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Photonic-band-gap structures and guide modes in two-dimensional magnetic photonic crystal heterostructures

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Abstract. We first investigate the band gap structures of two-dimensional magnetic photonic crystals (MPC) composed of rectangular (square) magnetic cylinders embedded in a host dielectric material in the rectangular (square) lattice, and we then study guide modes at interface of MPC heterostructures (MPCHs) by use of plane wave expansion method in combination with supercell technique. We find that both the mirror-symmetric MPCHs and the mixed-type MPCHs composed of square cylinders in a square lattice can produce the TM guide modes even without any lattice distortions. This feature is quite different from that of the non-magnetic PC heterostructures, in which the occurrence of the guide modes requires the relatively longitudinal gliding or transverse displacement of lattices. It may provide a new way to generate guide modes and apply to the device of light wave guides.

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1 Introduction

The band structures of photonic crystal (PC) have attracted great interest after the pioneering works of Yablonovitch and John [1,2]. The conventional non-magnetic photonic crystal (NMPC) is a periodical modulation structure of dielectric constant; its dispersion relation of photons exhibits some forbidden frequency regimes, i.e., photonic band gap (PBG) structures. The presence of PBGs provides a wide platform of many applications, for instance, the light wave guides used for controlling the propagation of light waves flexibly [3–5]. The light wave guides can be created by introducing line defects in an ideal PC. Recently, Li et al. have reported the band structures of a heterostructure composed of two semi-infinite two-dimensional PCs with different filling factors for circular cylinders [6]. They found that the interface states can be generated either by introducing relatively longitudinal gliding of the cylinders in the lattices on the two sides of the interface of heterostructure (referred to the longitudinally gliding of lattice), or displacing the cylinders in the lattices on the either sides of the interface, transversely leaving a distance about the interface (referred to the transverse displacement of lattices). Their work proposed a new way to create the guide modes. More recently, we suggested another style of PC heterostructures (PCHs) which are composed of rectangular (square) air cylinders, setting in a rectangular (square) lattice, with different rotation angles on the two sides of interface [7]. For instance, the rectangular cylinders in the left lattice and right lattice of the PCHs are rotated by an identical angle but in clockwise and anticlockwise, respectively. It exhibits mirror-symmetry with respect to the interface. A lot of TE (TM) guide modes are observed when the mirror-symmetric is broken, e.g. introducing the relatively longitudinal gliding or transverse displacement of the lattices together with cylinders. However, for the perfect mirror symmetric PCH, there is no any guide mode appearing within the PBGs. Therefore, it is an important and interesting topic how to find new kind of PCHs that can produce guide modes without making any relative shift of the Bravais lattices on the either sides of the interface of the PCH.

Many researchers have devoted to diversify the class of PCs, for instance, not only including dielectric medium but also involving other materials such as semiconductors [8], conductors, liquid-crystals [9,10] and magnetic materials [11–13]. It is worth pointing out that magnetic photonic crystal (MPC), as a new candidate of PC, has been widely studied theoretically [11–13]. One of the foci is the investigations of the effects of magnetic permeability on the frequency position and width of PBGs. As the MPC is composed of magnetic (dielectric) cylinders

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periodically embedded in dielectric (magnetic) materials, therefore, the wave impedance should bring significant influence on PBGs [14]. The effects of magnetic permeability may lead to a wide PBG located at low frequency regime, which results in a large gap-midgap ratio $\omega_R = \Delta\omega/\omega_g$, where ω_g denotes the central frequency of the PBG and $\Delta\omega$ the PBG width. The large $\Delta\omega$ and ω_R are favorable to the fabrication of the light waveguide.

In this paper, we study the properties of the guide modes in the MPCHs. We first calculate the band structures of two-dimensional MPCs which are composed of magnetic rectangular (square) cylinders in rectangular (square) lattice, and then investigate the guide modes of the heterostructures composed of two semi-infinite MPCs. The plane-wave expansion method in combination with a suppercell technique is employed. We find that the MPCHs with mirror-symmetric structures composed of square cylinders in square lattice or the mixed MPCHs composed of square cylinders in square lattice can produce the TM guide modes without modifying the original MPCHs.

The rest parts of this article are organized as follows. Section 2 describes the necessary formulas used in the calculations for the 2D MPCHs. The calculated results for prototype MPCs and the related heterostructures are presented and discussed in Section 3. Finally a brief summary is given in Section 4.

