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The equivalent structure and some optical properties of the periodic-defect photonic crystal

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The concept of the effective medium is used to deal with problems of defects in photonic crystals (PhCs) throughout this paper. First, scattering phenomena in PhCs with defects are investigated and can be very well replaced by those in an effective medium with effective defects in interesting frequency region. It is based on the fact that the Bloch wave in the defect-free PhC very approximates to the wave in the effective medium. Then a periodic-defect PhC created by adding periodic defects into the defect-free PhC is proposed. It can be replaced with an effective PhC by utilizing the concept of effective periodic defects embedded into an effective medium. We verify the equivalence between the periodic-defect PhC and the effective PhC by comparing their photonic band structure (PBS) and photonic band gaps (PBGs) as well as transmissions. Next, the effective PhCs instead of the periodic-defect PhCs are used to investigate the variance of the PBGs by applying different periodic defects. The substitution allows us successfully predicting the negative refraction in the periodic-defect PhC through the PBS of the effective PhC. Finally, the field distributions and Fourier coefficients of waveguide modes in the effective PhC and the periodic-defect PhC are equivalent by the supercell method confirmations. © *2011 American Institute of Physics*. [doi:10.1063/1.3567296]

I. INTRODUCTION

Photonic crystals (PhCs) are formed with dielectric periodic structures analog to solids and exhibit some properties, such as the photonic band structures (PBSs) which include photonic passing bands and photonic band gaps (PBGs), and complicate dispersion relations.[1,2] Generally speaking, PBSs have to be obtained before further discussing other applications of PhCs. They can be solved by the widely used plane-wave expansion method. Then the finite-difference time-domain (FDTD) method[3] is often used to calculate its real-time field and energy flow. If distributions of cylinders in the two-dimensional PhC are quasiperiodic or random, it needs a large supercell to calculate the PBS and a large PhC area for FDTD simulation. It is not only a time-consuming calculation, but also a challenge on hardware equipment such as computer memory. If optical properties of PhCs can be replaced with effective refractive indices, it is possible to design some special structures in PhCs and understand their optical performances based on the effective models. The problems on calculation time and equipments could be improved explicitly.

As we know, PBSs reveal different optical responses when light propagates inside the PhC at different frequencies. On the one hand, PhCs can be treated as an anisotropic material that presents negative refraction[4–6] and the superprism effect.[4,7] On the other hand, they can be treated as a homogeneous material with an effective dielectric constant under certain condition.[4] Several effective-medium methods (EMTs) about disordered PhCs or metamaterials[8–11] reveal the possibility that treats some PhCs as simple media with effective refraction indices for all incident angles in certain frequency regions. In our previous work, a high-transmission PhC heterostructure *Y* branch waveguide is proposed.[12] Unlike other defect-mode PhC waveguide operating at the photonic bandgap (PBG), the designed waveguide operates at photonic band region. It is composed of two different PhCs, each of them has different air-hole radius resulting in different effective refraction index within the first photonic band. Then these two effective media, just like the core and cladding of the conventional waveguide, confine light in the core region very efficiently. It can be explained by the mechanism of total internal reflection between two PhCs and the transverse resonance condition is also satisfied. Especially, the boundary between two PhCs does not support any interface mode. This result tells us that even in complicated structures such as PhCs and their compounds, the concept of effective medium still holds in certain frequency region without losing correctness of optical performances.

In other fields, Andrianov *et al*. have successfully used asymptotic homogenization method to calculate acoustic wave propagation in periodic composite materials in long-wavelength region.[13,14] This method uses multiple-scale asymptotic expansions in powers of a natural small parameter ε, which characterizes the rate of heterogeneity of the structure, to represent fields in a composite. It is successfully applied in micromechanics of composites whose coefficients are rapidly varying periodic functions in spatial coordinates, for example, the hexagonal array of cylindrical fibers. Besides, these results will remain correct for other kinds of transport coefficients such as electrical conductivity, diffusion, magnetic permeability, etc. From the concept of homogenization, the optical response of the PhC can be simplified that may help to design new composite materials

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for a large variety of engineering applications. It also points out that the homogenization method is useful and important for both fundamental and applied points of view.

In this paper, we use the concept of homogenization to verify the equivalence between the periodic-defect PhC and the effective PhC in certain frequency region. The starting point of our goal is the scattering phenomena. First, we discuss them in PhCs with some defects and compare with the results of the effective model composed of the effective medium and effective defects. Then the Fourier series expansion of the Bloch wave in the defect-free PhC is used to confirm the concept of the effective medium. Next, periodic defects are added into the defect-free PhC to form the periodic-defect PhC, and the effective PhC is proposed to replace with the former. We show that PBGs of the periodic-defect PhC are equal to those of the effective PhC. Due to the equivalence exists between the periodic-defect PhC and the effective PhC, it is easy to investigate tunability of the PBG through the PBS of the effective PhC by changing the distribution of periodic defects. We also predict the negative refraction from the PBS of the effective PhC and verify it by using the FDTD simulation. Finally, defect modes are investigated by removing a line of periodic defects in the periodic-defect PhC. The calculations show that field distributions and Fourier coefficients of the periodic-defect PhC is equivalent to those of an effective PhC.

II. SCATTERING PHENOMENA OF ONE AND TWO DEFECTS IN THE PHOTONIC CRYSTAL

A. One-defect scattering

Recently, the multiple-scattering theory has been used to study PBSs,[15,16] optical flows,[17] transmissions,[18] negative refractive phenomena,[19] and other topics[20,21] of PhCs. Because the PhC contain lots of periodic scatters, the wave in the PhC suffers multiple scattering processes by all scatters resulting in a spatially periodic distribution eventually. Due to the periodic distribution of the dielectric constant, the Bloch wave can exist in the PhC. In certain frequency regions, the PhC show a characteristic of a fixed effective refractive index for all angles. As a result, the Bloch wave propagating through the PhC is similar to the plane wave propagating through a homogeneous medium. If a cylindrical defect exists on the path of the propagation plane in the homogeneous medium, the wave is scattered by the defect and form concentric circles. The similar phenomenon should also take place in the PhC. The investigation of the scattering phenomenon by defects in an originally defect-free PhC is an intuitive way to initially verify the correctness of the PhC replaced by an effective medium.

Before discussing the concept of an effective medium, effective refraction indices varied with incident angles of the PhC have to be obtained first. The normal direction of the equifrequency surface (EFS) is the direction of the group velocity as well as the propagation direction of light in the PhC, so EFS can give the relation between the incident and the refractive angles.[4] According to the conservation rule, the incident and refractive wave vectors are continuous for the tangential components parallel to the interface. Given the incident wave vector $\bar{k}_i$ with a corresponding frequency ω and an incident angle θ_i, the refractive wave vector $\bar{k}_r$ and thus the refractive angle θ_r can be determined simultaneously. By using Snell's law, effective refraction indices varied with incident angles of the PhC are acquired.

