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Photonic band structures of two-dimensional photonic crystals with deformed lattices*

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Using the plane-wave expansion method, we have calculated and analysed the changes of photonic band structures arising from two kinds of deformed lattices, including the stretching and shrinking of lattices. The square lattice with square air holes and the triangular lattice with circular air holes are both studied. Calculated results show that the change of lattice size in some special ranges can enlarge the band gap, which depends strongly on the filling factor of air holes in photonic crystals; and besides, the asymmetric band edges will appear with the broken symmetry of lattices.

Keywords: photonic band gap, photonic crystal, plane-wave expansion method
PACC: 4270Q, 7820P, 7115B

1. Introduction

Photonic crystals (PCs) are artificial periodic structures with a period of the order of optical wavelength, which can be designed by using the photonic band theory. The existence of photonic band gap (PBG) may bring about some novel physical phenomena,[1] and many potential applications in several scientific and technical fields are implied such as filters, high-efficient light-emitting diodes,[2] cavities,[3] optical switches, waveguides,[4] design of low-threshold lasers,[5] fibres,[6] and wavelength division multiplexers,[7] etc. It is also proposed that such PCs may hold the key to the continued progress towards all-optical integrated circuits.[8]

Although three-dimensional (3D) photonic crystals which can be used to trap light in all three directions suggest the most interesting ideas for novel applications, the fabrication difficulty limits their applications. Despite the fact that rapid progress has been made in microfabrication technology, and many types of 3D PCs with a micrometer size have been reported on a layer-by-layer growth scheme, the fabrication of 3D PCs with a band gap in the visible or near-infrared regime is still a difficult and challenging task.[9,10] In contrast, the fabrications of two-dimensional (2D) PCs with near-IR band gaps[11,12] is much easier and these PCs could also find many important applications due to their strong angular reflectivity properties over a wide frequency band. For this reason, much attention has been drawn towards 2D lattice structures.

The band structures of 2D photonic crystals with various structures,[13−17] which are usually the triangular and the square lattices of air holes and dielectric rods with all kinds of cross sections, have been calculated using different methods. The search for new microstructure with larger gaps remains to be the important issue. The creation of a gap depends on many factors in the microstructure such as topology, dielectric constant ratio, lattice structure, and filling factor. The dielectric constant is often limited by material properties and causes a severe constraint to the search for photonic crystals with large gaps, particularly in the technologically important near-infrared region. To obtain a larger PBG, different methods have been used such as two sets of inclusions,[18] anisotropic inclusions,[19] insertion of metallic cylinders,[20] and

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reducing the structural symmetry of unit cells.[21−23] Although reducing the symmetry of the unit cells can be used effectively to obtain a large complete band gap for 2D PCs,[21,22] it is more difficult to transform the cross section of the unit cells than to change the lattice structure. So in this paper, we calculate and analyse the change of band structures of 2D photonic crystals arising from the deformation of lattices. One of our aims is to find whether and when the band gap will be enlarged with the deformed lattice.

Although there exist many studies of the absolute band gaps of photonic crystals, there are few discussions and demonstrations on the specific applications of wide band gaps. In particular, the usual statement that large absolute band gaps should be useful for functioning of photonic circuits is without good grounds. As a matter of fact, there is no sound reason to exploit the absolute band gaps in 2D structures unless the photonic-crystal circuits could guide light of both polarizations. In this paper, we only consider the TE mode band structures where the electric field is parallel to the 2D plane since only the TE modes are often concerned in the study of photonic crystal lasers.[24] Two typical types of 2D photonic crystals have been considered including the square lattice with square air holes and the triangular lattice with circular air holes.

2. Calculation method

A variety of methods have been used to calculate photonic band structures. Among these, there are plane-wave expansion method,[25] multiple-scattering theory (the Korringa–Kohn–Rostoker method),[26] tight-binding formulation,[27] transfer matrix method,[28] finite difference method,[29] generalized Rayleigh identity method,[30] averaged field approach,[31,32] etc. Each method has its own advantages and disadvantages, and one may choose a suitable method depending on a particular problem. Here we use the plane-wave expansion method for photonic crystal band structure computation, which could help us find the variation of band structure with the deformation of the lattice conveniently.

