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Band gap studies of triangular 2D photonic crystals with varying pore roundness

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Abstract

Photonic crystals (PCs) are theoretically studied in order to correlate the structural parameters with the resulting electromagnetic behaviour. Two-dimensional (2D) PCs of dielectric media are routinely assumed to be formed by circular rods or pores, respectively. Main topics of the paper are band gap modifications (TM- and TE-polarization) for pores of deteriorating roundness, approximated by ellipses of varying eccentricity. On the basis of Maxwell's equations and a 'plane wave expansion', band structures are computed for triangular 2D lattices of air columns in silicon. The results are compared with calculations for circular air columns of varying filling factors.

Keywords: A. Semiconductors; B. Nanofabrications; D. Band structure; D. Optical properties

1. Introduction

In recent years, the fabrication and physical characterization of photonic crystals (PCs) have gained increasing interest due to their extraordinary optical properties (see, e.g. Refs. [1–4]). Among possible candidates, Si-based macroporous PCs [5–7] combine a well-established technology with an appropriate high dielectric constant. The quality of the electro-chemically etched lattices of air columns in silicon, especially the size distribution and the roundness of the holes, has been inspected by scanning electron microscopy. A dedicated image processing technique revealed the individual pore areas. Applying the equation of a circle to all measured areas provides a mean pore radius and the corresponding error bar [8]. It turned out that there could be significant modifications of the circular pore geometry to other oval-shaped forms, caused by the electro-chemical pore formation process.

In photonic band structure (PBS) computations, two-dimensional (2D) lattices of triangular or square types are routinely assumed to be arranged from columns (holes or rods) of circular shape. The dispersion of the bands can be controlled by the lattice filling factor and the dielectric contrast between the columns and the background. In the present paper, numerical results are presented to study the influence of deteriorating column roundness on PBS data. The geometrical character of the single 'atoms' of the lattice has been approximated by ellipses with varying eccentricity and orientation in the lattice. The theory will only be indicated here, followed by the discussion of the results and practical conclusions.

2. Theory

The analytical formalism and the numerical background have been treated elsewhere in detail [9]. Solving Maxwell's equations for the magnetic field $\mathbf{H}_\omega$ yields the so-called "master equation" (cf. e.g. Refs. [10,11]):

$$\nabla \times \left(\frac{1}{\epsilon(\mathbf{r})} \nabla \times \mathbf{H}_\omega(\mathbf{r}) \right) = \left(\frac{\omega}{c} \right)^2 \mathbf{H}_\omega(\mathbf{r}), \tag{1}$$

with ω—frequency of the light and c—velocity of light.

The magnetic field $\mathbf{H}_\omega$ is expanded into plane waves of wave vector $\mathbf{k}$ with respect to the 2D reciprocal lattice vectors $\mathbf{G}$. The matrix Ξ in the resulting eigenvalue problem is defined by:

$$\Xi^{\mathbf{k}}_{\mathbf{G}\lambda,\mathbf{G}'\lambda'} = [(\mathbf{k}+\mathbf{G}) \times \hat{\mathbf{e}}_\lambda] \cdot [(\mathbf{k}+\mathbf{G}') \times \hat{\mathbf{e}}_{\lambda'}] \epsilon^{-1}(\mathbf{G},\mathbf{G}'). \tag{2}$$

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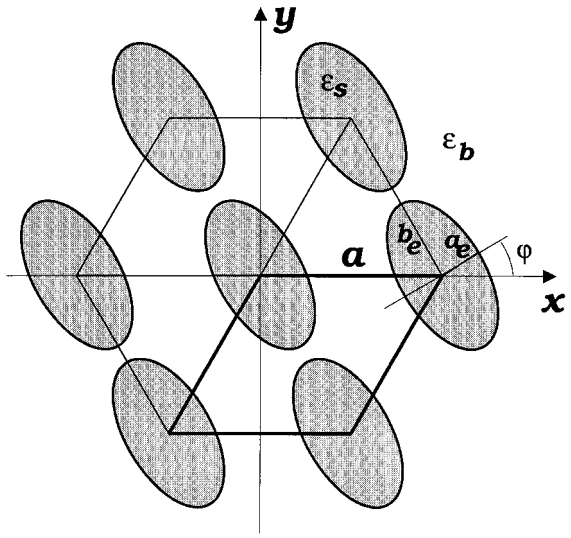

Fig. 1. Model of a PC (triangular lattice of elliptical pores).

