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Band-Gap Engineering and Defect Modes in Photonic Crystals with Rotated Hexagonal Holes

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Abstract—We study the band-gap structure of two-dimensional photonic crystals created by a triangular lattice of rotated hexagonal holes and explore the effects of the reduced symmetry in the unit-cell geometry on the value of the absolute band gap and the frequencies of localized defect modes. We reveal that a maximum absolute band gap for this structure is achieved for an intermediate rotation angle of the holes. This angle depends on the radius of the holes and the refractive index of the background material. We also study the properties of the defect modes created by missing holes and discuss the mode tunability in such structures.

During recent years, we have observed a rapidly growing interest in the design and fabrication of novel types of photonic-crystal structures possessing large absolute band gaps. The study of various geometries of three-dimensional photonic crystals and different ways to enlarge their absolute band gaps is a key issue in the physics of periodic dielectric structures, where different polarizations of light are coupled together and, therefore, the existence of an absolute band gap is crucially important for various applications of three-dimensional photonic crystals in optics (see. e.g., [1] and references therein).

However, for two-dimensional (2D) photonic crystals, Maxwell equations are known to decouple effectively for two polarizations, so that the study of a particular photonic band gap of such periodic structures can be carried out independently for both *E*-polarized and *H*-polarized electromagnetic waves. Accordingly, two types of photonic band gaps are usually distinguished to exist for different polarizations. When the band gaps for two different polarizations overlap, they create the combined band gap known as an absolute bandgap.

One of the main reasons to enlarge the absolute band gaps and to study the band-gap properties of 2D periodic photonic structures is the attractive possibility of creating novel types of tunable waveguides and circuits for applications of photonic crystals in integrated optics. In particular, the existence of a large absolute band gap would allow us to design waveguides in planar structures which can support propagating modes of both polarizations in the same frequency domain.

To date, a number of different approaches have been suggested for the enlargement of the absolute band gaps of 2D photonic-crystal structures. One of these approaches relies on the idea of using the photonic crystals created by a 2D lattice of noncircular holes and exploring the symmetry-reducing properties of 2D photonic crystals for the band-gap enlargement [2–12]. In particular, Wang *et al.* [11] demonstrated that the absolute band gap becomes maximal in the case of air holes of the same symmetry as the lattice symmetry. For example, the band gap takes a maximum value for a triangular lattice of rotated hexagonal holes. However, Qui *et al.* [10] suggested that a band gap as large as that demonstrated in [11] can be achieved in 2D photonic crystals created by air holes of more complex noncircular shape without any rotation.

In spite of many studies of the absolute band gaps of photonic crystals created by a lattice of noncircular holes, no specific applications of such large band gaps have been discussed and demonstrated. In particular, the usual statement that large absolute band gaps should be useful for the functioning of photonic circuits is not well grounded. As a matter of fact, there is no solid reason to exploit the absolute band gaps in 2D structures unless photonic-crystal circuits guide light of both polarizations, but the study of defect modes and waveguides in such structures is still incomplete or lacking.

The purpose of this paper is twofold. First, we explore further the concept of the enlargement of the absolute band gaps of 2D photonic crystals through reducing symmetry in the unit-cell geometry taking as an example a 2D dielectric periodic structure created by a triangular lattice of rotated hexagonal holes. In particular, we reveal that in such 2D structures large absolute band gaps can be achieved for an intermediate value of the rotation angle of the hexagonal holes. Second, we demonstrate that, by using 2D photonic crystals with a large absolute band gap, it is possible to create defects which can support localized modes for both polarizations of light, so that the waveguides based on such defects can guide light of both polarizations as well.

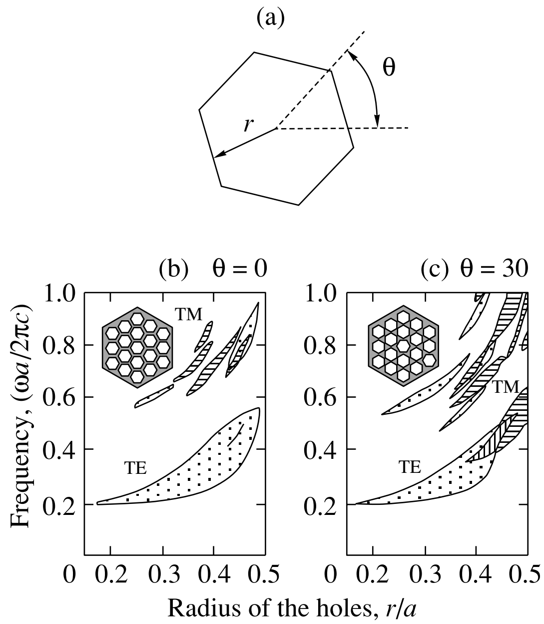

Fig. 1. Photonic band gaps of a triangular lattice of hexagonal holes with radius r, rotated by the angle θ [see (a)], in the dielectric with $\epsilon = 12$ (silicon or AsGa) for (b) conventionally oriented hexagonal holes ($\theta = 0°$), and (c) hexagonal holes rotated by the angle ($\theta = 30°$). Shown are the band gaps for both the TE (dotted areas) and TM (horizontally hatched areas) polarized waves, respectively. The absolute band gap (hatched vertically) appears as an overlap of two band-gap structures.