3. Results and discussion

In our calculation, we study two types of air holes arrays, and the dielectric constant of background is fixed at ε=13.

3.1. Square air holes in rectangular lattice

Firstly, we study a square lattice of square air holes with the half width L=0.47a, where a is the lattice constant of the crystal. In a perfect crystal ($a_x = a_y = a$; a_x and a_y represent the lattice constant in x and y direction respectively), a band gap opens at 0.43481 $(\omega a/2\pi c)$ − 0.48244$(\omega a/2\pi c)$ and the width of the gap is 0.04762 $(\omega a/2\pi c)$ (see Fig.1(a)). Then we stretch the lattice along x direction to $a_x = 1.05a$. In Fig.1(b), the band gap lies at 0.39007 $(\omega a/2\pi c)$ − 0.45513$(\omega a/2\pi c)$ and the width of the gap width is 0.06506$(\omega a/2\pi c)$ which is larger than that of the perfect PC in Fig.1(a). Moreover, comparing the band edge of the first and second bands in the two figures, we can find the degeneracy of band edge in x and y directions is relieved when the lattice is lengthened, which makes the gap in y direction larger than that in x direction. To measure the effect of different lattice size on the band gap, we calculate the scan map of the half width of the gap with the change of lattice constant in x direction (a_x) from 0.95a to 1.25a. The results are displayed in Fig.2. In this graph, we can find that with a_x varying from 1.0a to 1.05a, the band gap increases from 0.04762 $(\omega a/2\pi c)$ to 0.06506$(\omega a/2\pi c)$. And the gap is enlarged when the stretching of the lattice is less than 0.15a, as compared with that of a perfect photonic crystal. However, when the lattice is shrunk, the gap will decrease quickly. This conclusion could help explain the difference between experimental results and theoretical ones, since nonuniformities inevitably occur in the fabrication of photonic crystals of micrometer and submicrometre scales.

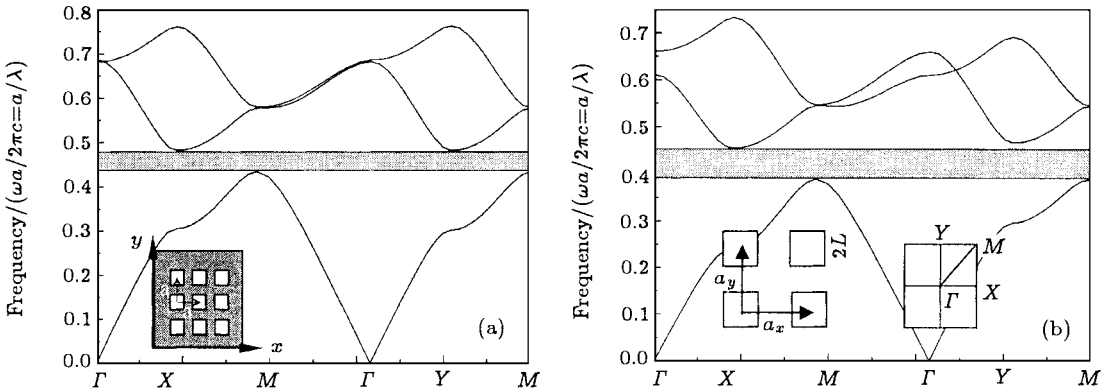


Fig.1. The band structures of the perfect and the distorted photonic crystals. The dielectric constant of the background is 13 and the half width of the square air hole is $0.47a$. (a) The band structure of the perfect photonic crystal; (b) the band structure of the photonic crystal with a_x=1.05a.

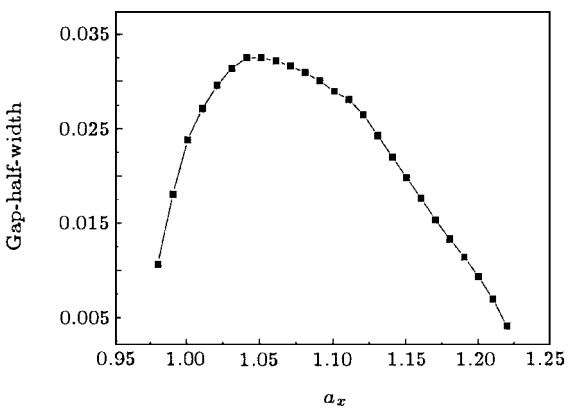


Fig.2. The scan map of the gap-half-width versus the change of lattice constant in x direction (a_x) from 0.95 to 1.25.

