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2003 J. Phys.: Condens. Matter 15 4109

(http://iopscience.iop.org/0953-8984/15/24/304)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **15** (2003) 4109–4118 PII: S0953-8984(03)59621-7

Guide modes in photonic crystal heterostructures composed of rotating non-circular air cylinders in two-dimensional lattices

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Received 10 February 2003, in final form 7 May 2003
Published 6 June 2003
Online at stacks.iop.org/JPhysCM/15/4109

Abstract
We investigate the properties of guide modes localized at the interfaces of photonic crystal (PC) heterostructures which are composed of two semi-infinite two-dimensional PCs consisting of non-circular air cylinders with different rotating angles embedded in a homogeneous host dielectric. Photonic band gap structures are calculated with the use of the plane-wave expansion method in combination with a supercell technique. We consider various configurations, for instance, rectangular (square) lattice–rectangular (square) air cylinders, and different rotating angles of the cylinders in the lattices on either side of the interface of a heterostructure. We find that the absolute gap width and the number of guide modes strongly depend on geometric and physical parameters of the heterostructures. It is anticipated that the guide modes in such heterostructures can be engineered by adjusting parameters.

1. Introduction

In the last decade there has been great interest in studies of photonic band gap (PBG) structures in materials with periodic dielectric modulation because of their remarkable features [1, 2]. One of the most important subjects is how to design photonic crystals (PCs) favourable for having specified PBGs at a predesignated frequency and large width of absolute band gaps in which the propagation of electromagnetic (EM) waves is inhibited for any propagation direction and polarization modes. This latter feature leads to extensive applications [3]. On the other hand, PC waveguides can be made by using gap modes, which can be produced from the local breaking of the periodicity of the lattice [4–9]—for example, the line defects produced by the removal of one or several rows of cylinders in an ideal two-dimensional (2D) lattice, or the localized modes at the interfaces of PC heterostructures. Recently, Li *et al* [10] revealed the properties of interface states in PC heterostructures which are composed of two semi-infinite

2D square lattices of circular air cylinders embedded in a homogeneous host dielectric. The lattice types, the shapes of scatterers, and the crystalline orientations in the two lattices are same, except for different filling fractions. For this kind of heterostructure, there exists an individual band gap for the TM/TE polarization mode (with the electric/magnetic field along the cylinder axis). However, no localized guide mode or interface mode are found when all the cylinders in the lattices on either side of the interface of the heterostructure are exactly centred at the square lattice sites. Only on introducing the relative lattice displacements parallel or perpendicular to interface are interface states produced [10].

To favour the creation of guide modes at the interfaces of heterostructures, we require special prototype PCs of heterostructures with much larger widths of absolute PBGs, because such PCs can then easily produce guide modes residing inside the wide PBGs. It is well known that PC symmetry plays an import role in the appearance of absolute PBGs [11], for example, in square lattices and honeycomb structures [12], and in group $4mm$ PCs [12]; on inserting small circular cylinders between the original circular cylinders, this leads to lowering of the symmetry of the PCs, and consequently the absolute PBGs appear. Using non-circular cylinders can also cause lowering of the symmetry of the PCs. Wang *et al* [13] suggested that by rotating square cylinders in a square lattice, the widths of absolute PBGs could be significantly enlarged. Recently, Wang *et al* [14] investigated the effects of shapes and orientations of scatterers as well as lattice symmetry on the PBG structures in 2D PCs. They found that for a given lattice symmetry, the largest absolute PBG may be achieved by employing scatterers with special shapes having the same symmetry as the lattice—for instance, hexagonal cylinders in triangular or honeycomb lattices, square cylinders in square lattices, and rectangular cylinders in rectangular lattices.

Motivated by these works, there is much interest in studying the guide modes in new PC heterostructures which are composed of two semi-infinite 2D rectangular/square lattices consisting of rotating rectangular/square air cylinders embedded in a homogeneous host dielectric. Two sets of lattices in a heterostructure have identical physical and geometric parameters but different rotating angles of the rectangular/square cylinders on either side of the interface of the heterostructure. We calculate the band gap structures for such heterostructures with the use of the plane-wave expansion method in combination with a supercell technique [5, 6]. We find that the guide modes are produced by introducing relatively longitudinal gliding of the cylinders in the lattices on either side of the interface of the heterostructure with the host dielectric along the interface, or displacing the cylinders in the lattices on either side of the interface individually away from their normal positions, transversely, leaving a distance from the host dielectric around the interface. The number of guide modes strongly depends on the rotation angles of the rectangular/square cylinders, the types of lattice, the shapes of air cylinders, and the relative displacements of the cylinders in the lattices on either side of the interface, etc. We present a detailed comparison of the PBG structures for different configurations of heterostructures.