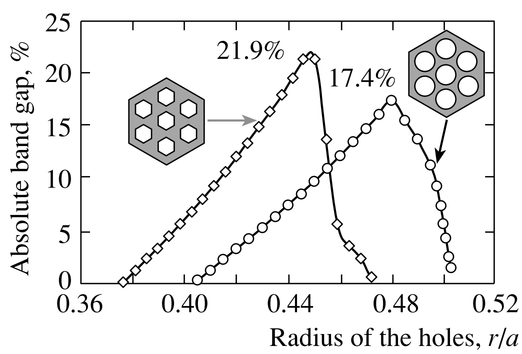

Fig. 2. Comparison between the absolute band gaps of two-dimensional photonic crystals created by a lattice of cylindrical (circles) and rotated hexagonal (diamonds) holes for different values of the hole radius r. For the hexagonal holes, the rotation is chosen to maximize the absolute band-gap at a given radius.

We consider a 2D photonic crystal created by a triangular lattice of hexagonal holes assuming an arbitrary rotation of the hole relative to the lattice symmetry axis, as shown in Fig. 1a. The photonic band gap is calculated by solving Maxwell equations by means of the plane-wave expansion method [13]. Two examples of the photonic band-gap structure of such a photonic crystal are shown in Figs. 1b and 1c for particular cases of the hole rotation, i.e., for $\theta = 0$ and $\theta = 30°$, respectively. Our main goal here is to study the effect of the hole rotation on the value of the (lowest order) absolute band gap. The results can naturally be compared with the band-gap spectra of the 2D structures created by circular holes, as well as with the case when the hexagonal holes are not rotated (see Fig. 1b).

In Fig. 2, we show the dependence of the normalized width of the absolute band gap for two types of triangular lattices created by circular and hexagonal holes as functions of the normalized radius r/a. We make this type of comparison for different values of the rotation angle of the hexagonal lattices, such that the rotation for the hexagonal holes is chosen to maximize the absolute band gap at a given radius. In all cases, we confirm that the hexagonal lattices possess a larger absolute band gap and that this band gap depends strongly on the hexagon orientation.

As a matter of fact, we observe that the absolute band gap can be enlarged dramatically by employing the concept of local symmetry reduction in the unit cell of the structure and by using hexagonal holes instead of circular holes to reduce the rotational symmetry. In this latter case, the band gap depends strongly on the rotation angle of the holes. In brief, our findings can be summarized as follows. First, the maximal band gap is achieved for some intermediate (critical) angle of rotation; in the case of the hexagonal holes in the material with $\epsilon = 12$, this critical angle is close to the value 24°. Second, the critical angle θ_{cr} depends on the value of the dielectric constant ϵ of the photonic-crystal material, but it varies slowly near this intermediate value. Figures 3a and 3b show the maximum value of the absolute band gap $\Delta\omega/\omega$ and the variation of the critical angle θ_{cr} of the rotated hexagonal holes on the value of the dielectric permittivity ϵ of the photonic-crystal material. It is therefore clear that this critical rotation angle is not a fundamental constant of the structure but is defined by some effective geometry and material properties corresponding to the maximum effect of the local symmetry reduction in the unit-cell geometry, similar to the effects discussed in [10] for a completely different problem. Moreover, the absolute band gap varies dramatically for relatively small values of ϵ, whereas it saturates for large ϵ, and the critical angle approaches the value 21°.

As we mentioned above, in the case of 2D periodic dielectric structures, both *E*- and *H*-polarization components of the electromagnetic field are decoupled. In this case, the existence of large absolute band gaps can be useful to support localized modes for both polarizations of light and the waveguides based on such defects can guide light of both polarizations as well. Therefore, in order to employ some practical advantages of using the properties of the absolute band gaps in 2D photonic structures, we should explore the properties of the defect modes and waveguides created in such types of photonic crystals. To be practically useful, such waveguides should be tolerant to the fabrication disorder, so 2D photonic structures created by a lattice of holes seem to be the best suited structures where defect modes and waveguides can be fabricated making some missing holes.

