Enlargement of Photonic Band Gaps and Physical Picture of Photonic Band Structures *

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(Received 1 December 2005)

Light propagation in a one-dimensional photonic crystal (PC), consisting of alternative slabs with refractive indices (layer thicknesses) n_1 (a) and n_2 (b), is investigated. An important optimal parameter matching condition, $n_1 a \approx n_2 b$, is obtained for the largest photonic band gap (PBG). Moreover, we find that the exact analytical solutions for the electric/magnetic field eigenmodes at the band edges are standing waves with odd or even symmetry about the centre of each layer. The electric/magnetic field eigenfunctions at the top and bottom of the nth band have n and n − 1 nodes in one period of PC, respectively. The PBG arises from the symmetric differences of the field eigenfunctions at the band edges.

PACS: 42. 70. Qs, 03. 50. De, 78. 67. Pt

Photonic crystals (PCs) are artificial microstructured materials with a periodically modulated dielectric function-ε. Intensive investigations on PCs have been carried out since the idea of PCs was proposed.[1,2] Up to now, most calculations of the photonic band structures and the corresponding electric/magnetic field distributions have been performed based on numerical methods, such as the plane wave expansion method and the finite-difference time-domain method. Some qualitative conclusions have been derived from the related numerical analysis. It is well known that the exact analytical solutions are quite useful for us to understand the physics of PCs. In a sense, the simplest one-dimensional (1D) PC with Kronig–Penney periodic dielectric structure[3−6] is the only exactly solvable theoretical model. The purpose is to draw new physics out of the 1D PC by means of the exact analytical solutions.

One of the most important properties of the PCs is the presence of photonic band gaps (PBGs), in which light propagation is prohibited. To design a new PC structure with large PBG has always been a key issue for the PC material and device applications and for the investigation of PC physics.[7−9] The behaviour of photons in PCs is analogous to the motion of electrons in periodic crystals. It has been known that the origin of the electron energy gap in a periodic crystal is due to the localization of the electrons in different regions, resulting in different values of the potential energy.[4] The origin of the PBGs has also been understood in a similar way.[10] The PBG arises from the difference in field location. The field eigenfunctions at the top of the nth band concentrate their energies in the higher-ε region. In contrast, the solutions corresponding to the bottom of the $(n+1)$th band concentrate their energies in the lower-ε region. To the best of our knowledge, a comprehensive physical picture of photonic band structures is still lacking at present. Our purpose here is to explain the physical origin of the photonic band structures from a new point of view by analysing the exact analytical solutions of the electric/magnetic field eigenfunctions at the band edges and to give theoretical guidance for designing a PC structure with a large PBG. Our picture is different from the well-known results.[10]

Let us now consider an electromagnetic (EM) wave propagating through a dielectric medium with no free charge and current. We take the x, y, and z axes to be perpendicular to each other and assume that the EM wave travels in the xy plane.

For the TM modes with the magnetic field parallel to the z axis, the following eigenvalue equation for H_z can be derived from Maxwell's equations:

$$\frac{\partial}{\partial x}\Big(\frac{1}{\varepsilon(x)}\frac{\partial}{\partial x}\Big)+\frac{\partial}{\partial y}\Big(\frac{1}{\varepsilon(x)}\frac{\partial}{\partial y}\Big)H_z(x,y) = -\frac{\omega^2}{c^2}H_z(x,y). \quad (1)$$

Similarly, for the TE modes, we have

$$\Big(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\Big)E_z(x,y) = -\frac{\omega^2}{c^2}\varepsilon(x)E_z(x,y). \quad (2)$$

In this Letter, we pay attention to light propagation in a 1D PC along the x-direction, consisting of alternative slabs with refractive indices (layer thicknesses) n_1 (a) and n_2 (b). The period of PC is $\Lambda = a + b$. By applying Bloch's theorem in the x-direction due to periodicity of PC, we can write the TM mode solutions as

$$H_{z,n}(k_x,k_y,x,y) = e^{ik_x x}e^{ik_y y}u_n(k_x,x), \quad (3)$$

where k_x is the reduced Bloch wave number within the first Brillouin zone: $-\pi/\Lambda < k_x \leq \pi/\Lambda$, k_y is a constant, and $u_n(k_x,x)$ is the periodic function in the x-direction: $u_n(k_x,x) = u_n(k_x,x+l\Lambda)$ $(l = 0, \pm1, \pm2, \cdots)$. The TE mode solutions can also be obtained similarly.