The outline of this paper is as follows. In section 2, we describe the necessary formulae used in the calculations and the model structures of PC heterostructures. The calculation results are presented in section 3 with analyses. Finally, a brief summary is given in section 4.

2. Formulae and model structures of heterostructures

The PBG structures of both the TM and TE polarization modes are usually determined by the following equation, to be satisfied by the magnetic field $\boldsymbol{H}(\boldsymbol{r})$ [15, 16]:

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

where $\epsilon(\boldsymbol{r})$ represents periodic modulation of the dielectric function in the 2D lattice. This equation can be solved numerically with the use of the plane-wave expansion method [11, 17] in combination with a supercell technique [4–6]. The size of supercells should be chosen large enough to guarantee the correctness of the results, i.e. the coupling effects between neighbouring supercells can be neglected; thus the plane-wave expansion method can still be approximately suited to the calculation of the PBG structures of heterostructures. The heterostructure considered here is composed of two semi-infinite 2D rectangular/square lattices containing rotating rectangular/square air cylinders, which are embedded in a homogeneous host dielectric of dielectric constant $\epsilon_b = 12.96$. The prototype PC of this heterostructure possesses the largest PBGs as reported in [14]. A sketch of the model heterostructures is displayed in figure 1(a). The lattice constants of the rectangular (square) lattices are denoted by $l_x(a)$ and $l_y(a)$ for the x- and y-axes, respectively. The long-side and short-side lengths of the individual rectangular cylinders are denoted by l_a and l_b, respectively. θ_r and θ_l represent the inclined angles of the long side of the rectangular cylinders against the x-axis for the right-hand and left-hand lattices around the interface, respectively. The y-axis is parallel to the interface. We also display the modified lattice structures of the heterostructure by introducing the relative displacements of the lattices on either side of the interface in figures 1(b) and (c): 1(b) for relatively longitudinal gliding of the cylinders in the lattices on either side of the interface of the heterostructure with the host dielectric along the interface; 1(c) for displacing the cylinders in the lattices on either side of the interface individually away from their normal sites, transversely leaving a distance from the host dielectric around the interface. We calculate the PBG structures of this heterostructure on the basis of rectangle lattices which consist of $m \times 1$ original unit cells from each side of the interface of the heterostructure. Thus, every unit cell of the supercells contains $2m \times 1$ original unit cells. The primary vectors of this supercell are $\boldsymbol{a}_1 = (2m, 0)l_x$ and $\boldsymbol{a}_2 = (0, 1)l_y$. The first Brillouin zone is a rectangle. The PBG structures of the heterostructure are determined by calculating the photonic density of states (DOS) only in the irreducible Brillouin zone of the supercell lattice.

3. Numerical results and analyses

Referring to [14], we first choose $l_y/l_x = 0.8$, $l_a/l_b = 0.84$, the filling factor $f = 0.688$, and the mirror-symmetric structure with $\theta_r = -\theta_l = 28°$. In this sample, the prototype PC has the largest width of the PBG [14] of $\Delta\omega = 0.402 - 0.362 = 0.040(2\pi c/l_y)$, where c is the speed of light in vacuum. In our calculations, we choose $m = 4$, and the number of plane waves in the expansion is $N = 1235$. According to the information from [10], these parameters are adequate for guaranteeing the correctness of the results for the interface states of heterostructures in 2D PCs.

At the beginning, we make calculations for the simplest heterostructure, in which all the air cylinders lie at the sites of a rectangular lattice without any displacement. There is an absolute PBG lying in the range $[0.366, 0.400](2\pi c/l_y)$, which is only slightly different from that ($[0.362, 0.402](2\pi c/l_y)$) for the prototype PC. This difference results from the existence of the interface of the heterostructure. We have not found any guide mode, consistently with the report of Li *et al* [10]. To produce interface states, we now consider the lattice longitudinal displacement effect. We introduce a relatively longitudinal gliding of the cylinders in the lattices on either side of the interface with the host dielectric along the interface by $\mathrm{d}y = 0.35l_y$ (the outcome is referred to as sample $1\mathrm{A}_{\mathrm{d}y}$); its calculated PBG is depicted in figure 2(a). For clarity, only a few bands around the PBG are shown in figure 2(a). The solid/dashed lines and the solid circle curves correspond to the TE/TM polarization modes and the TE guide modes, respectively. Two solid/dashed horizontal lines define the range of the PBG for the TE/TM