We consider the PhC composed of a two-dimensional triangular array of air cylinders on the x-y plane. The air cylinders with dielectric constant $\varepsilon_b = 1.0$ are embedded into a background medium with the dielectric constant $\varepsilon_a = 2.25$. ΓK and ΓM are parallel to x and y axes, respectively. The lattice constant of the triangular array is a and the radius r of all air cylinders is $0.20a$. A defect is created by removing an air cylinder which is denoted as the dotted circle in Fig. 1(a), so the dielectric constant ε_d of the defect is 2.25. To remove an air cylinder is also equivalent to add an additional medium with a dielectric constant $\varepsilon_a - \varepsilon_b$ at the defect place. The defect can perturb and scatter the propagating Bloch wave in the PhC. The EFS considered here is circular so that effective refraction indices n_{eff} are constant for all angles. In the following, an effective medium of which effective dielectric constant $\varepsilon_{\text{eff}} = n_{\text{eff}}^2$ and the relative permeability $\mu = 1$ is substituted for the defect-free PhC. At the same time, the defect with the radius $0.20a$ is treated as an effective defect, whose effective dielectric constant ε_d is equal to $\varepsilon_{\text{eff}} + \varepsilon_a - \varepsilon_b$. Then the structure of the PhC with a defect is replaced with an effective one which includes the effective medium and an effective defect. The distribution of the effective dielectric constant in the effective structure is shown in Fig. 1(b).

The scattering phenomenon in the one-defect PhC is shown by using the FDTD method. The frequency of the

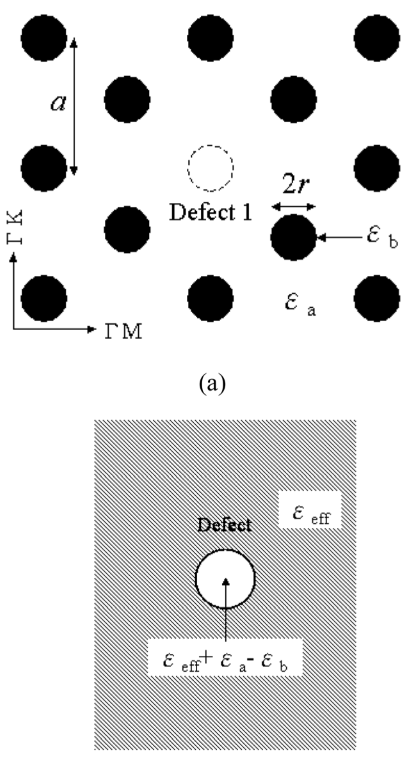
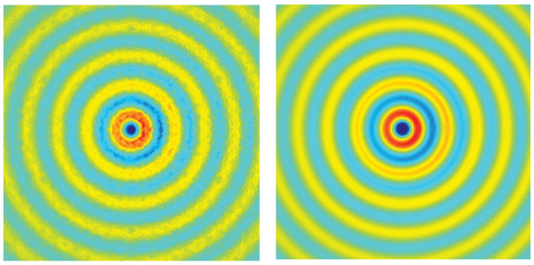


FIG. 1. (a) A defect within a two-dimensional triangular PhC. (b) Equivalent structure of an effective medium with an effective defect.



(a) (b)

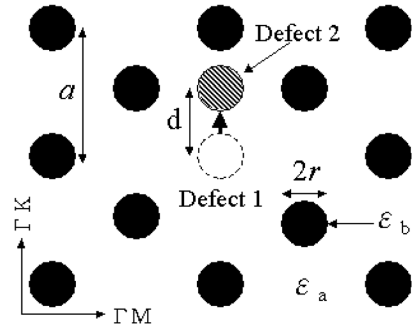
FIG. 2. (Color online) (a) The wave scattered by a defect in the PhC where ε_a, ε_b, ε_d, and r are 2.25, 1.0, 2.25, and 0.20a, respectively. (b) The wave scattered by the effective defect in the effective medium where $\varepsilon_{\mathrm{eff}}$, ε_d, and r are 2.0736, 3.3236, and 0.20a, respectively. A Gaussian beam with frequency 0.30(c/a) is incident in both (a) and (b) cases.

incident Gaussian beam with TM-polarization (E-field is parallel to the cylinder) is 0.30(c/a), where c is the speed of light in vacuum. The Gaussian beam is normally incident from air into the PhC and propagates along the ΓM direction. The distance between the defect and the PhC boundary has to be large enough for the reason that the incident beam needs passing through an enough distance to become the Bloch wave. This distance is 25a in our simulation. The effective index n_{eff} calculated from the EFS is 1.44, which indicates that $\varepsilon_{\mathrm{eff}}$ and ε_d are 2.0736 and 3.3236, respectively. The total wave ψ_{total} in the PhC is the sum of the incident wave ψ_{incident} and the scattered wave $\psi_{\mathrm{scattered}}$. So the scattered wave by the defect can be obtained by subtracting the incident wave from the total wave in the PhC as shown in Fig. 2(a). It is found out that the wave fronts of the scattered wave in the PhC form a series of near concentric circles away from the defect. Then we compare it with the corresponding scattering phenomenon in the effective structure. Figure 2(b) shows that the scattering wave is produced by the effective defect in the effective medium. Compare two scattered waves in Figs. 2(a) and 2(b), the scattered wave in an effective medium is very close to that in the PhC. The consistency reveals that the effective structure is a good approximation to deal with the scattering phenomenon by the defect in the PhC.

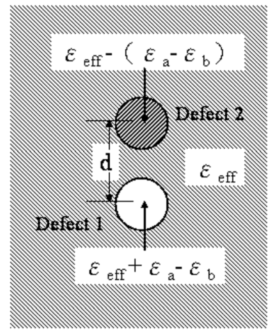
B. Two-defect scattering

In this section, the scattering phenomenon produced by two defects in the PhC is discussed. When the cylinder is shifted by a distance of d and does not overlap with other cylinders, the shifted cylinder can produce two defects within the PhC as shown in Fig. 3(a). One (defect 1) is located at the original position and the other (defect 2) is a distance of d away from the original position. Using the concept of effective defects, the effective dielectric constant of the defect 1 is $\varepsilon_a - \varepsilon_b$ more than $\varepsilon_{\mathrm{eff}}$, and that of the defect 2 is $\varepsilon_a - \varepsilon_b$ less than $\varepsilon_{\mathrm{eff}}$. The distribution of the effective dielectric constant in the effective structure is shown in Fig. 3(b).