* Supported by the National Natural Science Foundation of China under Grant Nos 60276004 and 60390073.

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By substituting Eq. (3) into Eq. (1), we have

$$u_n(k_x,x)=\begin{cases} e^{-ik_x x}(A_1 e^{i\alpha x}+B_1 e^{-i\alpha x}) & -b\le x<0,\\ e^{-ik_x x}(C_1 e^{i\beta x}+D_1 e^{-i\beta x}) & 0\le x<a. \end{cases} \tag{4}$$

Here $\alpha^2=n_2^2\omega^2/c^2-k_y^2$ and $\beta^2=n_1^2\omega^2/c^2-k_y^2$. By using Maxwell's boundary conditions at the $x=0$ and $x=a$ interfaces and applying Bloch's theorem, $H_z(a)=\exp(ik_x\Lambda)H_z(-b)$, we can obtain the photonic band equation as follows:

$$-\frac{1}{2}\Big(\gamma+\frac{1}{\gamma}\Big)\sin(\alpha b)\sin(\beta a)+\cos(\alpha b)\cos(\beta a) =\cos(k_x\Lambda), \tag{5}$$

where $\gamma\equiv n_1^2\alpha/n_2^2\beta$ (α/β) for the TM (TE) modes.

$$-\frac{1}{2}\Big(\delta+\frac{1}{\delta}\Big)\sin(\alpha b)\sin(\beta a)+\cos(\alpha b)\cos(\beta a) =\cos(k_x\Lambda), \tag{6}$$

For simplicity, we consider the case of $k_y=0$ and omit the band index n in the following discussions. By using the continuity of the tangential component of the electric and the magnetic fields at the $x=0$ interface, the TM eigenmodes in the period of $-b\le x<a$ can be written as

$$H_z(x)=\begin{cases} H_z(0)[\cos(\alpha x)+P\sin(\alpha x)] & -b\le x<0,\\ H_z(0)[\cos(\beta x)+\gamma P\sin(\beta x)] & 0\le x<a. \end{cases} \tag{7}$$

Moreover, based on the continuity of the tangential component of the electric and the magnetic fields at the $x=a$ interface and Bloch's theorem, we can obtain

$$P\equiv\frac{\cos(\alpha b)\exp(ik_x\Lambda)-\cos(\beta a)}{\gamma\sin(\beta a)+\exp(ik_x\Lambda)\sin(\alpha b)}. \tag{8}$$

According to Eqs. (5), (7) and (8), the following symmetry conditions can be obtained $|H_z(a/2+x)|=|H_z(a/2-x)|$, for $|x|\le a/2$; and $|H_z(-b/2+x)|=|H_z(-b/2-x)|$, for $|x|\le b/2$.

We can rewrite Eq. (5) as

$$\gamma=\frac{\cos(\alpha b)\cos(\beta a)-\cos(k_x\Lambda)}{\sin(\alpha b)\sin(\beta a)} \pm\frac{1}{\sin(\alpha b)\sin(\beta a)}\{[\cos(\alpha b)-\cos(k_x\Lambda)\cos(\beta a)]^2 -\sin^2(k_x\Lambda)\sin^2(\beta a)\}^{\frac{1}{2}}, \tag{9}$$

where $\pm$ indicates the two sets of solutions for γ, corresponding to odd- and even-bands. Furthermore, the solutions of the band edges at $k_x\Lambda=0$ or $k_x\Lambda=\pi$ can be derived from Eq. (9) as follows:

$$\gamma=\begin{cases} -\tan(\alpha b/2)\cot(\beta a/2) \quad \text{or}\\ -\cot(\alpha b/2)\tan(\beta a/2), \quad k_x\Lambda=0,\\ \tan(\alpha b/2)\tan(\beta a/2) \quad \text{or}\\ \cot(\alpha b/2)\cot(\beta a/2), \quad k_x\Lambda=\pi. \end{cases} \tag{10}$$