2 Formulas

We consider a two-dimensional PC composed of cylinders with dielectric constant $\epsilon(x, y)$ and magnetic permeability $\mu(x, y)$; both the dielectric constant and the magnetic permeability are homogeneous along the z-axis. The electromagnetic wave fields in the 2D PC are governed by the following equations [11]

$$\nabla\times\left[\frac{1}{\epsilon(x,y)}\nabla\times\left(\frac{1}{\mu(x,y)}\mathbf{B}(x,y)\right)\right] = \left(\frac{\omega}{c}\right)^2\mathbf{B}(x,y). \quad (1)$$

We now treat equation (1) by use of plane wave expansion method [11–15], i.e. consider a periodical modulation of magnetic induction function in the 2D MPC, and expand magnetic induction function in terms of plane waves as

$$\mathbf{B}(\mathbf{r}) = \sum_{\mathbf{G}}\sum_{\lambda=1}^{2} b_\lambda(\mathbf{G})\mathbf{e}_\lambda e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}, \quad (2)$$

where $\mathbf{r} = (x, y)$ and $\mathbf{G}$ denotes the reciprocal lattice vector of the 2D lattice, and $\mathbf{e}_1(\mathbf{e}_2)$ is the unit vector of the polarization direction of the TE(TM) modes. Substituting equation (2) into equation (1), we can derive two eigen equations as

$$\sum_{\mathbf{G}\mathbf{G}'} \epsilon^{-1}(\mathbf{G}_0 - \mathbf{G}')\mu^{-1}(\mathbf{G}'-\mathbf{G})(\mathbf{k}+\mathbf{G}_0)\cdot(\mathbf{k}+\mathbf{G}')b_1(\mathbf{G}) = \left(\frac{\omega}{c}\right)^2 b_1(\mathbf{G}_0), \quad (3a)$$

for the TE mode, and

$$\sum_{\mathbf{G}\mathbf{G}'} \epsilon^{-1}(\mathbf{G}_0 - \mathbf{G}')\mu^{-1}(\mathbf{G}'-\mathbf{G})(\mathbf{k}+\mathbf{G})\cdot(\mathbf{k}+\mathbf{G}')b_2(\mathbf{G}) \times \frac{|\mathbf{k}+\mathbf{G}_0|}{|\mathbf{k}+\mathbf{G}|} = \left(\frac{\omega}{c}\right)^2 b_2(\mathbf{G}_0), \quad (3b)$$

for the TM mode. $\epsilon(\mathbf{G})$ and $\mu(\mathbf{G})$ represent the Fourier transforms of $\epsilon(\mathbf{r})$ and $\mu(\mathbf{r})$, respectively. These equations can be numerically solved and used to calculate the PBG structures of MPCHs in combination with supercell technique [4–6]. The size of supercells should choose large enough to guarantee the correctness of the results, i.e., the coupling effects between neighboring supercells can be neglected, thus the plane-wave expansion method still can be approximately suitable to the calculation of the PBGs structures of heterostructures. The heterostructure considered here is composed of two semi-infinite 2D rectangular (or square) lattices with rectangular (or square) magnetic (or dielectric) cylinders embedded in a homogeneous dielectric (or magnetic) medium. A sketch of the model MPCH is shown in Figure 1a. The lattice constants of the rectangular (square) lattice are denoted by $l_x(a)$ and $l_y\,(a)$ for the x and y axes; the short-side and long-side lengths of the individual rectangular cylinders 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- and left-side lattices, respectively. The y axis is parallel to the interface. We also display the modified lattice structures of the MPCH after making the longitudinal gliding of the cylinders in the lattice on the either sides of the interface of heterostructure along the interface, as shown in Figure 1b. To determine the PBG structures of the perfect MPCs, we employ the plane wave expansion method, however, in the calculations of the dispersion curves of the MPCHs, we adopt the supercell method, in which the enlarged rectangle lattice consists of $m \times 1$ original unit cells from either sides of the interface of heterostructure. Thus, every unit cell of the supercells is composed of $2m \times 1$ original unit cells. The primary vectors of this supercell are chosen by $\mathbf{a}_1 = (2m, 0)l_x$ and $\mathbf{a}_2 = (0, 1)l_y$. The first Brillouin zone is of rectangle. The PBG structures of the heterostructure are determined from calculating the photonic density of states (DOS) only in the irreducible Brillouin zone of the supercell lattice. The number of the plane waves in the expansion should be large enough to guarantee the precision of numerical results.