Then we also use the FDTD method to compare the scattering phenomena in the PhC and the effective structure, respectively. The shifted distance d is chosen as 0.5a along the x (ΓK) direction. A Gaussian beam with the frequency 0.30 (c/a) is normally incident from air into the PhC and



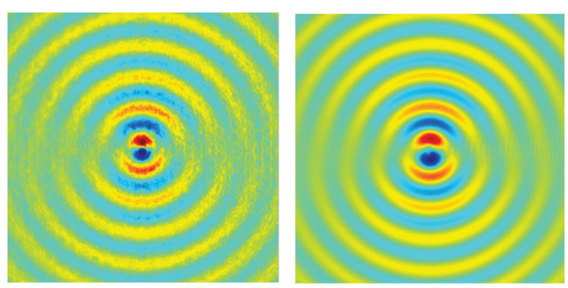
(a)



(b)

FIG. 3. (a) Two defects within a two-dimensional triangular PhC by shifting a cylinder a distance of d away from the original position. The shifting cylinder does not overlap with other cylinders. (b) Equivalent structure of an effective medium with two effective defects.

propagates along y (ΓM direction). In Fig. 4(a), the calculation shows that the scattered wave is indeed from two positions of these two defects. Next, we also simulate the same Gaussian beam incident on the effective structure, and compare with the calculation of the PhC case. The effective medium has an effective dielectric constant of 2.0736, and effective dielectric constants of the defect 1 and the defect 2 are 3.3236 and 0.8236, respectively. Both radii of two defects are still 0.20a. The scattered wave by these two defects in the effective structure is shown in Fig. 4(b), and it is also very close to that in the PhC.



(a) (b)

FIG. 4. (Color online) (a) The wave scattered by two defects whose dielectric constants ε_d are individually 2.25 and 1.0 in the PhC. ε_a, ε_b, and r are 2.25, 1.0, and 0.20a, respectively. (b) The wave scattered by two effective defects whose effective dielectric constants ε_d are individually 3.3236 and 0.8236 in the effective medium. $\varepsilon_{\mathrm{eff}}$ and r are 2.0736 and 0.20a, respectively. A Gaussian beam with frequency 0.30(c/a) is incident and the shifted distance d is 0.5a along the x (ΓK) direction in both (a) and (b) cases.

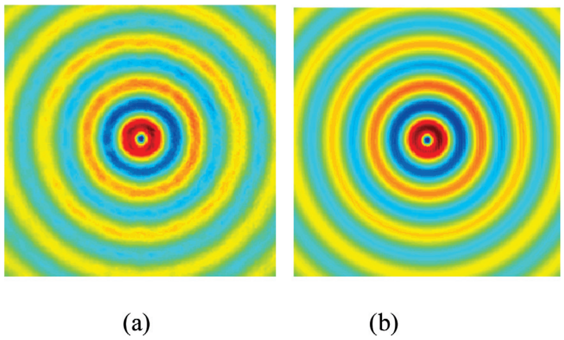


FIG. 5. (Color online) (a) The wave scattered by two defects whose dielectric constants ε_d are 2.25 and 16.0801 in the PhC. ε_a, ε_b, and r are 2.25, 1.0, and 0.20a, respectively. (b) The wave scattered by two effective defects whose effective dielectric constants ε_d are 3.3236 and 15.9037 in the effective medium. ε_{eff} and r are 2.07 and 0.20a, respectively. A Gaussian beam with frequency 0.30(c/a) is incident and the shifted distance d is 0.5a along the x (ΓK) direction in both (a) and (b) cases.

In order to verify that the effective structure can apply to defects with large dielectric constants, another demonstration is shown in Fig. 5(a), where two defects of Fig. 4(a) are changed to 2.25 and 16.0801. The scattering phenomenon produced by two effective defects in the effective medium is shown in Fig. 5(b) where effective dielectric constants of the defect 1 and the defect 2 are 3.3236 and 15.9037, respectively. In this case, the difference of the dielectric constant between the defect 1 and background medium is 1.25 and that for another defect is 13.83. According to the scattering formula of the 2D cylinder,[22] the scattered wave is proportional to the difference of the dielectric constant between the cylinder and the background medium. So the scattered wave from the large-dielectric-constant defect is eleven times larger than that from the small-dielectric-constant one. In Figs. 5(a) and 5(b), both scattered waves seem from one defect only. But in fact, they are produced by two defects. The scattered wave from the small-dielectric-constant defect is very weak so that it is covered by the scattered wave from the large-dielectric-constant one. The scattered wave in Fig. 5(b) is consistent with that in Fig. 5(a). As a result, both Figs. 4 and 5 show that effective structures can exhibit very similar scattering phenomena to those in PhCs.

C. Comparison of the Bloch wave in the PhC and the propagation wave in the effective medium

Above results show the effective structure is a good approximation to describe the scattering phenomena in the PhC, and they also imply that the Bloch wave should be very close to the propagation wave in the effective medium. Then a demonstration of the Bloch wave in the defect-free triangular PhC is calculated by the plane-wave expansion method.[23] The elementary reciprocal lattice vectors in the k-space are $\vec{G}_1 = 2\pi/a(1, -1/\sqrt{3})$ and $\vec{G}_2 = 2\pi/a(0, 2/\sqrt{3})$, respectively, and the reciprocal lattice vector is $\vec{G} = \vec{G}_{pq} = p\vec{G}_1 + q\vec{G}_2$, where p and q are integers. All parameters of the PhC are the same as above discussions, which are $\varepsilon_a = 2.25$, $\varepsilon_b = 1.00$, and $r = 0.20a$. The electric field E_z of the TM-polarization Bloch wave is expressed as sum of all Fourier series,[23]

$$E_{z,\vec{k}n}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} E_{z,\vec{k}n}(\vec{G}) e^{i\vec{G}\cdot\vec{r}}, \quad (1)$$

where $\vec{k}$ is the wave vector in the first Brillouin zone and n is a band index. The real part of E_z at 0.30 (c/a) and the Fourier coefficients $Ez,\vec{k}n(\vec{G})$ in Eq. (1) are shown in Fig. 6(a) and 6(b), respectively. The E_z distribution in Fig. 6(a) shows the wave propagates along the ΓM direction, in which circles represent air cylinders. By calculations, several coefficients more than 0.01 are denoted in Fig. 6(b) except for the $\vec{G}_{00}$ term, and all the other undenoted terms are very small which can be ignored. The $\vec{G}_{00}$ term is the maximum one, which is 0.9963. The Bloch wave can be approximately expressed as the summation of all these Fourier series whose coefficients $Ez,\vec{k}n(\vec{G})$ are more than 0.01. On the other hand, according to the effective medium approximation, the wave in the effective medium can be described by $\phi_{\text{eff}} = \exp(i\vec{k}_{\text{eff}}\cdot\vec{r}) = \exp(i\vec{k}\cdot\vec{r})$ with the wave vector $k = k_{\text{eff}} = 2\pi n_{\text{eff}}/a$. If Φ_{PhC} represents the Bloch wave in the PhC, we have the relation between Φ_{PhC} and Φ_{eff}:

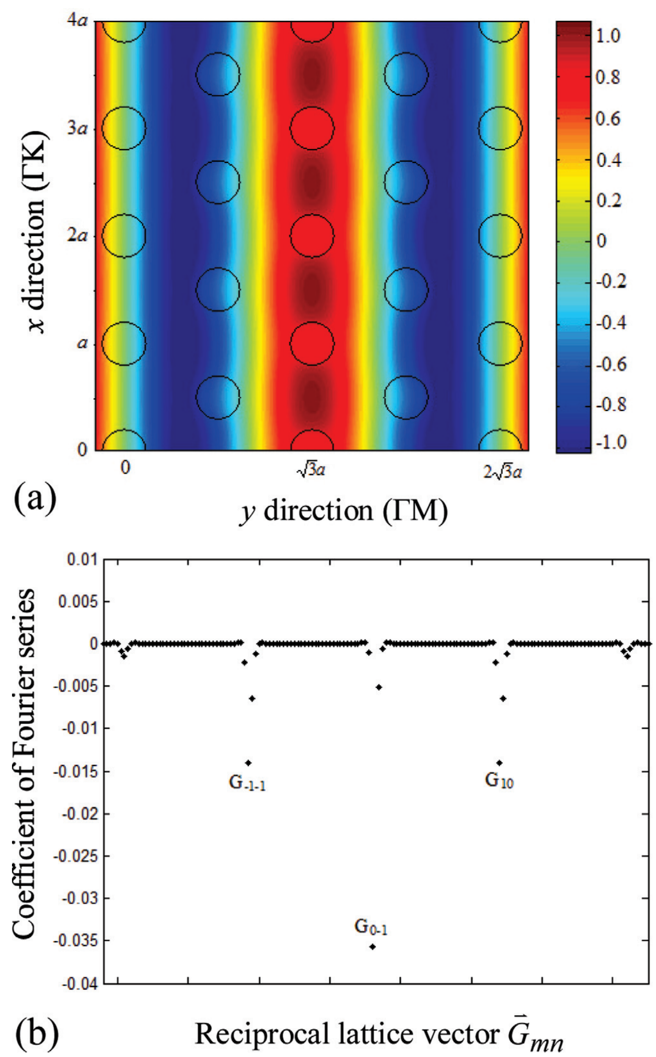


FIG. 6. (Color online) (a) The E_z field in the PhC where ε_a, ε_b, and r are 2.25, 1.0, and 0.20a, respectively. The frequency is 0.30(c/a) and the wave vector is 0.25(π/a) along the ΓM direction in the first Brillouin zone. (b) The coefficients $E_{z,\vec{k}n}(\vec{G})$ of the E_z field in (a).

$$\begin{aligned}\phi_{\mathrm{PhC}}(x,y) &\approx e^{i\bar{k}\cdot\bar{r}} * \left[0.9963 e^{i\bar{G}_{00}\cdot\bar{r}} - \left(0.0357 * e^{i\bar{G}_{0\,-1}\cdot\bar{r}}\right)\right. \\ &\quad - 0.0141 * (e^{i\bar{G}_{-1\,-1}\cdot\bar{r}} + e^{i\bar{G}_{1\,0}\cdot\bar{r}})] \\ &\approx \phi_{\mathrm{eff}}(x,y) * \left[0.9963 - \left(0.0357 * e^{-i\frac{4\pi}{\sqrt{3}a}y}\right)\right. \\ &\quad \left. - 0.0141 * \left(e^{-i\frac{2\pi}{a}\left(x+\frac{y}{\sqrt{3}}\right)} + e^{i\frac{2\pi}{a}\left(x-\frac{y}{\sqrt{3}}\right)}\right)\right]. \end{aligned} \quad (2)$$

From above equation, Φ_{PhC} is mainly composed of the $\vec{G}_{00}$-term harmonic wave. Other high-order harmonic ones comparing to the $\vec{G}_{00}$ term are very small so that they can be ignored and only the $\vec{G}_{00}$ term is left. Finally, we obtain $\phi_{\mathrm{PhC}}(x, y) \approx \phi_{\mathrm{eff}}(x, y)$. It means that Φ_{eff} is approximate to Φ_{PhC} with very high accuracy in this case.

III. PERIODIC-DEFECT PHOTONIC CRYSTAL

A. Effective photonic crystal

In Sec. II, the concept of the effective medium treats all defects in the PhC as effective defects in the effective medium. Following this concept, we can remove off some cylinders or replace some cylinders with different media to form periodic defects and then treat them as effective periodic defects or an array of effective dielectric cylinders. The periodic defects denoted by the empty circles are shown in Fig. 7(a). The PhC with periodic defects is called the periodic-defect PhC. By the concept of the effective medium, the periodic-defect PhC can be approximate to another representation, the effective PhC, which consists of an effective medium replacing the defect-free PhC, and an array of effective dielectric cylinders replacing periodic defects.

A periodic-defect PhC and its effective PhC are demonstrated here. The periodic defects are created by replacing air cylinders with a high refractive-index medium of $n_c = 4.01$ on a defect-free PhC, which is composed of a triangular array of air cylinders on a medium with the dielectric constant $\varepsilon_a = 2.25$. The radius r of each cylinder is $0.42a$. When the frequency is below 0.36 (c/a), $n_{\mathrm{eff}} = 1.20$ is a good value to represent the effective refraction index of the defect-free PhC for all angles. So the $\varepsilon_{\mathrm{eff}}$ of the effective medium is 1.44 and $\varepsilon_d = \varepsilon_{\mathrm{eff}} + \varepsilon_c - \varepsilon_b$ of each effective dielectric cylinder is 16.5201 in the effective PhC. The distance between two adjacent defects, which is called the defect lattice, is chosen as $2a$. Hence the new lattice constant of the effective PhC is also $2a$, and the ratio of the radius to the new lattice constant becomes 0.21. The effective dielectric cylinders form a triangular array, too. The distribution of the effective dielectric constant in the effective PhC is shown in Fig. 7(b).

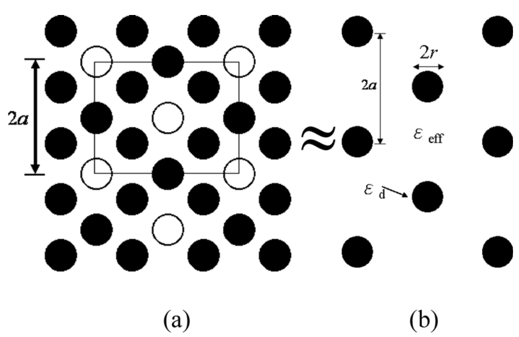


FIG. 7. (a) The periodic defects distribute in the PhC. (b) The distribution of the effective dielectric constant in the effective PhC.