The Fourier transform of the inverse dielectric constant $\epsilon^{-1}(\mathbf{G},\mathbf{G}') = \epsilon^{-1}(\mathbf{G}-\mathbf{G}')$ depends on the difference of the reciprocal lattice vectors, only. For 2D crystals and in-plane propagation the eigenmodes of the vector field decouple to modes of the electric field vector parallel or perpendicular to the pore axes, called TM- and TE-polarization, respectively. A large number of plane waves, typically up to 500, are necessary to attain convergence [12], if the dielectric contrast is high.

To quantify azimuthal etching variations of the air columns in PCs, analytical solutions have been derived for the Fourier transform of ϵ^{-1} for elliptical columns (cf. Fig. 1). ϵ_s is the dielectric constant of the columns, and ϵ_b is the dielectric constant of the background. The elliptical columns may show different orientations with respect to the lattice. The dimensions of the rods are given by the major and minor axes (b_e, a_e) resulting in an eccentricity of $e = a_e/b_e$. The Fourier transform $\epsilon^{-1}(\mathbf{G})$ for the real structure of Fig. 1 reads:

$$\epsilon^{-1}(\mathbf{G}) = \frac{1}{\epsilon_b}\delta_{\mathbf{G},0} + \left(\frac{1}{\epsilon_s} - \frac{1}{\epsilon_b}\right)\gamma_e \frac{2J_1(a_e\sqrt{g(\varphi)})}{a_e\sqrt{g(\varphi)}}, \qquad (3)$$

with J_1 being the Bessel function of the first kind. The factor $\gamma_e = 2\pi a_e b_e/(a^2\sqrt{3})$ stands for the 'filling factor', describing the ratio of the area of the column to the area of the total unit cell. Function $g(\varphi)$ describes the orientation of the column in the unit cell:

$$g(\varphi) = G_x^2\left(\cos^2\varphi + \left(\frac{b_e}{a_e}\right)\sin^2\varphi\right) + G_y^2\left(\sin^2\varphi + \left(\frac{b_e}{a_e}\right)\cos^2\varphi\right) + 2G_xG_y\cos\varphi\sin\varphi\left(1 - \left(\frac{b_e}{a_e}\right)\right). \qquad (4)$$

The dispersion properties of 2D PCs are basically determined by the dielectric contrast, the lattice type, i.e. square or triangular geometry, and the lattice filling ratio, scaled by the lattice parameter a. In this context it has to be noticed that Padjen et al. [13] analyzed the filling pattern dependence of band gaps for 2D triangular geometry, especially the influence of the aspect ratio of rectangular columns. Baba et al. [14] computed PBSs for 'optical atoms' built up from circles, hexagons, squares and triangles, where only lattices of circular holes showed notable complete band gaps (see also Ref. [15]).

3. Results

Fig. 2 shows the fundamental differences between band structures of circular and elliptical pores in triangular lattices with the air filling factor being identical in (a) and (b). The radius of the circular pores $r_{0\_max}/a = 0.468$ has been predetermined as that providing the maximum possible complete band gap of $\Delta f = 0.1603[\omega a/\pi c]$. For elliptical pores of the same area and an eccentricity of $a_e/b_e = 0.8$, the size of the gap decreases considerably. It has to be noted that **k**-lines Γ–**M**–**K**–Γ of 1/12 of the irreducible Brillouin zone are not sufficient to identify the minimum complete band gap for an arbitrarily oriented ellipse, because of the breakdown of symmetry laws (only inversion symmetry is kept).

For simulating the experimental process of electro-chemical pore formation, it is useful to distinguish two boundary cases of elliptical pore shape variations:

(i) the major axis b_e is constant (minor axis variations decrease the pore size);
(ii) the air filling ratio is constant ($a_e b_e$ = constant, pores have the same area).

Fig. 3 illustrates the variation of the attainable complete gap size, if the major diameter of the pores is the control parameter of the etching process. Then, axis b_e of the ellipse is kept constant, and the eccentricity (case (i)) is varied solely by a_e. The maximum complete gap of $\Delta f = 0.1603[\omega a/\pi c]$ is obtained for a circular hole of $r_0/a = 0.468$ (solid line, cf. Fig. 2). The decrease of the gap size, observable for $a_e/b_e < 1$ in Fig. 3, is a combined effect of the falling filling factor and roundness variations. The computed series has revealed that the size of the remaining complete band gap decreases mainly with the decrease of the air filling factor. For an increasing eccentricity one can find further maxima of band gaps for higher values of b_e (right hand side of Fig. 3). Since the air filling is reduced for $a_e/b_e = 0.95/0.9$, the attainable maximum gap decreases. The angular variations of the gap size are weak.