3 Numerical results

3.1 Band structures of prototype MPCs

We first calculate the density of states (DOS) of the MPC which is composed of rectangular pure magnetic cylinders setting in a rectangular lattice and embedded in a pure dielectric material. We set $\theta_r = \theta_l$(referred to sample A), the calculated result is shown in Figure 3a. From reference [15], it is known that this kind of the non-magnetic

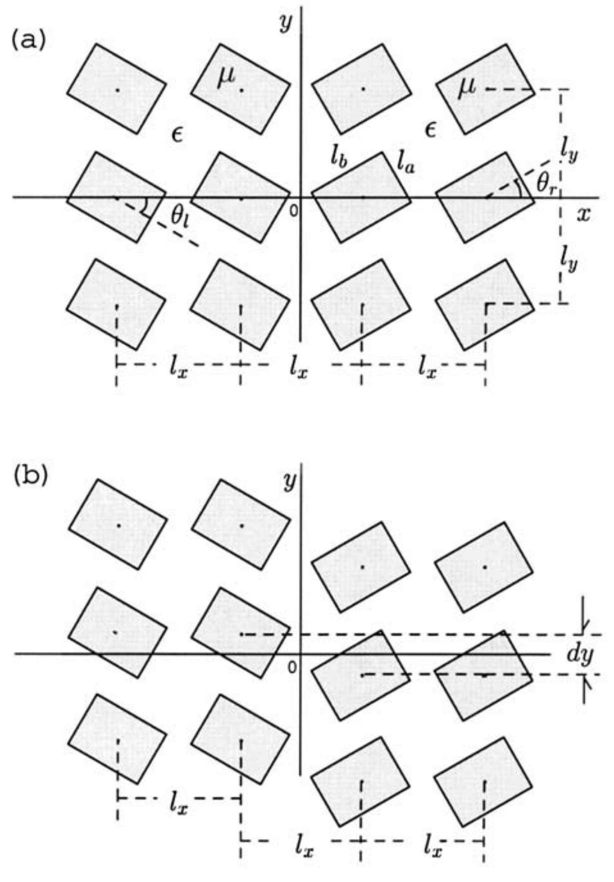

Fig. 1. Sketch of magnetic photonic crystal heterostructure (MPCH). The MPCH is composed of two semi-infinite 2D PCs with rectangular (square) lattice together with rectangular (square) pure magnetic cylinders embedded in a pure host dielectric. The lattice constants of the rectangular (square) lattice are denoted by $l_x(a)$ and $l_y(a)$ for the x and y axes; the short-side and long-side lengths of the rectangular magnetic cylinders by l_a and l_b, respectively. θ_r and θ_l are the inclined angles of the long-side of the rectangle cylinder against the x axis for the right and left lattices of the interface, respectively. (a) The perfect MPCH; (b) introducing relatively longitudinal gliding dy of the the lattices together with cylinders on the either sides of the interface of heterostructure to the host medium along the interface.

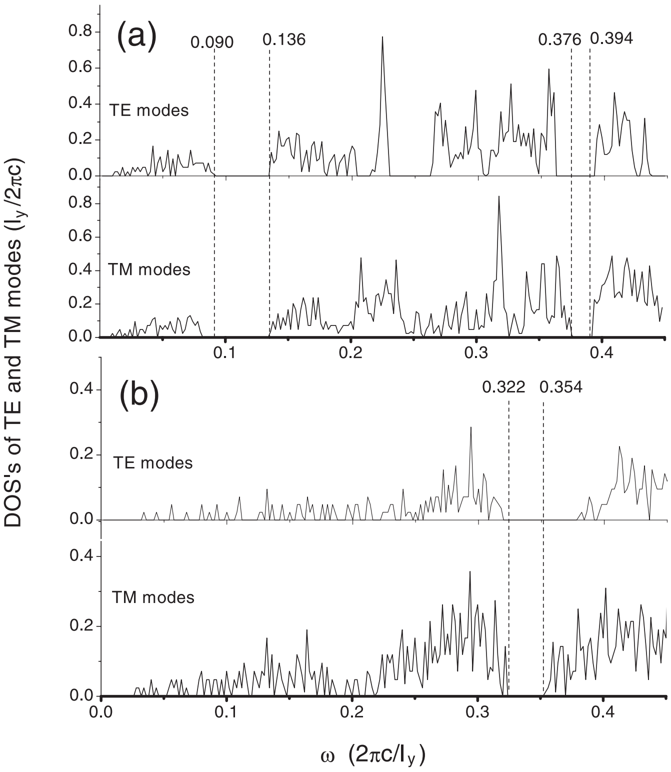

Fig. 2. DOSs of the MPC composed of rectangular magnetic cylinders embedded in a homogeneous dielectric medium in a rectangular lattice. The parameters used are as follows: The short-long side length ratio of lattice is $l_y/l_x = 0.8$; the short-long side length ratio of scatterer is $l_a/l_b = 0.84$; the filling factor is $f = 0.668$, and the rotation angle of rectangular cylinders is $\theta = 28°$ The dielectric constant is $\epsilon_b = 16.00$ and the magnetic permeability is (a) $\mu = 13.69$ and (b) $\mu = 1$.