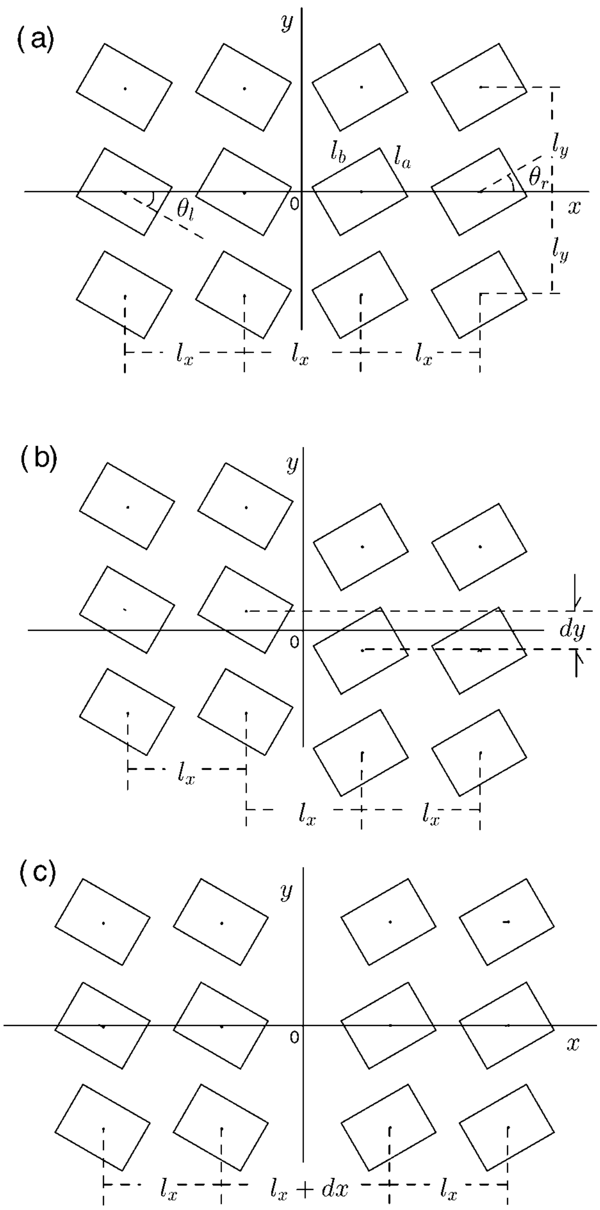

Figure 1. A schematic diagram of a mirror-symmetric PC heterostructure. It consists of two semi-infinite 2D rectangular/square lattices containing rotating rectangular/square air cylinders embedded in a homogeneous host dielectric of dielectric constant $\epsilon_b = 12.96$. The lattice constants of the rectangular (square) lattices are denoted by $l_x\,(a)$ and $l_y\,(a)$ for the x- and y-axes, respectively. The long-side and short-side lengths of the rectangular air cylinders are denoted by l_a and l_b, respectively. θ_r and θ_l are the inclined angles of the long side of the rectangle cylinders against the x-axis for the right-hand and left-hand lattices on the interface of the heterostructure, respectively. (a) The original PC heterostructure; (b) after introducing relatively longitudinal gliding dy of the cylinders in the lattices on either side of the interface of heterostructure with the host dielectric along the interface; (c) after displacing the cylinders in the lattices on either side of the interface individually away from their normal positions, transversely leaving a distance d$x/2$ from the host dielectric around the interface.

mode. Hereafter we always employ these line styles to plot the PC bands. We observe two TE guide modes lying in the first PBG in the range $[0.349, 0.398](2\pi c/l_y)$; the corresponding PBG width is $\Delta\omega = 0.049(2\pi c/l_y)$. As is well known, the larger gap width can strongly favour the existence of interface states. On increasing the amount of relatively longitudinal gliding, the TE gap modes are moved upward from the lower edge to the upper edge of the PBG. When $\mathrm{d}y = 0.35l_y$, two TE guide modes move in the middle of the PBG and they extend over the whole k_y-region, which is that of the favourable interface states having good stability, because they lie far away from the edges of bands. When $\mathrm{d}y = 0.5l_y$, the TE guide modes merge into the upper edge of the PC band completely. The PBG of the TM mode ranges over the frequencies $[0.373, 0.399](2\pi c/l_y)$. Combining the two PBGs of the TE and TM modes, we obtain an absolute PBG in the range $[0.373, 0.398](2\pi c/l_y)$ with a width of $\Delta\omega = 0.025(2\pi c/l_y)$, much smaller than that of the PBG of the TE mode, $0.049(2\pi c/l_y)$. In this absolute band gap, there are two TE guide modes now and they only appear in some k_y-regions.