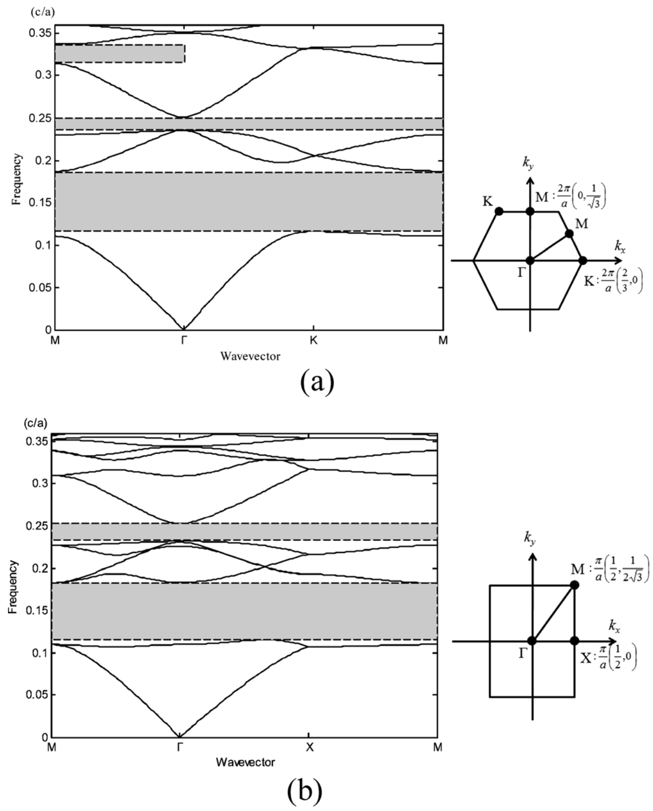


FIG. 8. (a) The PBS of the effective PhC where $\varepsilon_{\mathrm{eff}}$, ε_d, r and the defect lattice are 1.44, 16.5201, $0.42a$, and $2a$, respectively. (b) The PBS of the periodic-defect PhC is calculated by the supercell method where ε_a, ε_b, ε_c, and r are 2.25, 1.0, 16.0801, and $0.42a$, respectively. The area of the supercell is shown in Fig. 7(a). In (a) and (b), the right figures are the first Brillouin zones.

B. Photonic band structure and transmissions

The PBS of the effective PhC with $\varepsilon_{\mathrm{eff}} = 1.44$ and $\varepsilon_d = 16.5201$ is shown in Fig. 8(a) where the first Brillouin

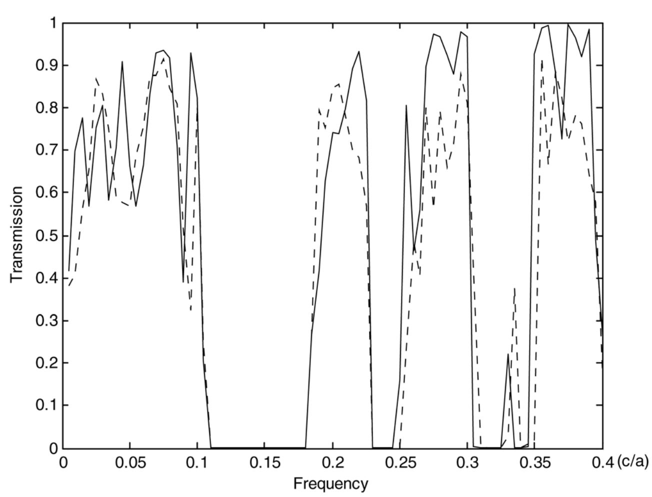


FIG. 9. Transmissions of the periodic-defect PhC (dashed line) and the effective PhC (solid line), respectively.

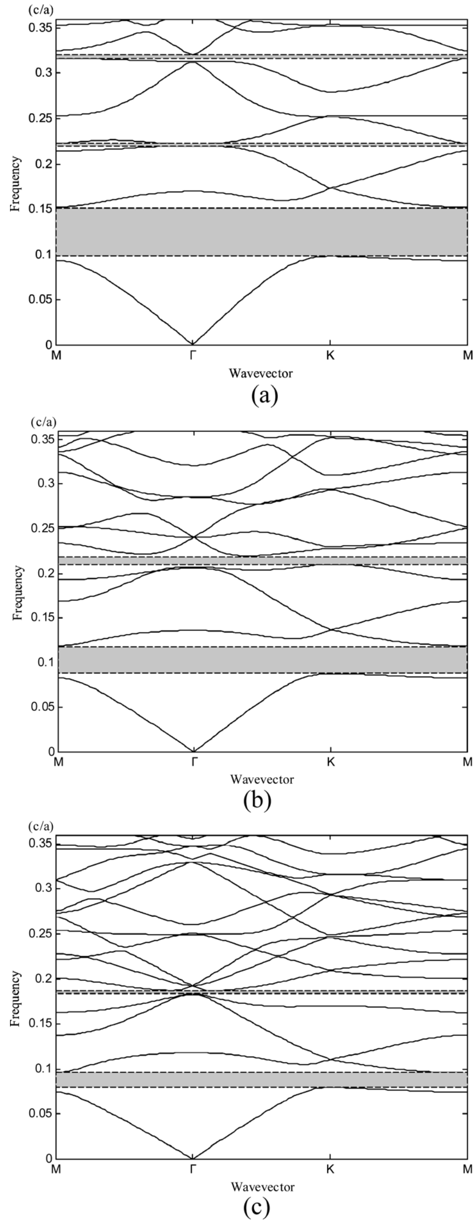


FIG. 10. The PBSs of three effective PhCs with $\varepsilon_{\text{eff}} = 1.44$, $\varepsilon_d = 16.5201$, and $r = 0.42a$ where the defect lattices are (a) $3a$, (b) $4a$, and (c) $5a$, respectively.

zone is at right side. From the calculation, two full PBGs denoted as gray regions exist below frequency of 0.36 (c/a). These two frequency regions are from 0.116 to 0.187 (c/a) and from 0.236 to 0.251 (c/a), respectively. Next, the supercell method[24] is used to calculate the PBS of the periodic-defect PhC. The PBS with the first Brillouin zone is shown in Fig. 8(b). The area of a supercell in the periodic-defect PhC is a rectangular region which is enclosed by solid line in Fig. 7(a). By comparing Fig. 8(a) with Fig. 8(b), the positions of the full PBGs almost coincide with each other.

In addition, the FDTD method is further used to calculate transmissions of the periodic-defect PhC and the effective PhC, respectively. Gaussian beams are normally incident from air into both PhCs and then propagate along the ΓM direction. In Fig. 9, the dashed and solid lines represent transmissions of the periodic-defect PhC and the effective PhC, respectively. Both transmissions at the frequencies from 0.11 to 0.18 (c/a) and from 0.23 to 0.25 (c/a) are very close to zero. These zero-transmission regions just correspond to full PBGs in Figs. 8(a) and 8(b). Besides, frequencies from 0.315 to 0.33 (c/a) are another zero transmission region because it belongs to the local PBG, which is denoted as the left-upper gray block in Fig. 8(a). From above discussions, PBGs of the effective PhC are coincident with those of the periodic-defect PhC. Except for these zero-transmission regions, both transmissions are also close to each other.