In the following figures the horizontal axes are calibrated in terms of r_0/a, which is the fictive radius of a circle having the same area as the ellipse considered. In Figs. 4 and 5, PCs

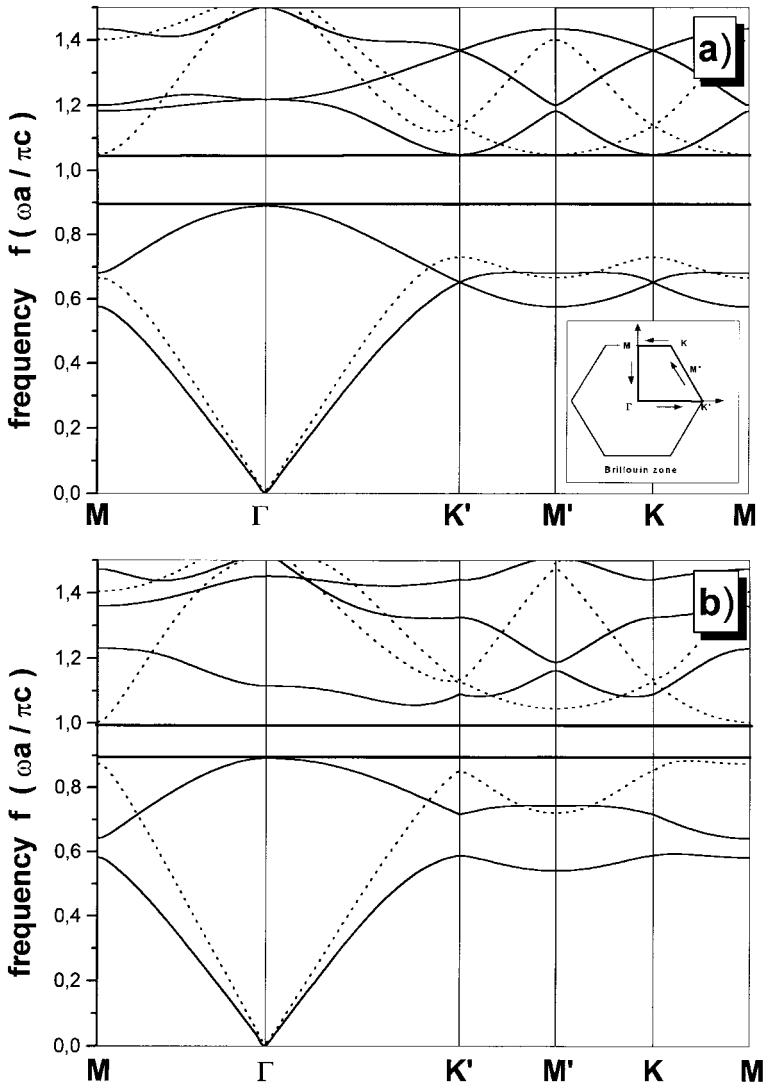

Fig. 2. PBSs for TM- (solid lines) and TE-mode (dotted lines) of a triangular lattice of air pores in Si ($\epsilon = 11.7$), $r_0/a = 0.468$, $\gamma_e = 0.7945$, 535 plane waves. (a) $a_e/b_e = 1$—circle; and (b) $a_e/b_e = 0.8$, $\varphi = 0°$ (complete gaps are marked by horizontal lines!).

of the same air filling ratio but of varying eccentricity and orientation (case (ii)) are directly compared. Fig. 4 represents the size of the complete band gap for exactly circular pores as a solid line. Elliptical pores of smaller r_0/a can partially increase the gap size for selected angles, e.g. for $\varphi = 0°$ (see Figs. 1 and 5). On the other hand, there is a considerable fall of the gap around $r_0/a = 0.45$ for $a_e/b_e = 0.8$ and $\varphi = 30°$. Since the air filling ratio is kept constant for compared abscissa values, the graph exclusively reveals the shape effect of eccentricity and orientation. Above the maximum gap at $r_0/a = 0.468$ the maximum eccentricity becomes gradually limited to attain 'non-overlapping atoms'.

After this review of the r_0/a-behaviour, the angular dependence is studied in more detail for $r_0/a = 0.45$ and 0.475. Starting at circular pores ($a_e/b_e = 1.0$, solid line) of the radius of $r_0/a = 0.45$ (see Fig. 5(a)) the orientation φ of the ellipses in the Brillouin zone and the eccentricity a_e/b_e are systematically varied. The air filling ratio has been kept constant at the level of $\gamma_e = 0.7346$ during the shape variations. It turned out that the size of the complete gaps showed a 60° angular oscillation behaviour of more or less pronounced extent. The variations of the size of the band gap are minor, if the eccentricity is small ($a_e/b_e > 0.90$). If the a_e-axis of the ellipse has an angle of $\varphi = 30°$ in the lattice, the gap size decreases up to 15% for an eccentricity of $a_e/b_e = 0.8$. Fig. 5(b) shows the behaviour of the complete band gaps at $r_0/a = 0.475$ ($\gamma_e = 0.8185$), which is clearly above the circular maximum. If the elliptical axis quotient goes down to 0.9, the band gap size is within the