We now study the effects of displacing the cylinders in the lattices on either side of the interface individually away from their normal sites, leaving a distance $\mathrm{d}x/2 = +0.35l_y/2$ from the host dielectric around the interface on the PBGs. We refer to this version as sample $1\mathrm{A}_{\mathrm{d}x}$; there is an absolute PBG in $[0.388, 0.426](2\pi c/l_y)$; the gap width is $\Delta\omega = 0.038(2\pi c/l_y)$, as shown in figure 2(b). This gap width is larger than that of the previous sample $1\mathrm{A}_{\mathrm{d}y}$. There exist two TE guide modes and one TM guide mode (marked by the open circle curve). These guide modes only extend over some k_y-regions. Meanwhile, there is one broader band gap for the TM polarization mode, which is located at $[0.207, 0.261](2\pi c/l_y)$, in which there exist two TM guide modes. When scanning the transverse displacement $\mathrm{d}x$ from $0.05l_y$ to $0.45l_y$, with the use of a step length of $\mathrm{d}x = 0.05l_y$, we find that when $\mathrm{d}x = 0.20l_y$, two TE guide modes begin to enter into the absolute PBG from the upper edge of the PC band; when $\mathrm{d}x = 0.35l_y$, these two guide modes survive over the whole frequency range of the absolute PBG. When $\mathrm{d}x = 0.45l_y$, one TE guide mode goes back to the upper edge of the absolute PBG again and finally merges into the upper band. As a result, we can artificially control the guide modes by adjusting the relatively transverse displacement of lattices in a heterostructure.

We conclude that the frequency and the width of the PBG are remarkably varied on introducing relatively longitudinal gliding of the cylinders or relatively transverse displacement of the cylinders in the lattices on either side of the interfaces of the heterostructures. These results can be well understood: as the supercell unit contains many cylinders, on imposing longitudinal gliding or transverse displacement with respect to the host dielectric about the interfaces, the positions of the cylinders inside the supercell unit undergo relative shifts; this should cause changes of the band gap structures (in frequency and width). The source of the production of the gap states localized at the interface of the PC heterostructures can be understood as follows: on introducing the relatively longitudinal gliding of the cylinders or making a transverse displacement of the cylinders in the lattices on either side of the interface with the host dielectric around the interface, there is an enlargement of the size of the resonant cavity consisting of these cylinder shifts around the interface; therefore, the frequencies of these resonant cavity modes are lower than those of the edges of the PBGs of the original PC heterostructure, and thus the gap states appear inside the PBGs now.

We turn to investigating other examples of heterostructures composed of two semi-infinite 2D square lattices containing rotating square air cylinders embedded in a homogeneous host dielectric. According to [14], the prototype PC of this kind of heterostructure possesses a large absolute PBG—its width is $\Delta\omega = 0.063(2\pi c/a)$ and it has a gap–mid-gap (gm) ratio $\omega_R = \Delta\omega/\omega_g = 14.9\%$, where ω_g denotes the frequency in the middle of the gap and $\Delta\omega$ the frequency width of the gap, when the filling factor is $f = 0.680$ and the rotating angle