Following the same procedure, we have also investigated the band gap of PCs with rectangular lattice (a_x=1.05a) of air holes (L=0.47a) as a function of the refractive index (in the range of 2.0$\leq$ n $\leq$4.0). The calculated results show that the width of the band gap increases as the refractive index increases, and reaches its maximum value when the refractive index is around 2.6. The band gap then decreases as the refractive index further increases. This result is shown in Fig.3.

The cases of different width of the square air holes are considered also. Calculated results show that a range of lattice size where the band gap will be enlarged does not always exist. When the half width of the square air holes is 0.42a, the width of band gap will decrease no matter how the length of the lattice changes. And if we take the half width of the square air holes to be 0.4a, the largest band gap appears at a_x=0.98a, but the enhancement is so small that it can be neglected.

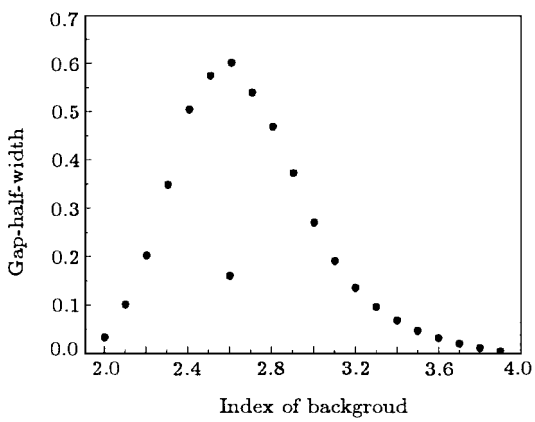


Fig.3. The gap-half-width of the photonic crystal with a_x = 1.05a as a function of index of the background.

From Fig.4, we can find that when the length of the lattice in x direction is changed from 0.92a to 1.03a, the width of the band gap is almost unchanged as the site of the band gap moves to the lower frequency region slowly. This result agrees with the conclusion put forward by Li *et al* that the reduction of the ground band gap is negligibly small at weak disorder of the site arrangement of unit cells.[33]

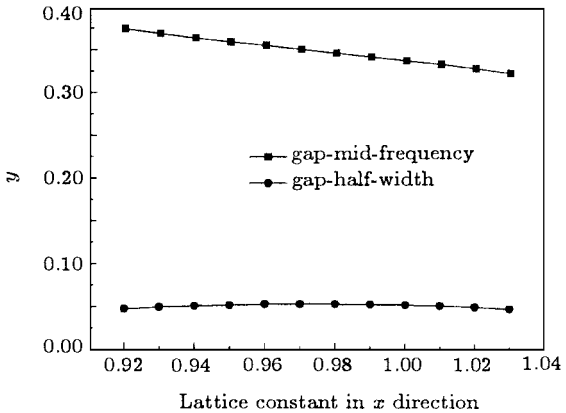


Fig.4. The scan map of the gap-half-width and the gap-mid-frequency as functions of lattice constant in x direction, for the half width of the square air holes $L = 0.42a$. Filled circles and squares denote the gap-half-width and the gap-mid-frequency.

In order to make clear the effect of the filling factor on the band gap of PC with rectangular lattice, we compare the scan map of band gaps in rectangular lattice ($a_x = 1.05a$ and $a_x = 0.95a$), shown as a function of filling factor, with that in a perfect square lattice. The results are illustrated in Figs.5(a) and 5(b) respectively. In Fig.5(a), we can find that the width of the band gap always decreases for $a_x = 1.05a$ until the width of square air holes becomes more than $0.94a$. In Fig.5(b), it can be seen that the shrinking of the lattice also can increase the gap in special ranges such as $0.7a \leq 2L \leq 0.8a$, but it is so small that we can consider the band gap is almost steady in the range of $0.54a \leq 2L \leq 0.8a$.