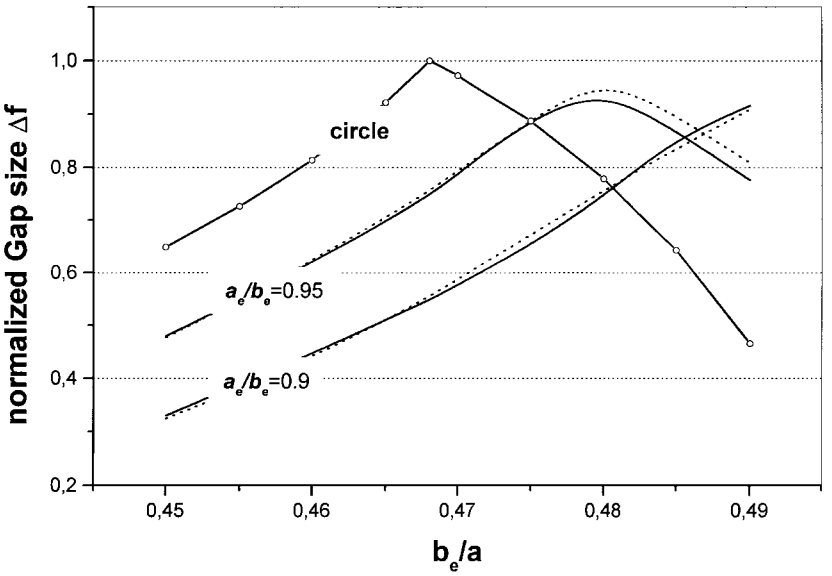

Fig. 3. Complete band gap variations for a triangular lattice of elliptical air holes in Si ($\epsilon = 11.7$), b_e-axis fix, 535 plane waves. $a_e/b_e = 0.95$, 0.9. Angle $\varphi = 0°$ (solid) and $\varphi = 30°$ (dotted).

interval $\Delta f \in [0.133\ (\varphi = 30°),\ 0.122\ (\varphi = 0°)]$, showing considerable angular variations, with the general tendency to a decrease of the gaps. Summing up Figs. 4 and 5 shows that there is no case of an elliptical pore lattice, which can surpass the size of the maximum complete band gap related to a PC of perfectly circular columns.

4. Discussion and conclusions

In this work theoretical studies on 2D PCs have been introduced. PCs of triangular lattice type show complete band gaps, if the dielectric contrast is sufficiently high. The corresponding band structures have been calculated

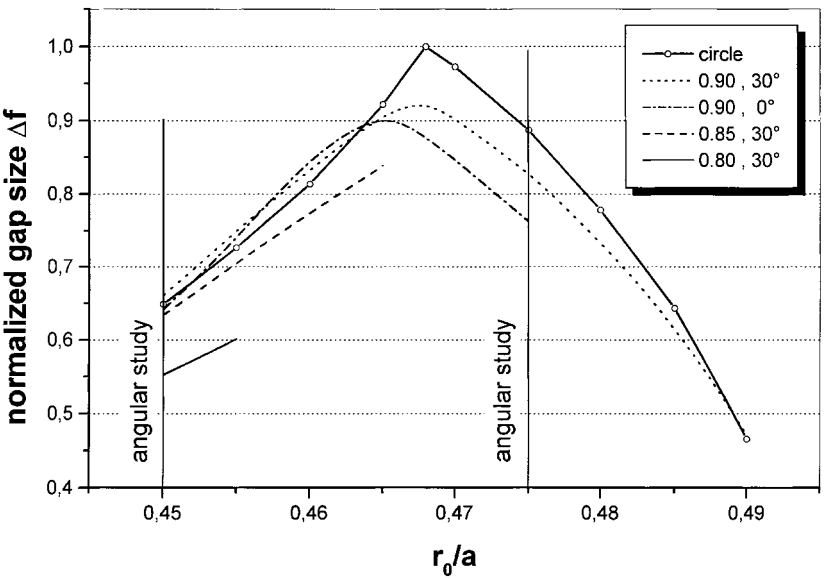

Fig. 4. Complete band gap variations for a triangular lattice of elliptical air holes in Si ($\epsilon = 11.7$), fill factor fix, 535 waves. Values of $a_e/b_e = [0.8,\ 1.0]$ and angle φ in the legend.