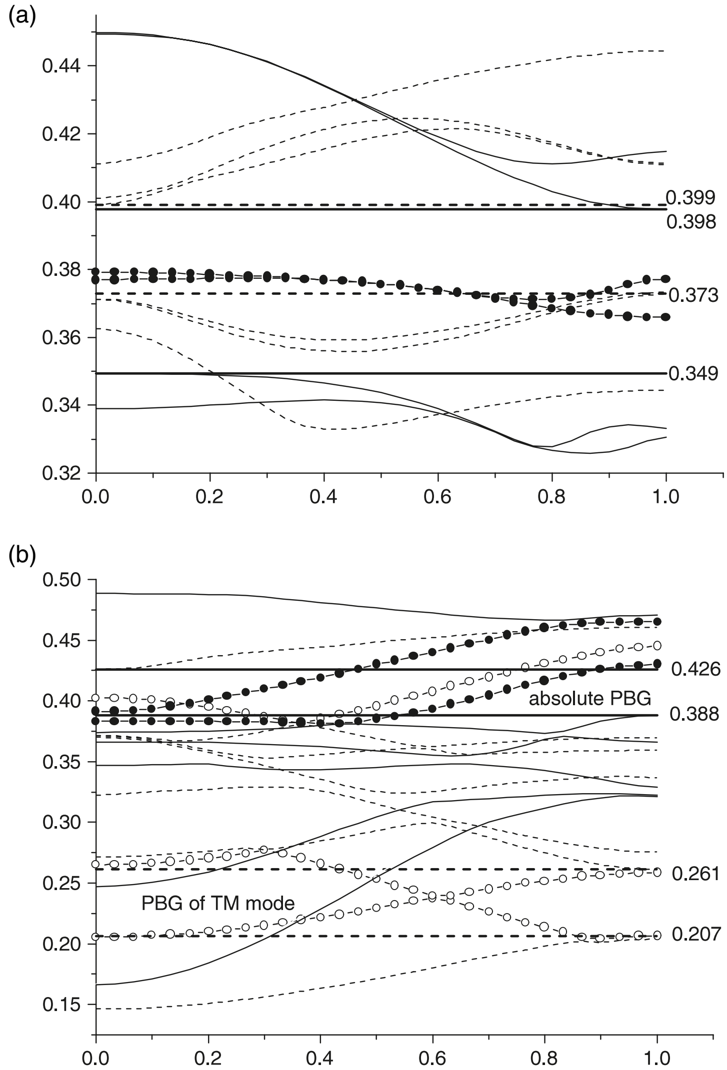

Figure 2. PBG structures of the mirror-symmetric PC heterostructure composed of two semi-infinite 2D rectangular lattices containing rotating rectangular air cylinders which are embedded in a homogeneous host dielectric of dielectric constant $\epsilon_b = 12.96$. The parameters used are as follows: $l_y/l_x = 0.8$; $l_a/l_b = 0.84$; filling fraction $f = 0.688$; $\theta_r = -\theta_l = 28°$. The solid lines, dashed lines, solid circle curves, and open circle curves correspond to the TE polarization modes, TM polarization modes, TE guide modes, and TM guide modes respectively; (a) after introducing a relatively longitudinal gliding of the cylinders in the lattices on either side of the interface of the heterostructure along the interface by $\mathrm{d}y = 0.35l_y$—two solid (dashed) horizontal lines define the range of the PBG for the TE (TM) mode; (b) after displacing the cylinders in the lattices on either side of the interface individually away from their normal sites, transversely leaving a distance of $\mathrm{d}x = 0.35l_y$ from the host dielectric around the interface.

of the square cylinders is $\theta = 30°$. Here a denotes the lattice constant of the square lattice. We consider a mirror-symmetric structure with $\theta_r = -\theta_l = 30°$. For this PC heterostructure (referred to as sample $3A_0$), there is only one PBG lying in the range $[0.395, 0.457](2\pi c/a)$ and its width is $\Delta\omega = 0.062(2\pi c/a)$; we do not observe any guide mode. However, on introducing relatively longitudinal gliding of the cylinders in the lattices on either side of the interface with the host dielectric along the interface by $\mathrm{d}y = 0.3a$ (the outcome is referred to as sample $3\mathrm{A}_{\mathrm{d}y}$), two TE guide modes and two TM guide modes appear inside the absolute PBG in the range $[0.388, 0.436](2\pi c/a)$; its gap width is $\Delta\omega = 0.048(2\pi c/a)$—larger than that ($\Delta\omega = 0.025(2\pi c/l_y)$ and $\omega_R = 11.6\%$) of sample $1\mathrm{A}_{\mathrm{d}y}$, as shown in figure 3(a). The modes extend continuously over the whole k_y-region. In view of this benefit and the width of the absolute PBG, we can safely say that the properties of this heterostructure (sample $3\mathrm{A}_{\mathrm{d}y}$) are better than those of sample $1\mathrm{A}_{\mathrm{d}y}$. We also observe similar variation of the frequency position of the guide modes with increase of $\mathrm{d}y$, shifting the edge of the upper band gap upward. When $\mathrm{d}y = 0.50a$, the guide modes disappear from the absolute PBG. In the lower-frequency region, there exists one TM polarization mode gap in the range $[0.224, 0.257](2\pi c/a)$, but no guide mode appears inside this gap.