PCs (NMPCs) can produce the largest absolute PBG in the frequency range of $[0.363, 0.405](2\pi c/l_y)$ when choosing the following parameters : $l_a/l_b = 0.84$, $l_y/l_x = 0.8$, $\epsilon = 12.96$, filling factor $f = 0.688$, and rotating angle $\theta = 28°$. Fixing $l_a/l_b = 0.84$ and $l_y/l_x = 0.8$, i.e., retaining the rectangular shape of the cylinders and the lattice, we consider the magnetic cylinders and scan the permeability in combination with the change of the other parameters such as the rotation angle, the filling factor, and the dielectric of the host material, to find optimal parameters. Finally, the largest absolute PBG in the range of $[0.090, 0.136](2\pi c/l_y)$ can be obtained for the parameters of $f = 0.668, \theta = 28°$, and $\epsilon = 16.00, \mu = 13.69$, as shown in Figure 2a. These values of ϵ and μ are completely compatible with realistic materials. Here 400 k-points in the 2D first BZ have been involved in the calculations of the DOS. For validating the precision, we checked the absolute PBG of sample A by the band structure calculation directly and find that the relative deviation is less than 1%. Therefore, we believe that this number of k-points is sufficient large enough for determining the PBG range. From Figure 2a, we obtain that the gap width is $\Delta\omega = 0.046(2\pi c/l_y)$, the frequency position of the midgap is $\omega_g = 0.113(2\pi c/l_y)$, and the large gap-midgap ratio is $\omega_R = \Delta\omega/\omega_g = 40.7\%$. This gap is referred to the first absolute PBG. Besides it, the second absolute PBG stands at a higher frequency regime. However, comparing to the corresponding NMPC sample presented in reference [15], there exists an absolute gap located at a higher frequency position of $\omega_g = \frac{1}{2}(0.405 + 0.363) = 0.384(2\pi c/l_y)$. It is evident that the gap-midgap ratio in the MPC now is larger than that in the NMPC. To reveal the effect of the permeability of cylinders on the band structures of PC, we recalculate the PBGs for another sample quite similar to sample A only except for the permeability $\mu = 1$ of cylinders, fixed other parameters. The corresponding

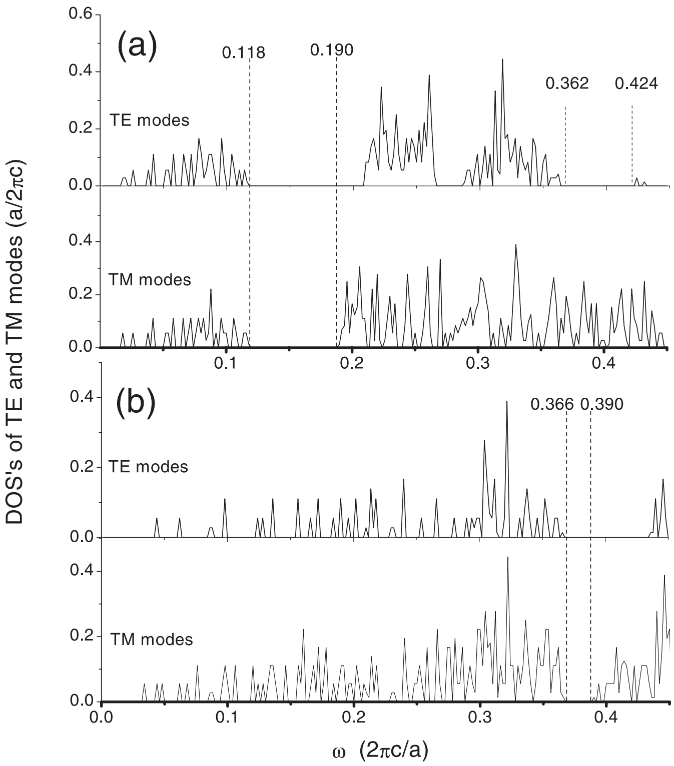

Fig. 3. Same as Figure 2 except only for the pure magnetic square cylinders setting on a square lattice. The parameters used are: $f = 0.59$, $\theta = 30.5°$, $\epsilon_b = 12.96$, (a) $\mu = 8.41$ and (b) $\mu = 1$.