C. Tunability of the photonic bandgap due to periodic defects

Next, the effects of the periodic-defect distribution on the PBGs are discussed. Since the effective PhC is equivalent to the periodic-defect PhC, it is convenient to discuss the effects through the effective PhCs. The PBSs of three effective PhCs with defect lattices of $3a$, $4a$, and $5a$ are calculated and shown in Figs. 10(a), 10(b), and 10(c), respectively. The

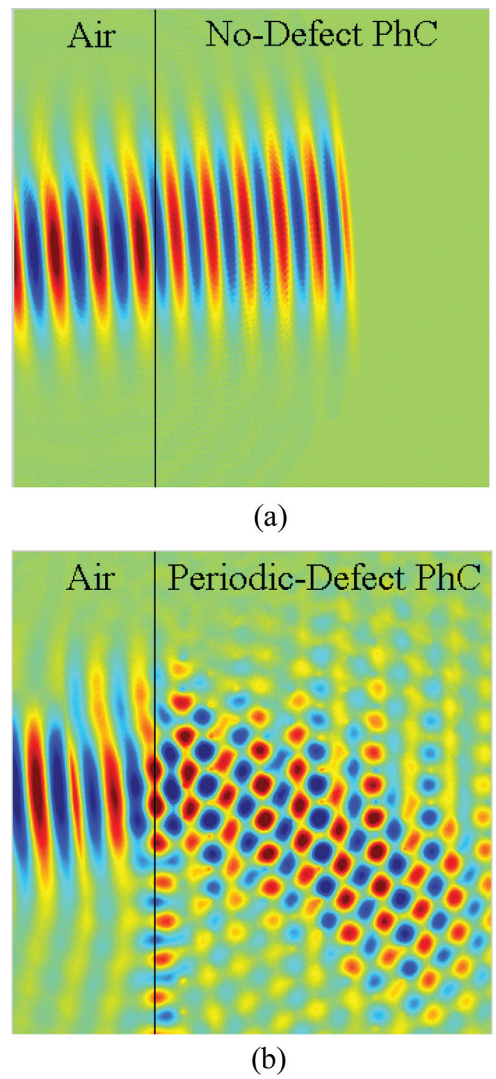


FIG. 11. (Color online) The refractive phenomena when the Gaussian beam with frequency of 0.15(c/a) incident from air into (a) the defect-free PhC where ε_a, ε_b, and r are 2.25, 1.00, and $0.42a$, respectively, and (b) the periodic-defect PhC where ε_a, ε_b, ε_d, r, and the defect lattice are 2.25, 1.0, 16.0801, $0.42a$, and $5a$, respectively.

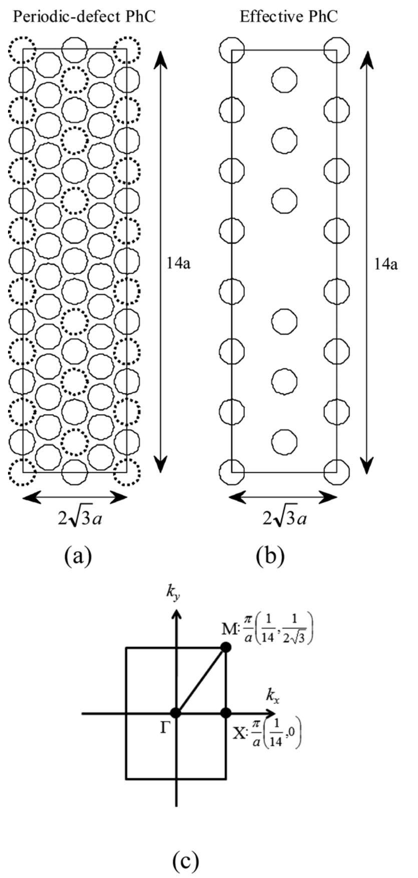


FIG. 12. (a)The supercell with size of $14a \times 2\sqrt{3}a$ in the periodic-defect PhC. (a)The supercell with size of $14a \times 2\sqrt{3}a$ in the effective PhC. (c) The first Brillouin zone for both (a) and (b). The band structures are calculated along M-Γ-X-M.

effective dielectric constants of $\varepsilon_{\mathrm{eff}} = 1.44$ and $\varepsilon_d = 16.5201$ are used, and the effective periodic defects are formed in a triangular array as that in Sec. III.B. Three PBGs exist below 0.36 (c/a) in the $3a$ case. Those are from 0.098 to 0.152 (c/a), from 0.220 to 0.221 (c/a), and from 0.317 to 0.321 (c/a), respectively. When compare with the $2a$ case, the position of the lowest PBG shifts 0.018 (c/a) downward and the width of it is narrowed down to 0.016 (c/a). In the $4a$ case, two PBGs are from 0.087 to 0.119 (c/a) and from 0.210 to 0.219 (c/a), respectively. In the $5a$ case, those are from 0.079 to 0.095 (c/a) and from 0.183 to 0.187 (c/a), respectively. The positions of the lowest PBG for the $3a$, $4a$, and $5a$ cases show the trend of shifting downward. It can be seen that the widths of the second PBG are decreased from 0.011 to 0.004 (c/a) as the defect lattice is increased from $3a$ to $5a$. When the defect lattice is more than $7a$, no any full PBG exists below 0.36 (c/a) by the calculation conclusion.

IV. NEGATIVE REFRACTION IN THE PERIODIC-DEFECT PHOTONIC CRYSTAL

From the PBSs of effective PhCs in Figs. 10(a), 10(b), and 10(c), the photonic bands become denser when the defect lattice becomes larger. Due to the periodic defects, the optical characteristic of the periodic-defect PhC becomes more complex and is very different from that of the defect-free PhC. For example, when the defect lattice is $10a$, more than 100 photonic bands are below 0.36 (c/a). In the following, the FDTD method with a Gaussian beam is used to investigate the difference of the refractions between the defect-free and periodic-defect PhCs. The negative refractions can be predicted through the PBS of the effective PhC.

The Gaussian beam with frequency of 0.15 (c/a) is incident from air into the defect-free and periodic-defect PhCs at the incident angle 6°. The defect-free PhC is the same as the one used in Sec. III. In Fig. 11(a), the refractive phenomenon in the defect-free PhC shows a normal case as the Gaussian beam incident into a right-handed medium. When periodic defects are added into the defect-free PhC, the refractive phenomenon displays dramatic change. The defect lattice considered here is $5a$ so the incident frequency locates at the third band as shown in Fig. 10(c). At this photonic band, the EFS shrinks as the frequency increase. It belongs to the negative refraction region[4] and predicts that negative refraction takes place at 0.15 (c/a). In Fig. 11(b), the Gaussian beam is incident with angle 6° into the periodic-defect PhC. The refractive phenomenon shows that the incident beam is deflected to the same side of the normal and the negative refraction takes place. It indicates that the PBS of the effective PhC can predict the refractive phenomenon very well, which is hard to figure out from the PBS of the periodic-defect PhC calculated by the supercell method. In this case, although the periodic defects only occupy $2\pi r^2/25\sqrt{3}a^2$ of