We now study the effects of the relatively transverse displacement of the cylinders in the lattices on either side of the interface of the heterostructure away from their normal positions, leaving a distance $\mathrm{d}x$ from the host dielectric around the interface. The calculated results are displayed in figure 3(b). When $\mathrm{d}x = 0.2a$ (this version is referred to as sample $3\mathrm{A}_{\mathrm{d}x}$), there is an absolute PBG lying in $[0.425, 0.476](2\pi c/a)$ with a large width of $\Delta\omega = 0.051(2\pi c/a)$. Two TE guide modes and three TM guide modes are formed inside this absolute band gap, in which one TE guide mode and two TM guide modes span over the whole k_y-region continuously. Considering the absolute gap width and the number of guide modes, we believe that sample $3\mathrm{A}_{\mathrm{d}x}$ is the most favourable candidate material for serving as a light waveguide.

To further reveal the characteristics of the proposed PC heterostructures, we carry out systematic calculations of the PBG structures for various configurations. We first consider the mirror-symmetric heterostructures: different combinations of lattice type and shape of the air cylinders—for instance, the rectangular (square) lattice with rotating square (rectangular) air cylinders for different relatively longitudinal (transverse) shifts $\mathrm{d}y$ ($\mathrm{d}x$) of the cylinders in the lattices on either side of the interface, and different rotating angles of the air cylinders around the symmetric axis of the cylinder. Of course, we always fixed $\theta_r = \theta_l$ to preserve the mirror symmetry. The optimal parameters and the optimal PBG structures are tabulated in table 1. All the frequencies are measured in units of $2\pi c/l_y$ (or $2\pi c/a$) for the rectangular (or square) lattice, and we fixed $l_b/l_a = 0.84$ for the rectangular air cylinders. ω_R is the gm ratio. 'Num. of gm' (TE or TM) denotes the number of the TE or TM guide modes inside the absolute PBG of the heterostructure. For comparison, we also present the results for non-mirror-symmetric heterostructures with parameters identical to those of the corresponding mirror-symmetric heterostructure except that $\theta_r = \theta_l$ now. The favourable results obtained are listed in table 2. The structures of samples $1\mathrm{B}_0$ and $2\mathrm{B}_0$ are almost the same apart from different normals of the interfaces; i.e. the interface of sample $1\mathrm{B}_0$ is parallel to the short side of the lattice, while in contrast, the interface of sample $2\mathrm{B}_0$ is parallel to the long side of the lattice. When the displacement is zero, the interface does not have any effect on the band gap structures; therefore, these two samples possess similar band gap structures, i.e. there is a PBG lying in the range [0.363, 0.402] $(2\pi c/l_y)$. In contrast, sample $1\mathrm{A}_0$ ($2\mathrm{A}_0$) has different band gap structures to its counterpart $1\mathrm{B}_0$ (or $2\mathrm{B}_0$) because samples $1\mathrm{A}_0$ and $1\mathrm{B}_0$ correspond respectively to mirror-symmetric and non-mirror-symmetric configurations even if the relative displacement of the cylinders in the lattices on either side of the interface with the host dielectric is zero.

It is clearly seen from two tables that:

(i) The largest absolute gap width of the PC heterostructure can reach the value of the prototype PC; for instance, the width of the PBG in the prototype PC is $0.063(2\pi c/a)$,