DOSs are plotted in Figure 2b. The absolute PBG is located at $[0.322, 0.354](2\pi c/l_y)$ below the second absolute PBG of the MPC, comparing Figures 2a and 2b. When increasing the permeability of cylinders, this absolute gap is gradually shifted upward the higher frequency regime, approaching the second absolute gap of sample A in Figure 2a, and meanwhile, its gap width is substantially narrowed. In addition, a new absolute gap is opened at a lower frequency regime. When $\mu = 13.69$, the new gap is opened at $[0.090, 0.136](2\pi c/l_y)$, which now is re-referred to the first absolute gap, while the original absolute gap at a higher frequency of $[0.376, 0.394](2\pi c/l_y)$ now is re-referred to the second absolute gap, as shown in Figure 2a. It is worth pointing out that the width ($0.046\ 2\pi c/l_y$) of the first absolute gap is much larger than that ($0.018\ 2\pi c/l_y$) of the second absolute gap.

We now change the shape of the cylinders and the lattice. Figure 3a displays the DOSs of square lattice containing square magnetic cylinders (referred to sample B). The optimal parameters can be found by consulting to reference [15] and scanning the related parameters over a large range to search for the maximal absolute PBG width, fixed the shape of square cylinders and the square lattice. The optimal parameters are found to be $\epsilon = 12.96$, $\mu = 8.41$, $f = 0.59$, and $\theta = 30.5°$. Sample B has a broad absolute PBG lying in $[0.118, 0.190](2\pi c/a)$; the width is $\Delta\omega = 0.072(2\pi c/a)$, and $\omega_R = 46.8\%$, compared to sample A. Here a denotes the lattice constant of square lattice. Similar to sample A, using magnetic cylinders can lead to the opening of a new gap at low frequency regime. A major difference between samples A and B is that only an absolute PBG of lower frequency exists in sample B. Although the second absolute gap of higher frequency for the TE modes exists in the range of $[0.362, 0.424](2\pi c/a)$ in Figure 3a when $\mu = 8.41$, the narrow width gap of the TM mode now is closed. Therefore, the second absolute gap of the higher frequency disappears now, as seen in Figure 3a. For a comparison, we also plot the DOSs for a sample quite similar to sample B except only for $\mu = 1.0$, as shown in Figure 3b. It is seen that only one absolute PBG lies at the higher frequency region of $[0.366, 0.390](2\pi c/a)$. When increasing μ, this absolute gap is closed gradually. It leads to only the survival of the lower frequency absolute gap.

The above results are calculated by a plane-wave expansion method with the use of the number $N = 1235$ of the plane waves and $m = 4$. To confirm the correctness of the results, we increase this number to $N = 1679$ and recalculate the PBG structures of Sample B. The obtained results show that the absolute PBG is lying in a range of $[0.115, 0.186](2\pi c/a)$. The relative deviation between two calculated results for $N = 1235$ and 1679 is 1.39% for $\Delta\omega$ and 0.33% for ω_g.

3.2 Guide modes in MPCH with rectangular (square) cylinders in a rectangular (square) lattice

We now turn to study the characteristics of the guide modes of the MPCH composed of two magnetic PCs, as shown in Figure 1. Two semi-infinite 2D MPCs on both sides of the interface have the physical and geometric parameters as the same as those of sample A, i.e., $l_a/l_b = 0.84$, $l_y/l_x = 0.8$, $\epsilon_b = 16.00$, $\mu = 13.69$, $f = 0.668$,and $\theta = 28°$ except only for different rotation angles of rectangular (square) cylinders. The rotation angle of the rectangular cylinders on the either sides of the interface is opposite, i.e., θ_l and $\theta_r(= -\theta_l)$, respectively, as shown in Figure 1a. It forms a mirror-symmetric structure with respect to interface. The obtained dispersion spectrum is similar to the mirror-symmetric NPCHs, that is, rotating the rectangular cylinders on two semi-infinite PCs in opposite directions can not generate any guide mode when not introducing relatively longitudinal gliding or transversely displacing of lattices together with cylinders. In this heterostructure, we only observe an absolute PBG at $[0.089, 0.133](2\pi c/l_y)$, it is a little narrower than the PBG at $[0.090, 0.136](2\pi c/l_y)$ of the corresponding prototype MPC, i.e., sample A. When introducing relatively longitudinal gliding of the lattice together with cylinders on the either sides of the interface of heterostructure to the host medium by a distance of $dy = 0.5l_y$, the original mirror symmetry of structure is broken now, two TM guide modes appear inside the absolute PBG. The band structure is shown in Figure 4. Here the solid (dashed) lines correspond to the TE (TM) modes; the two solid horizontal lines indicate the edges of absolute PBG, and the open circles denote the TM guide modes. Hereafter, we always employ these line styles to plot the PC band structures.