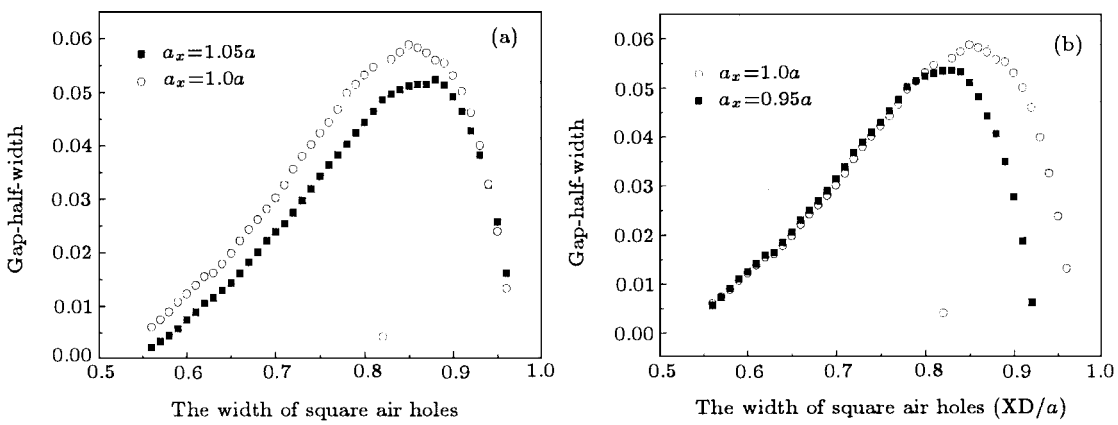


Fig.5. The scan map of the gap-half-width of the photonic crystal with different a_x as a function of the width of the square air holes, compared with that of the perfect square lattice photonic crystal with a_x=1.0a (empty circles) (a) a_x=1.05a (filled squares); (b) a_x=0.95a (filled squares).

From the above analysis, we can find that the effect of band gap produced by the deformation of the lattice in square lattice structure with the square air holes strongly depends on the size of the air holes.

3.2. Triangular lattice with circular air holes

For triangular lattice with circular air holes we have carried out similar calculations and analyses. We calculate the band structures of photonic crystals with different angle α, which is taken as a parameter of the change of the lattice. For a perfect crystal, α=30°; if the lattice is stretched, $\alpha < 30°$, otherwise, $\alpha > 30^0$ (see Fig.6).We take the radius of the circular air holes to be r/a=0.48. When α is in the range of 30°–28°, the band gap will be enlarged. And when α=29°, the gap is the largest. But when the angle is larger than 30°, the gap will decrease quickly (see Fig.6). Moreover, there will be a narrow gap in high frequency region when $\alpha \leq$25°. Figures 7(a) and 7(b) are the band structures for α=30° and 25° respectively. It can be seen that the ground band gap becomes narrower when α=25°, as compared with that of α=30°, at this point the second gap appears in high frequency region.

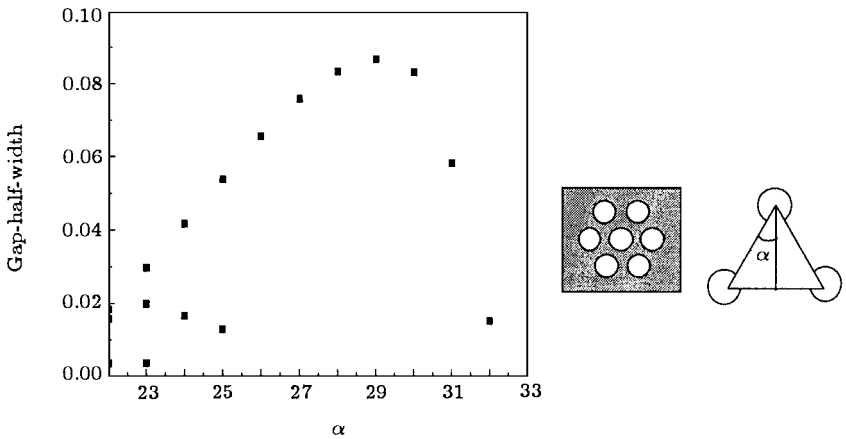


Fig.6. Variation of gap-half-width of the triangular lattice versus α. In this calculation, we take ε_0=13, r/a=0.48.