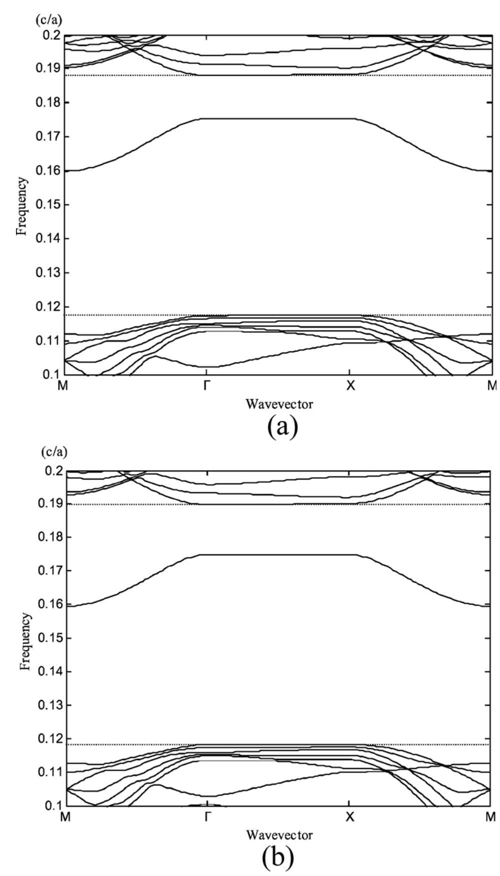


FIG. 13. (a) Defect modes exist between 0.1599 and 0.1754 (c/a) in the structure of Fig. 11(a), where ε_a, ε_b, ε_c, and r are 2.25, 1.0, 16.0801, and $0.42a$, respectively. (b) Defect modes exist between 0.1595 and 0.1749 (c/a) in the structure of Fig. 11(b), where $\varepsilon_{\mathrm{eff}}$, ε_d, r, and the defect lattice are 1.44, 16.5201, $0.42a$, and $2a$, respectively.

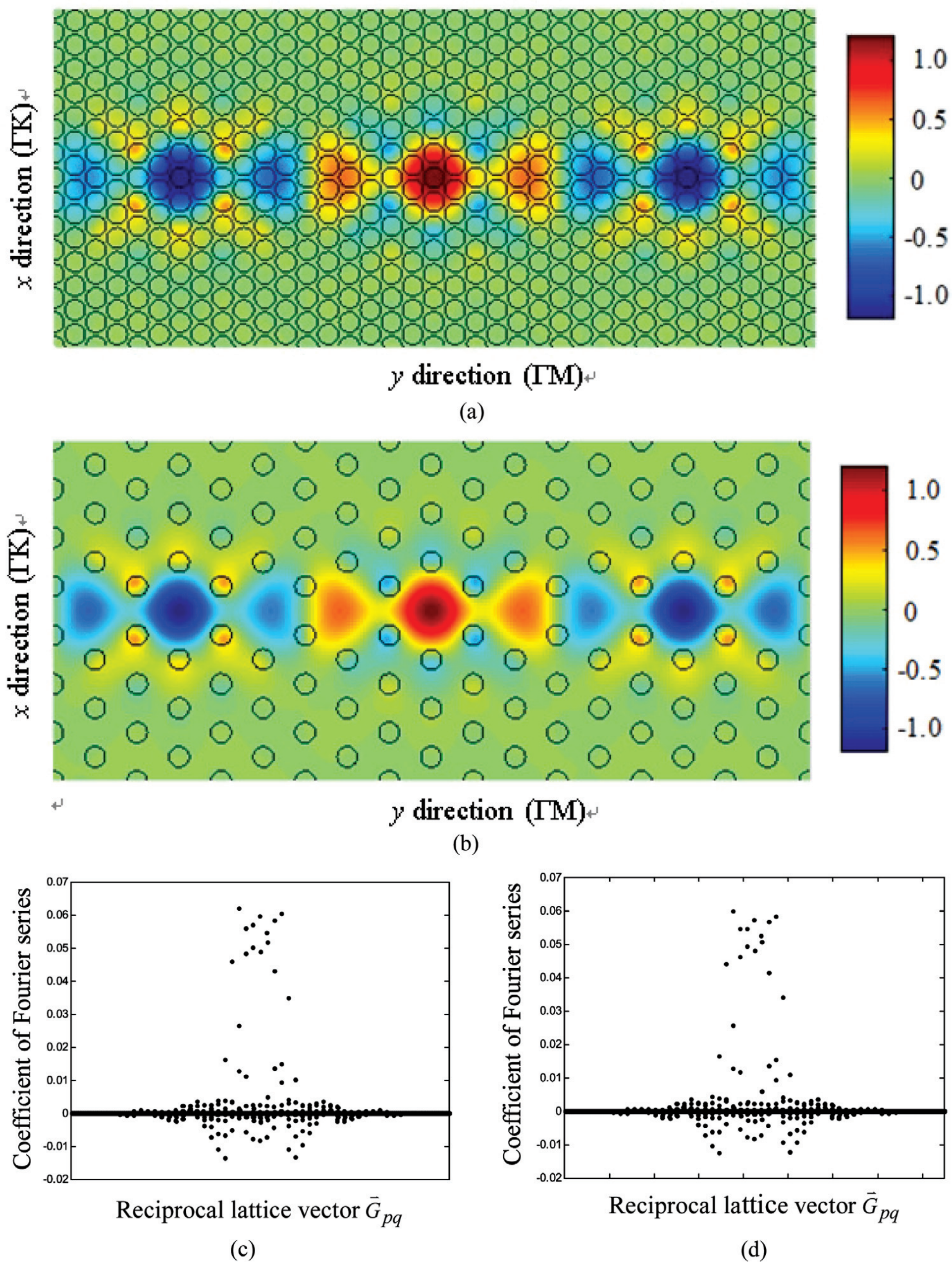


FIG. 14. (Color online) When the frequency is $0.17(c/a)$, field distributions of the defect mode (a) along the waveguide in the periodic-defect PhC and (b) along the waveguide in the effective PhC, and coefficient distributions of the defect mode (c) in the periodic-defect PhC and (d) in the effective PhC.

the PhC, which is about 2.56%, the refraction is very different from that of the defect-free PhC.

V. DEFECT MODES IN THE PERIODIC-DEFECT PHOTONIC CRYSTAL AND IN THE EFFECTIVE PhC

When a disorder is introduced to the PhC, defect modes would be created in the PBG region. In the PhC, if a row or a line of air-hole cylinders are removed, a photonic waveguide can be formed. Since previous results show that the periodic-defect and the effective PhCs have much similar performances in the interesting frequency region, we further discuss the defect modes in both PhCs by using the supercell method, and check whether the effective PhC still works here. The PhC waveguide is created by removing a line of periodic defects. The size of the supercell is chosen as $14a \times 2\sqrt{3}a$ in the periodic-defect PhC shown in Fig. 12(a). In the periodic-defect PhC, dashed-line circles represent periodic defects with dielectric constant $\varepsilon_c = 16.0801$ and solid-line circles represent air-hole cylinders, where the background dielectric constant $\varepsilon_a = 2.25$. Both radii of periodic-defect and air-hole cylinders are $0.42a$. One of those periodic defects at the center of the supercell is removed so that defect modes can be produced within the PBG region. The effective structure of Fig. 12(a) is shown in Fig. 12(b) where periodic effective cylinders with dielectric constant $\varepsilon_d = 16.5201$ and radius $r = 0.42a$ are embedded in the effective medium with dielectric constant $\varepsilon_{\text{eff}} = 1.44$. The new lattice constant is $2a$ and the ratio of radius to the lattice constant is 0.21. An effective cylinder at the center of the supercell is also removed in order to match the structure in Fig. 12(a). The size of the supercell remains $14a \times 2\sqrt{3}a$. The first Brillouin zone for both supercells is shown in Fig. 12(c). The PBSs are calculated along M-Γ-X-M.