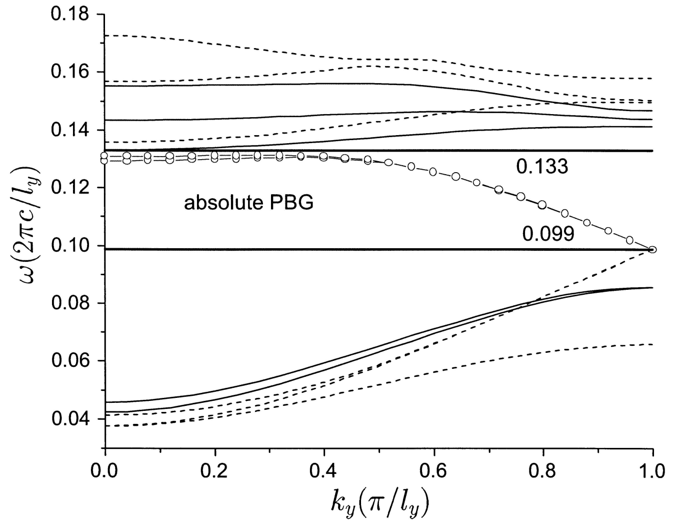

Fig. 4. Band structures of the MPCH composed of rectangular magnetic cylinders in a rectangular lattice when introducing relatively longitudinal gliding of the lattices together with cylinders by $dy = 0.5l_y$. The parameters are the same as those in Figure 2a except for the rotation angle of rectangular cylinders $\theta_r = -\theta_l = 28°$ now. The solid lines, dashed lines, and opened circles correspond to the TE modes, TM modes, and TM guide modes, respectively.

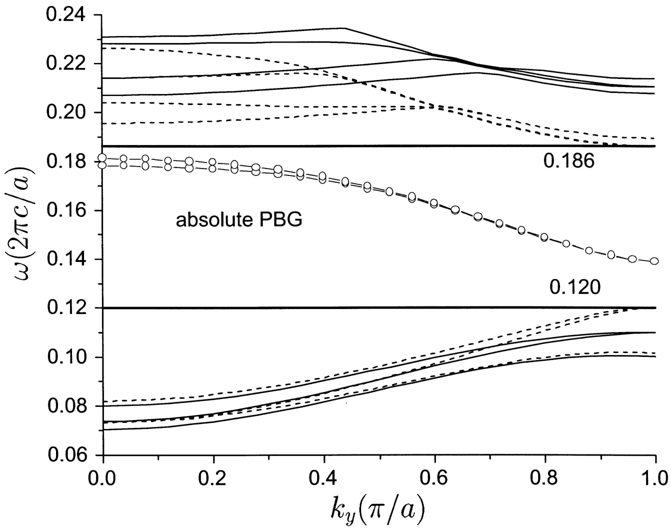

Fig. 5. Band structures of the MPCH composed of square magnetic cylinders in a square lattice. The parameters are as the same as those in Figure 3a except for $\theta_r = -\theta_l = 30.5°$.

For clarity, only several bands around the first absolute PBG are plotted in Figure 4. It is seen from Figure 4 that the absolute PBG locates at $[0.099, 0.133](2\pi c/l_y)$ with a ratio of $\omega_R = 29.3\%$ and a width of $\Delta\omega = 0.034(2\pi c/l_y)$ narrower than that of the perfect MPCH. It is evident that $\Delta\omega$ and ω_g in the perfect MPCH are much larger than those in the corresponding NMPCH with the same gliding distance of $d_y = 0.5l_y$. In the later case, we observe an absolute PBG at $[0.373, 0.399](2\pi c/l_y)$ [7] with $\Delta\omega = 0.025(2\pi c/l_y)$ and $\omega_R = 6.5\%$. When changing the gliding distance, the frequency of the guide modes can be shifted accordingly.