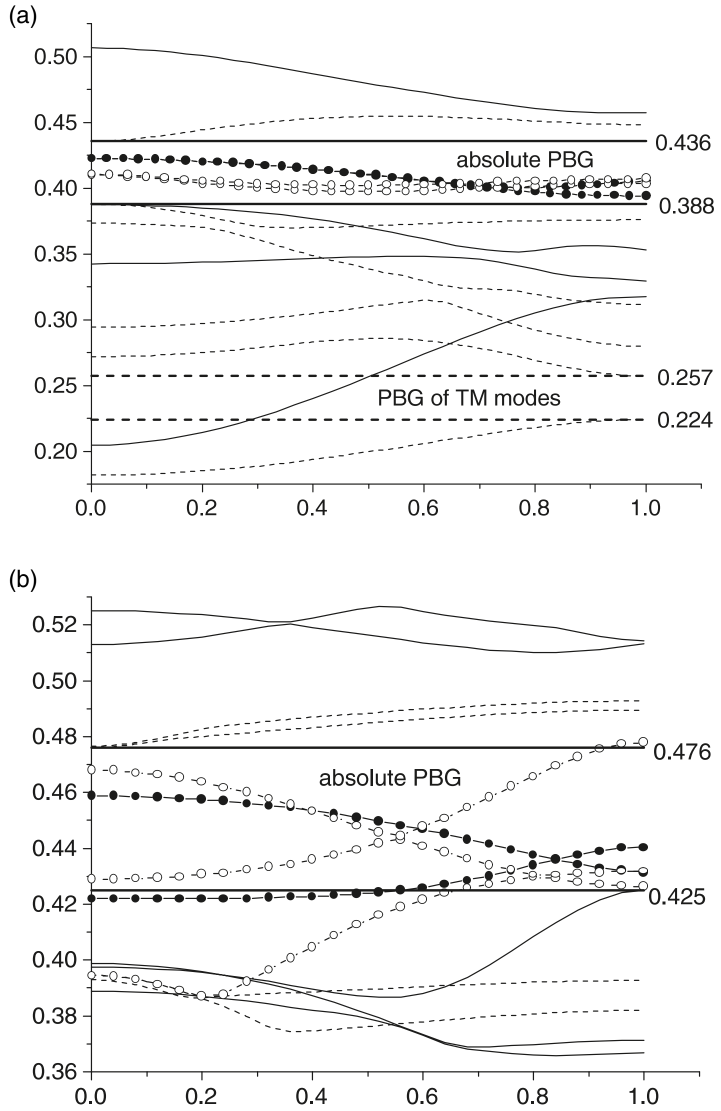

Figure 3. As figure 2, except that the rectangular lattice and rectangular cylinders are replaced by a square lattice and square cylinders. The parameters are: filling fraction $f = 0.680$; $\theta_r = -\theta_l = 30°$. (a) After introducing a relatively longitudinal gliding of the cylinders in the lattices on either side of the interface by $\mathrm{d}y = 0.30a$; (b) after making a relatively transverse displacement of the cylinders in the lattices on either side of the interface by $\mathrm{d}x = +0.20a$.

while sample $3\mathrm{A}_0$ has a width of the PBG of $0.062(2\pi c/a)$; the PBG width in sample $2\mathrm{A}_{\mathrm{d}y}$ is $0.064(2\pi c/l_y)$; the PBG width in sample $3\mathrm{B}_0$ is $0.066(2\pi c/a)$.

(ii) The samples in table 1 possess more guide modes than the samples in table 2. This result can be easily understood: as is well known, broken symmetry always favours the creation of localized states. The mirror-symmetric heterostructures possess more strongly broken symmetry on the interface than the non-mirror-symmetric samples.

As indicated above, when employing the plane-wave expansion method to calculate the PBG structures of the heterostructures, the size of the supercells should be chosen large enough

Table 1. PBGs and guide modes for mirror-symmetric PC heterostructures.

Sample	Lattice type	Shape of air cylinders	f	$\|\theta\|$ (deg)	dx	dy	$\Delta\omega$ ($2\pi c/l_y$ or $2\pi c/a$)	ω_R (%)	Num. of gm (TE)	Num. of gm (TM)
$1A_0$	Rectangle[a]	Rectangle	0.688	28	0	0	$0.400 - 0.366 = 0.034$	8.9	0	0
$1A_{dy}$					0	$0.35l_y$	$0.398 - 0.373 = 0.025$	6.48	2	0
$1A_{dx}$					$0.35l_y$	0	$0.426 - 0.388 = 0.038$	9.3	2	1
$2A_0$	Rectangle[b]	Rectangle	0.688	118	0	0	$0.476 - 0.452 = 0.024$	5.2	0	0
$2A_{dy}$					0	$0.30l_y$	$0.508 - 0.444 = 0.064$	13.4	2	4
$2A_{dx}$					$0.25l_y$	0	$0.523 - 0.464 = 0.059$	11.2	2	2
$3A_0$	Square	Square	0.680	30	0	0	$0.457 - 0.395 = 0.062$	14.6	0	0
$3A_{dy}$					0	$0.30a$	$0.436 - 0.388 = 0.048$	11.7	2	2
$3A_{dx}$					$0.20a$	0	$0.476 - 0.425 = 0.051$	11.3	2	3
$4A_0$	Square	Rectangle	0.585	45	0	0	$0.402 - 0.364 = 0.038$	9.9	0	0
$4A_{dy}$					0	$0.30a$	$0.402 - 0.361 = 0.041$	10.7	2	2
$4A_{dx}$					$0.35a$	0	$0.417 - 0.386 = 0.031$	7.7	3	2

[a] $l_y/l_x = 0.8$.
[b] $l_y/l_x = 1/0.8$.