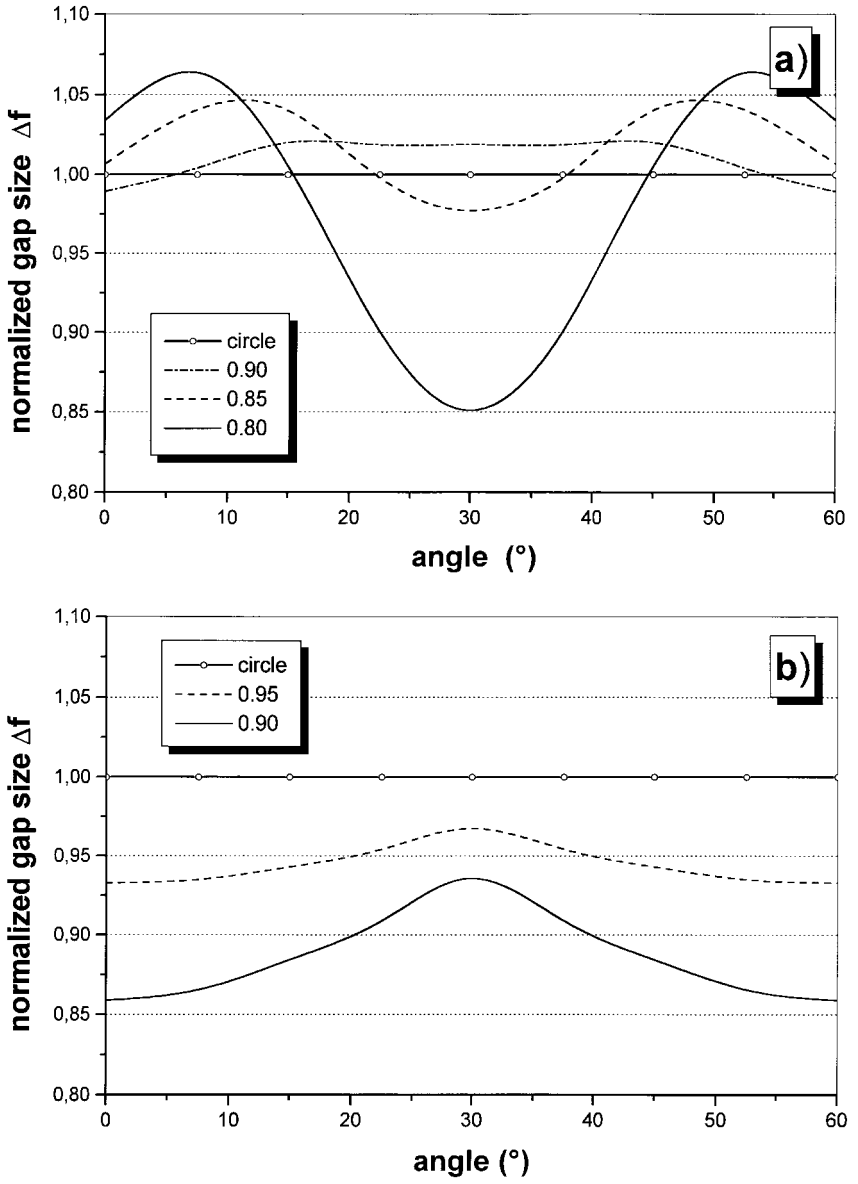

Fig. 5. Angular variations of complete band gaps for a triangular lattice of elliptical air holes in Si ($\epsilon = 11.7$) : (a) below ($r_0/a = 0.450$), and (b) above ($r_0/a = 0.475$) the maximum circular pore gap, fill factor fix, 535 waves.

on the basis of Maxwell's equations in a plane wave approach. The known band structure of circular pore lattices and the features of the related complete band gaps are used as the basis of the argumentation presented. The paper has introduced a quantitative description of the influence of elliptical pore modifications on the band structures of triangular 2D PCs, being experimentally relevant.

If the air filling factor, i.e. the area of all contributing elliptical pores, is constant after the etching, increasing eccentricity shows different behaviour below and above the radius r_{0_max}/a related to the maximum circular gap. Above r_{0_max}/a there is generally a gap reduction, whereas below the circular maximum the gap size oscillates with the orientation angle, having a period of 60°. With the major pore diameter being the fixed process parameter during the crystal fabrication, the decrease of the gap size above r_{0_max}/a can be reduced. To summarize, if there are roundness deficiencies in the preparation process of the PCs, the major pore diameter should exceed the circular optimum according to the derived procedure to compensate the decrease of air filling.

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