We now turn to consider another structure. We choose two pieces of sample B (square cylinders in the square lattice with $\epsilon = 12.96, \mu = 8.41, f = 0.59, \theta = 30.5°$) to construct a mirror-symmetric MPCH. We find that two TM guide modes appear in the absolute PBG. The band structures are plotted in Figure 5. The absolute PBG stands at the range of $[0.120, 0.186](2\pi c/a)$ with a width of $\Delta\omega = 0.066(2\pi c/a)$ and $\omega_R = 43.1\%$. Two TM guide modes extend over a full region of k_y, which is favorable for light waveguides. More interesting feature of this MPCH is that the occurrence of the guide modes does not request any lattice distortion. This property is quite different from that of the NMPC heterostructures (NMPCHs) composed of the air circular cylinders in a square lattice with different filling factors on the either sides of the interface [6] or the air rectangular (square) cylinders in a rectangular (square) lattice with different rotation angles of cylinders [7]. In these NMPCHs, to produce guide modes, the relatively longitudinal gliding or transverse displacement of lattices is necessary [7].

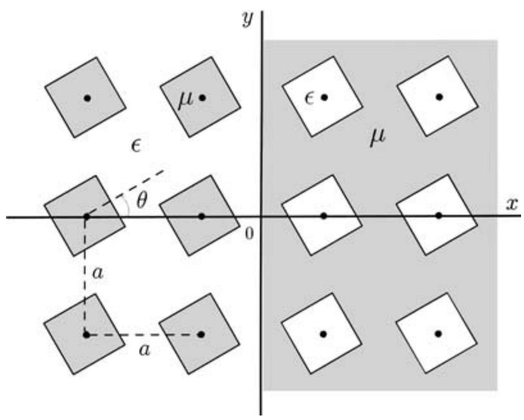

Fig. 6. Sketch of the mixed-type MPCH. The shadows and blank areas represent the pure magnetic material with permeability μ and the pure dielectric with the dielectric constant ϵ, respectively.

3.3 Guide modes in the mixed MPCH

We now consider another type of MPCHs, the so-called mixed type MPCH is schematically shown in Figure 6. The semi-infinite MPC on the left (right) side of the interface is composed of square pure magnetic (pure dielectric) cylinders embedded in a pure dielectric (pure magnetic) background medium in a 2D square lattice. The magnetic (dielectric) material, wherever it appears in the left side of the interface as the scatterers (background) or in the right side as the background (scatterers), always possesses the same permeability (dielectricity). The square cylinders in the two semi-infinite MPCs have identical rotation angle. We choose the parameters as $\epsilon = 12.96, \mu = 8.41, \theta = 30.5°$, and $f_l = f_r = 0.59$. Here f_l and f_r denote the filling factors in the left and the right MPCs, respectively. Namely, the PC on the left of interface just corresponds to the prototype structure of

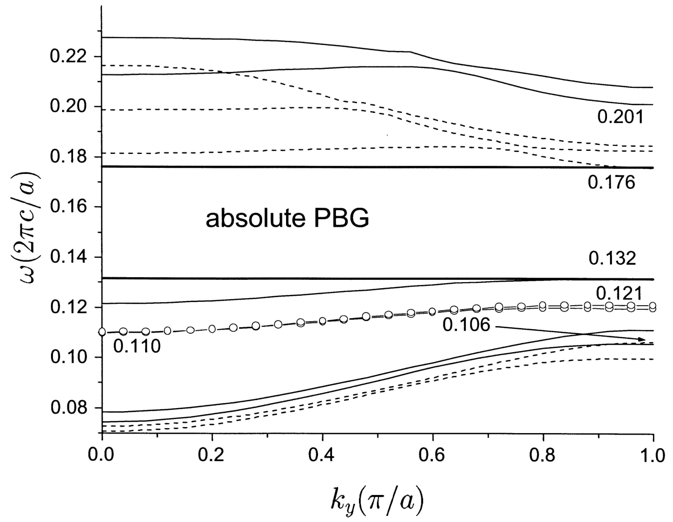

Fig. 7. Band structures of the mixed-type MPCH composed of square cylinders in a square lattice with $\epsilon_b = 12.96$, $\mu = 8.41$, and the filling factor is $f_l = f_r = 0.59$.