Based on Eqs. (8) and (10), the solutions for the TM modes at the band edges can be further written as

$$H_z(x)=\begin{cases} B_0\sin[\alpha(x+b/2)] & -b\le x<0,\\ D_0\sin[\beta(x-a/2)] & 0\le x<a, \end{cases} \tag{11}$$

for $\gamma=-\tan(\alpha b/2)\cot(\beta a/2)$ and $k_x\Lambda=0$, and

$$H_z(x)=\begin{cases} A_0\cos[\alpha(x+b/2)] & -b\le x<0,\\ C_0\cos[\beta(x-a/2)] & 0\le x<a, \end{cases} \tag{12}$$

for $\gamma=-\cot(\alpha b/2)\tan(\beta a/2)$ and $k_x\Lambda=0$, and

$$H_z(x)=\begin{cases} A_0\cos[\alpha(x+b/2)] & -b\le x<0,\\ D_0\sin[\beta(x-a/2)] & 0\le x<a, \end{cases} \tag{13}$$

for $\gamma=\cot(\alpha b/2)\cot(\beta a/2)$ and $k_x\Lambda=\pi$, and

$$H_z(x)=\begin{cases} B_0\sin[\alpha(x+b/2)] & -b\le x<0,\\ C_0\cos[\beta(x-a/2)] & 0\le x<a, \end{cases} \tag{14}$$

for $\gamma=\tan(\alpha b/2)\tan(\beta a/2)$ and $k_x\Lambda=\pi$. Here $A_0=H_z(0)/\cos(\alpha b/2)$, $B_0=H_z(0)/\sin(\alpha b/2)$, $C_0=H_z(0)/\cos(\beta a/2)$ and $D_0=-H_z(0)/\sin(\beta a/2)$.

Equations (11)–(14) clearly indicate that the TM mode eigenfunctions corresponding to band edges at $k_x\Lambda=0$ or $k_x\Lambda=\pi$ have definite parities. We can easily see from Eqs. (11) and (12) that the parities of the magnetic field eigenfunctions in the regions of $-b\le x<0$ and $0\le x<a$ are identical in the case of $k_x\Lambda=0$. On the contrary, Eqs. (13) and (14) show that the magnetic field eigenfunctions have the opposite parities in the adjacent layers for one period of PC if $k_x\Lambda=\pi$. These results can be understood based on Bloch's theorem. This is because the phase difference between $H_z(-b)$ and $H_z(a)$ is required to be 0 or π at the band edges. Moreover, it is more interesting to note that the two sets of solutions corresponding to $k_x\Lambda=0$, i.e., Eqs. (11) and (12), always have opposite parities. This conclusion is also applicable to Eqs. (13) and (14) in the case of $k_x\Lambda=\pi$. It is the opposite parities of the eigenfunctions at the band edges that directly leads to the different localization of the field energy and the appearance of the PBG in PCs, as discussed earlier. Generally, the eigenfunctions corresponding to $k_x\Lambda\ne0$ and π have mixed parities, although all the eigenfunctions at the band edges have definite parities.

The exact analytical solutions for the electric field eigenfunctions $E_y(x)$ for the TM modes at the band edges can also be obtained by substituting Eqs. (11)–(14) into Maxwell's equations.

The corresponding analytical solutions for the TE modes can also be exactly derived in a similar way.

In order to obtain the optimal parameter matching condition for the largest PBGs [the largest width $(\Delta\omega)_{\max}$ or the largest relative width $(\Delta\omega/\omega_m)_{\max}$ with ω_m the middle frequency of the PBG], we have solved Eq. (5) numerically. The optimal parameter matching condition is quite useful for designing PC materials and devices with a large PBG. Moreover, we have also calculated the field eigenfunctions at the band edges. A comprehensive physical picture of

the photonic band structures is given from a standing wave point of view based on our calculations.

First, we calculate the relative PBG width $\Delta\omega/\omega_m$ as a function of the refractive index ratio n_2/n_1. We find that $\Delta\omega/\omega_m$ increases monotonically with increasing of n_2/n_1 when a and b are fixed. The rate of increase for $\Delta\omega/\omega_m$ tapers as n_2/n_1 increases. This implies that, in order to design a PC with large relative PBG width, we can simply increase n_2/n_1.