Because the supercells in Figs. 12(a) and 12(b) are very large, total 6241 plane waves are used to calculate the PBSs and defect modes. The results are shown in Figs. 13(a) and 13(b), respectively. Between two dashed lines are the PBG regions. Defect modes exist between 0.1599 and 0.1754 (c/a) in the periodic-defect PhC, and those exist between 0.1595 and 0.1749 (c/a) in the effective PhC. Both defect modes are located at the PBG region. The error between two calculations in Figs. 13(a) and 13(b) is less than 0.3%. It can be said that defect modes of the periodic-defect PhC are coincident with those of the effective PhC. Next, demonstrations of field distributions are shown to verify the point of view. When the frequency is $0.17(c/a)$, the field distributions along the waveguide (ΓM or y direction) by using Eq. (1) are shown in Figs. 14(a) and 14(b), respectively. In both cases, the defect modes are mostly confined in the lateral range of $10a$. Coefficient distributions of Fourier series in these two cases are shown in Figs. 14(c) and 14(d). The field distribution in Fig. 14(a) is much similar to that in Fig. 14(b) because coefficient distributions between two cases are also much close to each other. As a result, it exhibits again that the effective PhC is equivalent to the periodic-defect PhC in the discussions of PhC waveguides in the interesting frequency region.

VI. CONCLUSION

The concept of the effective medium is used to deal with problems of defects in PhCs throughout this paper. Scattering phenomena by defects in PhCs are an intuitive way to initially confirm this concept. It is found out that they are very similar to scattering phenomena in the effective structure composed of the effective medium and the effective defects in interesting frequency regions. Then we further discuss the reason why the effective medium can substitute for a defect-free PhC. It is the factor that the Bloch wave in the defect-free PhC is mainly composed of the $\vec{G}_{00}$-term harmonic wave and all other higher-order ones can be ignored. The $\vec{G}_{00}$-term harmonic wave is the same as the wave in the effective medium. If the Bloch wave is replaced with the $\vec{G}_{00}$-term wave, the approximation is as high as 99%. So it is a very good approximation to substitute the effective medium for the defect-free PhC.

Since scattering phenomena in PhCs are similar to those in effective media, it is reasonable to presume that there is an equivalence existing between the periodic-defect PhC and the effective PhC. Two fully PBGs and transmissions calculated by the FDTD method verify this equivalence in the interesting frequency region. So the concept of the effective medium is successfully extended from few defects in the PhC to periodic defects in the PhC. It allows us changing the defect lattice to investigate the variance of the PBGs of the effective PhC instead of the period-defect PhC. Furthermore, the PBS of the effective PhC with defect lattice $5a$ successfully predicts the negative refraction when Gaussian beam propagates through the period-defect PhC. The difference of the FDTD calculations between the defect-free PhC and the periodic-defect PhC points out the optical performance can be dramatically changed by the periodic defects. Finally, waveguide modes in the periodic-defect PhC and the effective PhC exhibit again that the effective PhC is equivalent to the periodic-defect PhC in the interesting frequency region.

In summary, the concept of the effective medium is important for both fundamental and applied points of view. The PhC can display different effective refraction indices by varying radii of air-hole cylinders. It is similar to semiconductor materials which change their refraction indices by doping different concentrations of impurities. The PhC can be treated as an artificially material whose optical performance different from the background medium and cylinders. So the effective representation of a PhC is much helpful to design optical devices composed of some materials not in nature.

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[1] S. John, Phys. Rev. Lett. **58**, 2486 (1987).
[2] A. Z. Genack and N. Garcia, Phys. Rev. Lett. **66**, 2064 (1991).
[3] A. Taflove and S. C. Hagness, *Computational Electrodynamics*, 2nd ed. (Artech House, Norwood, 2000).
[4] M. Notomi, Phys. Rev. B **62**, 10696 (2000).
[5] S. Foteinopoulou and C. M. Soukoulis, Phys. Rev. B **67**, 235107 (2003).
[6] A. Martínez and J. Martí, Phys. Rev. B **71**, 235115 (2005).
[7] N. Malkova, D. A. Scrymgeour, and V. Gopalan, Phys. Rev. B **72**, 045144 (2005).
[8] G. Boedecker and C. Henkel, Opt. Express **11**, 1590 (2003).
[9] D. Felbacq and G. Bouchittè, Waves Random Media **7**, 245 (1997).
[10] V. Yannopapas, J. Opt. Soc. Am. B **23**, 1414 (2006).
[11] V. Yannopapas, Phys. Rev. B **75**, 035112 (2007).
[12] Ting-Hang Pei and Yang-Tung Huang, J. Appl. Phys. **109**, 034504 (2011).
[13] A. L. Kalamkarov, I. V. Andrianov, and V. V. Danishevs'kyy, Appl. Mech. Rev. **62**, 030802 (2009).
[14] I. V. Andrianov, V. I. Bolshakov, V. V. Danishevs'kyy, and D. Weichert, Proc. R. Soc. A **464**, 1181 (2007).
[15] X. Wang, X. G. Zhang, Q. Yu, B. N. Harmon, Phys. Rev. B **47**, 4161 (1993).
[16] K. M. Leung and Y. Qiu, Phys. Rev. B **48**, 7767 (1993).
[17] L. -S. Chen, C. -H. Kuo, and Z. Ye, Phys. Rev. E **69**, 066612 (2004).
[18] L. -M. Li and Z. –Q. Zhang, Phys. Rev. B **58**, 9587 (1998).
[19] C. -H. Kuo and Z. Ye, Phys. Rev. E **70**, 026608 (2004).
[20] F. Zolla and S. Guenneau, Phys. Rev. E **67**, 026610 (2003).
[21] P. Mallet, C. A. Guérin, and A. Sentenac, Phys. Rev. B **72**, 014205 (2005).
[22] Kiyotoshi Yasumoto, *Electromagnetic Theory and Applications for Photonic Crystals* (Taylor & Francis, London, 2006).
[23] K. Sokoda, *Optical Properties of Photonic Crystals*, 2nd ed. (Springer, Berlin, 2005).
[24] W. Zhi, R. Guobin, L. Shuqin, and J. Shuisheng, Opt. Express **11**, 980 (2003).