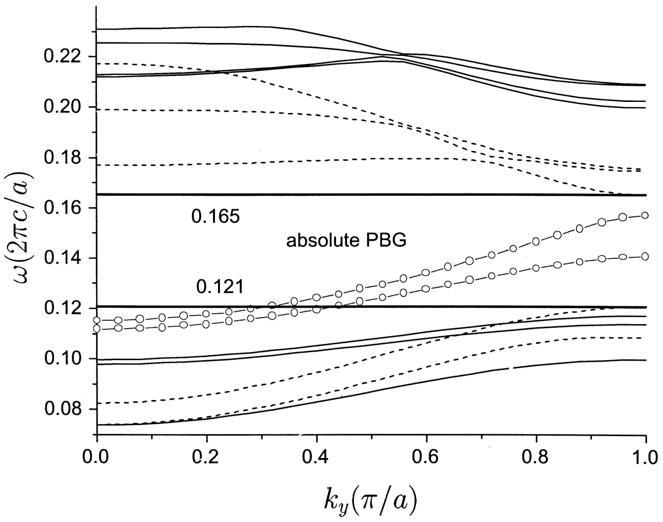

Fig. 8. Same as Figure 7 except only for the left filling factor of $f_l = 0.320$ and the right filling factor of $f_r = 0.600$.

sample B that possesses a large PBG, as shown in Figure 3. The calculated PBG spectrum is displayed in Figure 7. In this mixed MPCH, the PBG of the TM modes is located at the frequency range of $[0.106, 0.176](2\pi c/a)$, while the PBG of the TE mode is located at the frequency range of $[0.132, 0.201](2\pi c/a)$. In other words, the absolute PBG is formed in $[0.132, 0.176](2\pi c/a)$. Two TM guide modes span over the frequency range from 0.110 to $0.121(2\pi c/a)$. Thus, these two TM localized modes are out of the frequency range of the absolute gap and they do not generate any guide mode now.

To produce the guide modes, we adjust the related parameters, and find that the change of the filling factors f_l and f_r can effectively shift the frequency position of the localized modes and create guide modes. For instance, we choose $f_l = 0.320$ and $f_r = 0.600$, the absolute PBG shifts down to the frequency range of $[0.121, 0.165](2\pi c/a)$ and meanwhile two localized modes go upward entering the PBG, as shown in Figure 8. The guide modes now appear in the region of k_y from 0.4 to 1.0 $(2\pi/a)$. The PBG width is $\Delta\omega = 0.044(2\pi c/a)$ and the gap-midgap ratio is $\omega_R = 30.8\%$ in this special mixed-type MPCH.

As indicated in reference [6], the NMPCH composed of circles cylinders with different filling factors on either sides of the interface can not create any guide mode when not introducing the relatively longitudinal gliding or transverse displacement of lattices. This conclusion still remains for the NMPCH when the scatterers are square air cylinders. We confirm this conclusion by the calculations with the use of various filling factors in the lattices on the either sides of the interface. For instance, when scanning the filling factor from 0.59 to 0.73 with an increment of 0.01, no any interface state can be observed. However, in the mixed-type MPCH, the difference of filling factors of the PCs on the either sides of the interface can generate guide modes even without making any longitudinal gliding or any transverse displacement of lattices together with cylinders. We also calculate the PBGs of the mixed-type MPCH composed of rectangular cylinders in the rectangular lattice. There is no any guide mode for the perfect MPCH.

4 Summary

We have calculated the DOSs of the MPCs and the PBG structures of the MPCHs with the use of the plane-wave expansion method in combination with a supercell technique. The large absolute PBGs in the MPCs, which are composed of rectangular (square) pure magnetic cylinders embedded in a pure dielectric medium background with rectangular (square) lattice, can be obtained by choosing proper parameters. Based on the obtained PBGs structures, we constructed two kinds of MPCHs and investigated the properties of the guide modes. In mirror-symmetric MPCHs, we find that, when square cylinders are set on the square lattice, two TM guide modes can be created even without making any longitudinal gliding or transverse displacement of lattice together with cylinders. Regarding to the mixed-type MPCHs composed of two pieces of semi-infinite MPCs in which the PC on the left (right) side of the interface consists of square pure magnetic (pure dielectric) scatterers embedded in a pure dielectric (pure magnetic) background medium in a 2D square lattice. The magnetic (dielectric) material, whenever it appears in the left side of the interface as cylinders (background) or in the right side as background (cylinders), possesses the same permeability (dielectricity). When using different filling factors for the PCs on the opposite side of the interface, we find that two TM guide modes can be generated without introducing any lattice distortion. It is expected that introducing magnetic material into the PCs should diversify the candidate of the PCs in practical applications.

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