Figure 4a shows the spectrum of localized defect modes supported by a triangular lattice of hexagonal holes for the case when the lattice is created by the holes rotated by 23.7° and the band gap takes its maximum value. As follows from these results, the defect created by a missing rotated hole can support simultaneously localized modes of both TE and TM polarizations, allowing for an effective manipulation of light in photonic-crystal circuits based on this type of defect. Additionally, in Fig. 4b, we show how the absolute band gap and the defect frequencies vary with a change in the rotation angle θ at a fixed value of the hole radius $r/a = 0.43$ defined in Fig. 1a. From the results presented in Fig. 4b, it follows that the frequencies of the defect modes inside the absolute band gap are almost constant for all angles.

Our results show that similar features are observed for the waveguides created in the lower symmetry photonic crystals possessing a large absolute photonic band gap: the possibility to enlarge the band gap in a 2D photonic structure created by rotated hexagonal holes allows such waveguides to support the guided modes of both polarization, and their bandgap properties can be easily manipulated. This problem will be addressed in our future publications.

In conclusion, we have presented the results of engineering of the absolute band gaps in 2D photonic crystals for photonic-circuit applications for the example of a photonic crystal created by a triangular lattice of hexagonal holes. We have revealed that the maximum value of the absolute band gap in this structure can be achieved when all hexagonal holes are rotated by a finite angle, and this rotation angle takes an intermediate value between the values corresponding to the simplest symmetries of the lattice. The critical rotation angle depends on the parameters of the photonic crystals, but it is shown to be almost constant for large values of the dielectric permittivity. Moreover, the frequencies of the defect modes which can be supported by missing holes in such structures do not vary much with hole rotation and a change in the value of the absolute band gap.

We believe that our results will be important for the design of photonic-crystal waveguides and circuits supporting propagating guided modes of both polarizations in the same frequency domain, as well as for the study of nonlinear waveguides where the intensity-induced coupling between modes of different polarization can be controlled through the rotation of holes or noncircular defects. In addition, we believe that our results can be useful for the design of novel types of coupled-resonator optical waveguides with properties which can be tuned by using rotated hexagonal holes instead of circular holes.

In addition, we would like to mention that large absolute band gaps can be very useful for exploring nonlinear properties of photonic crystals, when the

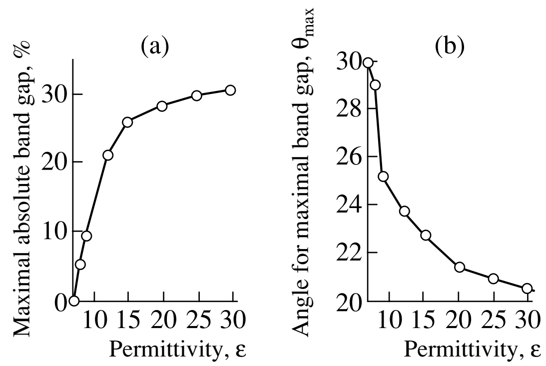

Fig. 3. (a) The maximum value of the absolute band gap $\Delta\omega/\omega$ and (b) the corresponding critical rotation angle θ_{cr} as functions of the dielectric permittivity ϵ of the photonic-crystal material.

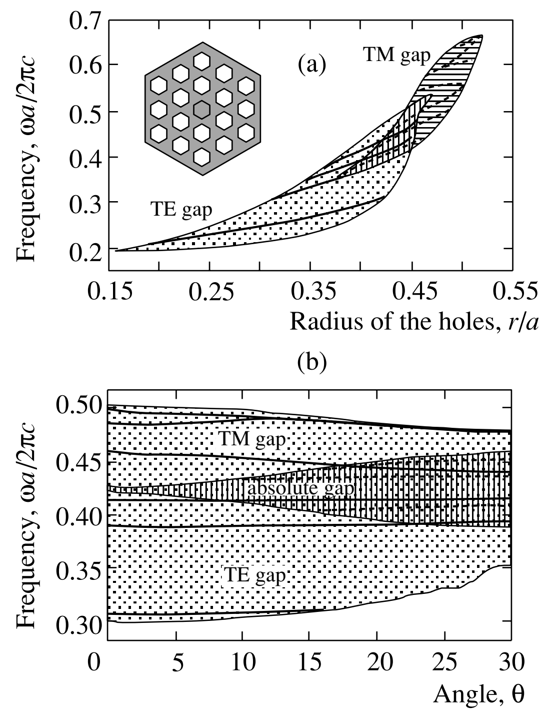

Fig. 4. Spectrum of localized defect modes in a triangular lattice of rotated hexagonal holes (a) as a function of the normalized hole radius r/a at a fixed value of rotation, θ = 23.7°, and (b) as a function of the rotation angle θ for a fixed value of the hole radius, $r = 0.43a$. The defect is created by nonetching of a single hole, as shown in the inset.

intensity-dependent refractive index of the waveguides can be employed to couple the field polarizations. In this case, we can create nonlinear photonic-crystal circuits where one polarization is used for the signal transmission and the other polarization is employed for controlling the signal propagation, in order to realize switching between different transmission regimes, etc.

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