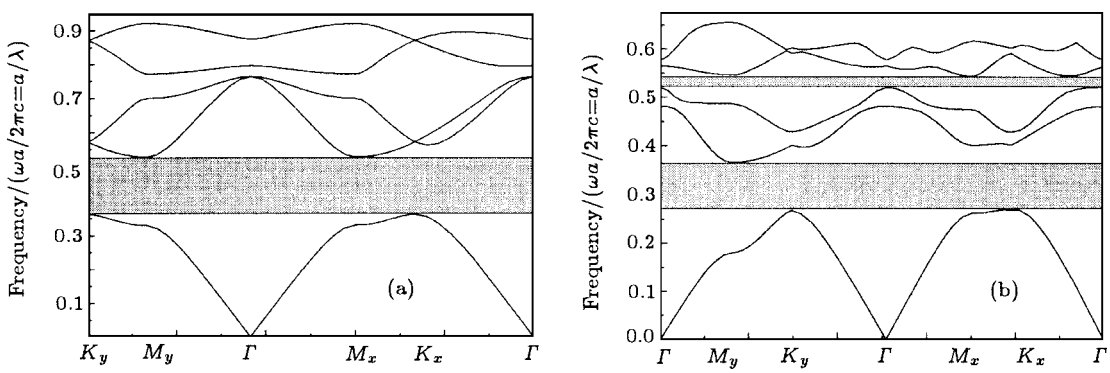


Fig.7. The band structures of photonic crystal with perfect triangular lattice for α=30° (a) and the stretched lattice for α=25° (b).

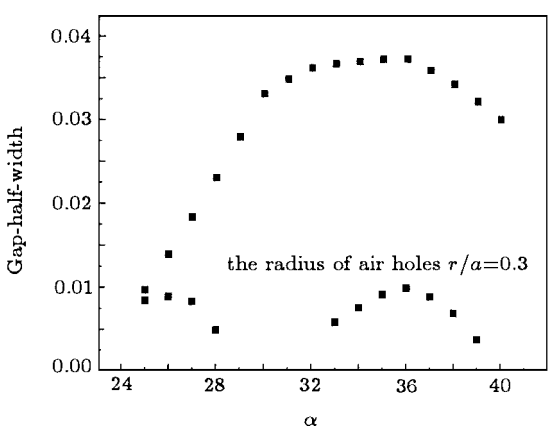


Fig.8. The scan map of the gap-half-width of the triangular lattice as a function of α. In this calculation, we take ε_0=13, r/a=0.3.

We change the radius of the air holes to $0.3a$ and repeat the same scan of α. The result is shown in Fig.8. With the increase of α, the gap reaches its maximum value $0.07466\omega a/2\pi c$ when $\alpha = 36°$. Furthermore, a narrow gap will appear in high frequency region if the lattice is shrunk and its maximum value is also at $\alpha = 36°$. However, when the lattice is stretched, the band gap will decrease quickly.

In Figs.9(a), (b) and (c), we compare the band gaps of photonic crystals at α=36°, 29°, 25° with those of the perfect photonic crystal (α=30°). In Fig.9(a), it can be seen that when α=36°, the band gap becomes wider in the range of $0.22 \leq r/a \leq 0.38$ and there will be a narrow band gap in high frequency region in the range of $0.29 \leq r/a \leq 0.39$. In Fig.9 (b) is the scan map of band gap for α=29°, which shows that the band gap will be enlarged until $r/a \geq 0.47$. But when $\alpha = 25°$, the band gap will decrease regardless of the size of the air holes, which can be seen in Fig.9(c).

In summary, for a system of PCs with fixed background materials, lattice structure and unit cell cross-section, we can obtain a band gap width map as a function of filling factors. Then the influence on the band gap, produced by the change of lattice structure, will depend strongly on the filling factors. We take the filling factor that can give the largest gap in a perfect

lattice as a critical point f_c. If the filling factor of deformed photonic crystals $f = f_c$, the change of lattice must make the gap narrower; If $f > f_c$, the stretch of the lattice could enlarge the gap in some special situations, and if $f < f_c$, the shrink of lattice may enlarge the gap.

