO_2 film estimated from the Auger parameter", *Phys. Rev*. **B67**, 195313 (2003).