We further investigate the relationship between the absolute PBG width $\Delta\omega$ and the refractive index ratio n_2/n_1 if the layer thicknesses a and b are fixed. Our results show that $\Delta\omega$ will reach its maximum for a given value of n_2/n_1. This opens a way for us to design a PC with large PBG.

Moreover, we can see from Table 1 that both the largest PBG width $(\Delta\omega)_{\max}$ and the corresponding refractive index ratio n_2/n_1 increase if a or the filling factor $f = a/\Lambda$ increases. Since the refractive index ratio n_2/n_1 is always a finite value, we therefore need to choose a group of appropriate parameters a, b and n_2/n_1 to design a PC structure with the largest PBG. For example, if choosing $a = 375\,\text{nm}$, $b = 175\,\text{nm}$, and $n_2/n_1 = 2.991$, we can obtain an maximum PBG width $(\Delta\omega)_{\max} = 6.699 \times 10^{14}\,\text{rad/s}$ and $\omega_m = 1.041 \times 10^{15}\,\text{rad/s}$.

Table 1. Variations of the maximum absolute width $(\Delta\omega)_{\max}(\times 10^{14}\,\text{rad/s})$ of the first PBG and the corresponding refractive index ratio n_2/n_1 with the layer thickness a in the case of $\Lambda = a + b = 550\,\text{nm}$.

a (nm)	75	125	175	225	275	325	375	425
$(\Delta\omega)_{\max}$	0.975	1.704	2.496	3.362	4.325	5.418	6.699	8.265
n_2/n_1	1.801	1.857	1.942	2.072	2.251	2.534	2.991	3.871

Figure 1 illustrates that the relative PBG width varies with the filling factor f when n_2/n_1 and Λ are fixed. We can easily find from Fig. 1 that the largest relative PBG width $(\Delta\omega/\omega_m)_{\max}$ can be obtained if the following optimal parameter matching condition is satisfied:

$$n_1 a \approx n_2 b. \tag{15}$$

Equation (15) is first obtained on the basis of our PBG calculations in 1D PCs. Moreover, we know from Eq. (15) that the filling factor corresponding to $(\Delta\omega/\omega_m)_{\max}$, i.e. $\widetilde{f}$, is determined by

$$\widetilde{f} \approx \frac{n_2/n_1}{n_2/n_1 + 1}. \tag{16}$$

Both Eqs. (15) and (16) are quite useful in practice, indicating an important direction for us to design a PC with the largest PBG.

Equation (16) shows that $\widetilde{f}$ is only a function of the refractive index ratio n_2/n_1, which is independent of the period Λ or the layer thicknesses a and b of the PC. In order to know the universality of Eqs. (15) and (16), we further calculate the relative PBG width as a function of the filling factor for many other PCs with different parameters a, b, and n_2/n_1. Our results clearly indicate that both Eqs. (15) and (16) are universal for an arbitrary 1D PC.