Table 2. PBGs and guide modes for non-mirror-symmetric PC heterostructures.

Sample	Lattice type	Shape of air cylinders	f	$\|\theta\|$ (deg)	dx	dy	$\Delta\omega$ ($2\pi c/l_y$ or $2\pi c/a$)	ω_R (%)	Num. of gm (TE)	Num. of gm (TM)
$1B_0$	Rectangle[a]	Rectangle	0.688	28	0	0	$0.402 - 0.363 = 0.039$	10.5	0	0
$1B_{dx}$					$0.35l_y$	0	$0.424 - 0.387 = 0.037$	9.1	1	1
$2B_0$	Rectangle[b]	Rectangle	0.688	118	0	0	$0.502 - 0.452 = 0.050$	10.5	0	0
$2B_{dx}$					$0.25l_y$	0	$0.530 - 0.475 = 0.055$	10.9	1	1
$3B_0$	Square	Square	0.680	30	0	0	$0.458 - 0.392 = 0.066$	15.5	0	0
$3B_{dx}$					$0.30a$	0	$0.478 - 0.414 = 0.064$	14.3	2	1

[a] $l_y/l_x = 0.8$.
[b] $l_y/l_x = 1/0.8$.

Table 3. Comparison of frequencies and the widths of PBG for some samples when using small and large sizes of the supercells and numbers of plane waves.

Sample	Lattice type	Shape of air cylinders	f	$\|\theta\|$ (deg)	dx	dy	$\Delta\omega$ ('old'[a]) ($2\pi c/a$)	$\Delta\omega$ ('new'[b]) ($2\pi c/l_y$)
$3A_{dy}$	Square	Square	0.068	30	0	$0.30a$	$0.436 - 0.388 = 0.048$	$0.440 - 0.392 = 0.048$
$3B_0$	Square	Square	0.068	30	0	0	$0.458 - 0.392 = 0.066$	$0.458 - 0.394 = 0.068$
$3B_{dx}$					$0.30a$	0	$0.478 - 0.414 = 0.064$	$0.474 - 0.409 = 0.063$

[a] 'old' means that the size of supercells is $m = 4$ and the number of plane waves is 1235.
[b] 'new' means that the size of supercells is $m = 8$ and the number of plane waves is 1679.

to guarantee that the effect of coupling between neighbouring supercells is negligible. To confirm the correctness of our results, we recalculated the PBG structures after enlarging the unit size of the supercells from $m = 4$ to 8 and increasing the number of plane waves from 1235 to 1679 for some samples—for instance, sample $3A_{dy}$ in table 1 and samples $3B_0$, $3B_{dx}$ in table 2. The results obtained are displayed in table 3, in which 'old' results correspond to $m = 4$ and $N = 1235$, and the 'new' ones correspond to $m = 8$ and $N = 1679$. It is clearly seen that two results only show small changes in the frequency and the gap width. The maximal relative errors are less than 1.03% for the frequency position of the gap and 3.08% for the gap width. Consequently, we believe that our results are reasonable.

As regards the possible fabrication of the proposed PC heterostructures using state-of-the-art of technology: it is possible to produce them. For instance, various patterns in heterostructures can be designed by computer, or using polymer templates pattered either by holographic [18] or x-ray lithography [19]. PC heterostructures with specified patterns may then be fabricated directly on a dielectric material by focused-ion-beam micromachining [20] with computer control or by chemically assisted ion-beam etching technology [21].

4. Summary

In this paper, we have investigated the properties of guide modes localized at the interfaces of mirror-symmetric or non-mirror-symmetric heterostructures of PCs. We calculate the PBGs for various configurations of the heterostructures using the plane-wave expansion method in combination with a supercell technique. We find that the absolute gap width and the number of guide modes strongly depend on the geometric and physical parameters of the heterostructures. The mirror-symmetric heterostructures can support more guide modes inside broader PBGs than the non-mirror-symmetric heterostructures. It is expected that the guide modes in such heterostructures could be artificially tailored by changing relevant parameters of systems.

Acknowledgments

This work was supported by Chinese National Key Basic Research Special Fund and by the Natural Science Foundation of Beijing, China.

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