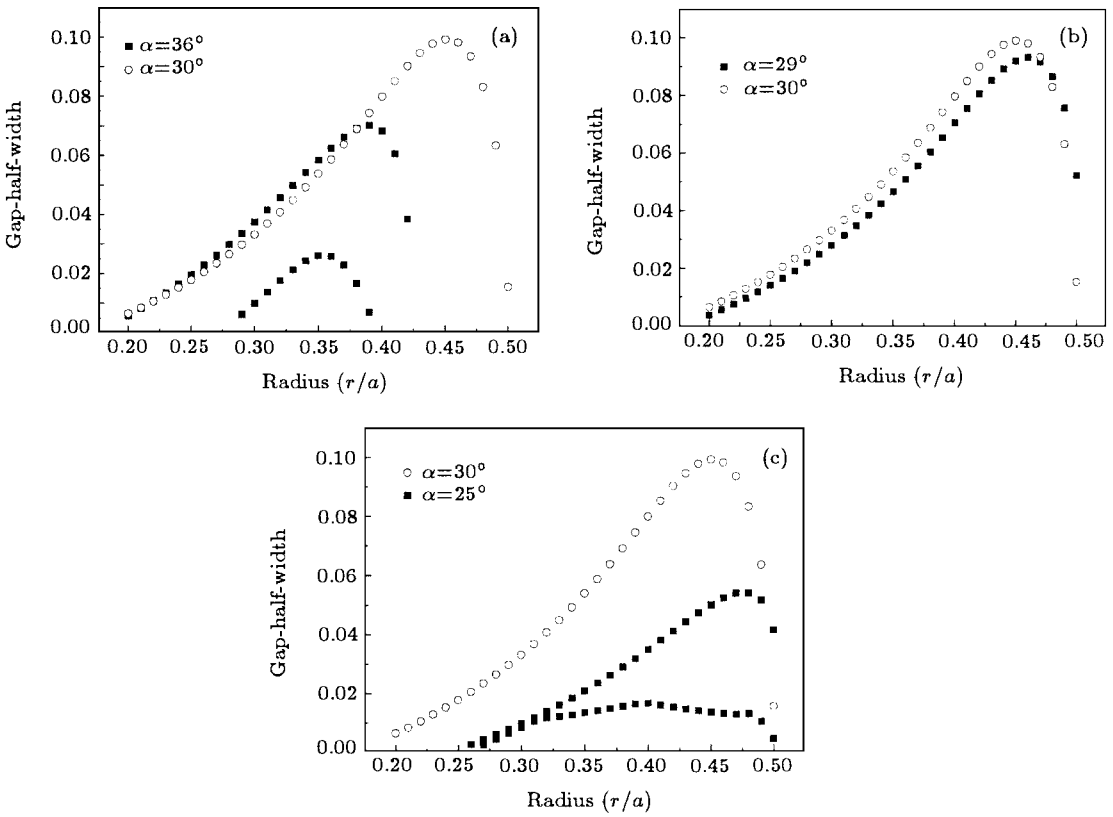


Fig.9. The scan map of the gap-half-width of the photonic crystal with different α as a function of the radius of the air holes, compared with that of the perfect photonic crystal with α=30° (empty circles): (a) α=36° (filled squares); (b) α=29° (filled squares); (c) α=25° (filled squares).

4. Conclusions

We have investigated the influences of the stretching or shrinking of lattice structures on the band gaps in 2D photonic crystals. Two types of photonic crystals are considered, including square air holes in square lattice and circular air holes in triangular lattice. Using the plane-wave expansion method, we calculate and analyse the changes of width and site of band gaps with the variation of lattices. Through comparing the band gap of deformed photonic crystal with that of perfect one, we find that the band gap can be enlarged in some special situations for these two types of structures. And the change of the band gap in deformed photonic crystal depends strongly on the filling factor of air holes. In other words, with different filling factor, the influence of the change of lattices on band gaps is different. This conclusion is useful for the understanding of the difference between the experimental and the theoretical results. And it could be helpful in designing photonic crystals, since nonuniformities will inevitably occur in the fabrication of photonic crystals in micrometer and submicrometre scales.

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