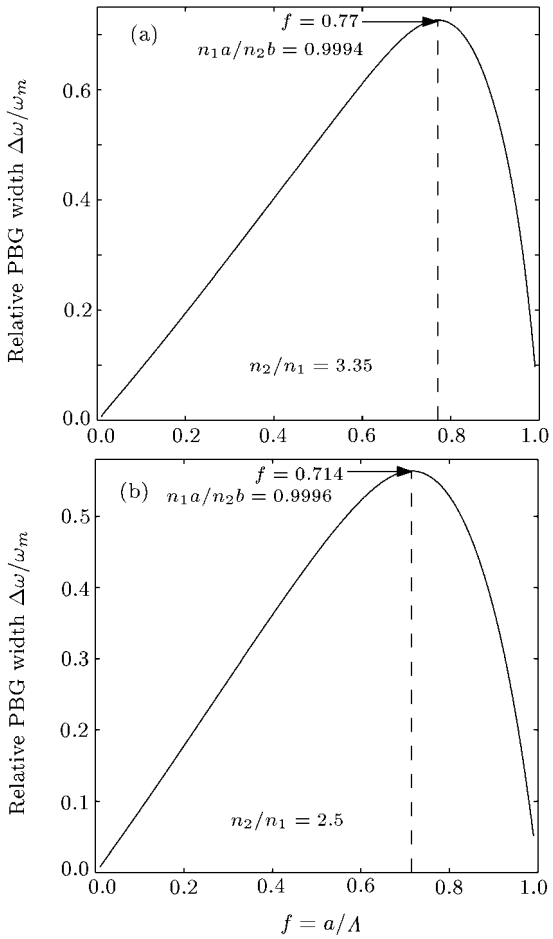

Fig. 1. The relative width $\Delta\omega/\omega_m$ for the first PBG as a function of filling factor f for the 1D PC with $\Lambda = 550\,\text{nm}$.

In Fig. 2, the electric field eigenfunctions $E_y(x)$, corresponding to the bottom and the top of each band, are presented for the $n = 1, 2, 3, 4, 5$ bands. We can see from Fig. 2 that the electric field eigenfunctions at the top and bottom of the nth band have n and $n-1$ nodes in the period of $-b \le x < a$, respectively. Hence, the two corresponding standing waves have different wavelengths and energies.[11] Moreover, the electric field eigenfunctions, corresponding to the top of the nth band and the bottom of the $(n+1)$th band, have n nodes. Naturally, one may ask a very interesting question. Why are the energies different between the top of the nth band and the bottom of the $(n+1)$th band although they have the same number of nodes? What is the physical origin of the PBG? The answer can be easily found from Eqs. (11)–(14). The two sets of solutions corresponding to the band edges always have opposite parities, leading to the field energy location in different regions and the formation of the PBG. In order to understand the localization of the field further, let us now define a parameter P_E to denote the localization of the

electric field energy in the high-ε region as: $P_E \equiv E_b/(E_a+E_b)$. Here $E_a = \int_0^a \varepsilon_0\varepsilon(x)|E_y(x)|^2dx/2$ and $E_b = \int_{-b}^0 \varepsilon_0\varepsilon(x)|E_y(x)|^2dx/2$. The calculated values of P_E for our 1D PC are 0.252, 0.459, 0.466, 0.463, 0.523, 0.475 for the bottoms of the 2nd–7th bands, and 0.871, 0.629, 0.626, 0.622, 0.566, 0.611 for the tops of the 1st-6th bands. The above data show that $P_{\mathrm{E1\,max}} > P_{\mathrm{E2min}}, P_{\mathrm{E2max}} > P_{\mathrm{E3min}}, \cdots, P_{\mathrm{E6\,max}} > P_{\mathrm{E7min}}$. In general, we have $P_{\mathrm{Enmax}} > P_{\mathrm{E}(n+1)\mathrm{min}}$. This implies that when a forbidden gap is formed between the nth band and the $(n+1)$th band, the corresponding eigenfunctions become two standing waves with the same number of nodes and two different frequencies $\omega_{n\,\max}$ and $\omega_{(n+1)\,\min}$. The electric field energy corresponding to the mode with $\omega_{n\,\max}$ is localized in the high-ε region. On the contrary, the mode with $\omega_{(n+1)\,\min}$ is in the low-ε dielectric material. We therefore know that the gap arises from the opposite symmetry of the eigenfunctions at the band edges, giving rise to the difference in field energy location. The low-frequency modes concentrate their electric field energies in the high-ε region, and the high-frequency modes concentrate their energies in the low-ε region.

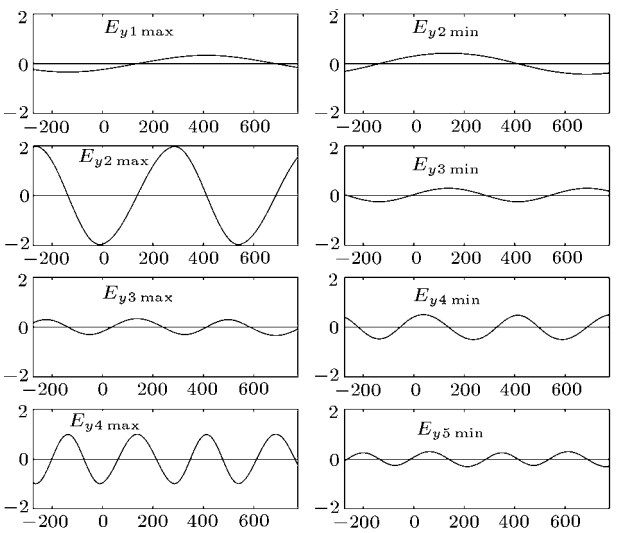

Fig. 2. Electric field eigenfunctions of the TM modes at the band edges for a 1D PC with $a = b = 275\,\mathrm{nm}$, $n_1 = \sqrt{12}$ and $n_2 = \sqrt{17}$. Here $E_{yi\max}$ ($E_{yj\min}$) is the electric field eigenfunction corresponding to the top (bottom) of the ith (jth) band.

We further find from our numerical calculations that the magnetic field eigenfunctions at the top and bottom of the nth band have n and $n-1$ nodes in one period of PC, respectively. Our results show that the magnetic field energy corresponding to the standing wave solution at the top of the nth band with the frequency $\omega_{n\,\max}$ is localized in the low-ε region. On the contrary, the solution at the bottom of the $(n+1)$th band with $\omega_{(n+1)\,\min}$ is in the high-ε dielectric material. Moreover, we can conclude that the localizations of the electric and the magnetic field eigenfunctions at the same band edge are completely opposite.

In conclusion, both the dispersion relations of the TM and TE modes and the electric/magnetic field eigenfunctions of the TM modes at the band edges have been derived analytically in a 1D PC. The important conclusions can be summarized as follows.

(1) An important and useful optimal parameter matching condition for the largest PBG, i.e. Eq. (15), is obtained. This opens a way for us to design PCs with large PBGs.

(2) We give a comprehensive physical picture of the photonic band structures from a new point of view. A series of standing waves can exist when the EM wave propagates in PCs. The electric/magnetic field eigenfunctions at the top and bottom of the nth band are naturally standing waves and have n and $n-1$ nodes in one period of PC, respectively. The more the standing wave nodes there are, the higher the corresponding frequency/energy. Furthermore, we find that all of the standing wave solutions at the band edges have definite parities. The eigenfunctions corresponding to the top of the nth band and the bottom of the $(n+1)$th band always have opposite parities. It is the opposite symmetry of the eigenfunctions at the top of the nth band and the bottom of the $(n+1)$th band that gives rise to formation of the PBG. Hence the gap can be attributed to different symmetries of the field eigenfunctions at the band edges, which leads to the localization of the field energy in different regions. It has been found that the eigenfunctions corresponding to the band top concentrate their electric (magnetic) field energies in the high (low)-ε region, and the corresponding solutions at the band bottom concentrate their electric (magnetic) field energies in the low (high)-ε region. The physical picture of photonic band structures given in the above is different from the known results.[10]

We believe that the present results are significant for designing PCs with large PBGs. Many interesting problems in the field of photonic crystal physics can be understood based on our physical picture of photonic band structures.

References

[1] Yablonovitch E 1987 *Phys. Rev. Lett.* **58** 2059
[2] John S 1987 *Phys. Rev. Lett.* **58** 2486
[3] Mishra S and Satpathy S 2003 *Phys. Rev.* B **68** 045121
[4] Kittel C 1996 *Introduction to Solid State Physics* (New York: Wiley)
[5] Pan S H and Feng S M 1991 *Phys. Rev.* B **44** 5660
[6] Cho H S and Prucnal P R 1987 *Phys. Rev.* B **36** 3237
[7] Feng Z F et al 2005 *Chin. Phys. Lett.* **22** 1941
[8] Li Z Y et al 2005 *Chin. Phys. Lett.* **22** 2585
[9] Wang Y Q et al 2004 *Chin. Phys. Lett.* **21** 324
[10] Joannopoulos J D, Meade R D and Winn J N 1995 *Photonic Crystals* (Princeton: Princeton University Press)
[11] Schiff L I 1968 *Quantum Mechanics* (New York: McGraw-Hill) p 38