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Modulation of Photonic Bandgap and Localized States by Dielectric Constant Contrast and Filling Factor in Photonic Crystals*

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Abstract: The band structure of 2D photonic crystals (PCs) and localized states resulting from defects are analyzed by finite-difference time-domain (FDTD) technique and Padé approximation. The effect of dielectric constant contrast and filling factor on photonic bandgap (PBG) for perfect PCs and localized states in PCs with point defects are investigated. The resonant frequencies and quality factors are calculated for PCs with different defects. The numerical results show that it is possible to modulate the location, width and number of PBGs and frequencies of the localized states only by changing the dielectric constant contrast and filling factor.

Key words: photonic crystals; photonic bandgap; defect states; FDTD

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1 Introduction

Recently, photonic crystals (PCs) in which the refractive index changes periodically have attracted a lot of attentions[1~8]. A complete photonic bandgap (PBG) can be formed in 3D PCs, which has 3D periodicity, and the propagation of electromagnetic waves with frequencies in the PBG is prohibited for all wave vectors. Various important scientific and engineering applications such as control of spontaneous emission, zero threshold lasing, very sharp bending of light, trapping of photons, and so on, are expected by utilizing the PBG and the artificially introduced defect states. All these are important in ultrasmall optical integrated circuits.

Much theoretic and experimental research works on the 2D PCs, 3D PCs and photonic crystal slab have been reported. Plihal[1] used the plane wave method to calculate the PBG of 2D PCs; Villeneuve and Qiu[4,5] calculated the defect modes in 2D PCs and focused on the resonant frequencies versus radius of defect; Steven[6] analyzed the guided modes in photonic crystal slabs and considered the effect of multiplayer structure on the third dimension; Ochiai[7] used the group theory and FDTD technique to investigate the dispersion relation and optical transmittance of photonic crystal slab. Song[8] analyzed the band structure of photonic crystal superlattice, and found the energy band fold in it.

However, the systemic investigations on the effect of dielectric constant contrast and filling factor on PBG have been reported seldom. Effect of different defects on the quality factors of localized states is also seldom discussed. In this paper, the

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FDTD technique combined with the Padé approximation[9~11] is used to analyze the PBG in a perfect 2D square lattice PCs and the localized states introduced by different defects. The multi-PBG in perfect PCs is analyzed, the width and the position of PBG for PCs with different parameters are calculated. Transmission spectrum is used in the analysis of defect states in PCs with different defects. The simple point source is used in FDTD calculation and the results are same as that of other groups are obtained.

2 Method

The FDTD technique is a powerful tool to simulate PCs because it is more convenient than the plane wave expansion method in modeling complicated structures. In this paper, we used the 2D FDTD algorithm to calculate the PBG and defect states in 2D PCs.

In this paper, we analyzed 2D PCs consisting of a square array of circle dielectric rods surrounded by air with the lattice constant a and the radius of dielectric rods r. Since the structure of PCs is periodic, a unit cell of lattice was naturally chosen as the finite computation domain in FDTD simulation to calculate the band structure. The periodic boundary condition was used at the boundary of the computation domain, which extends the computation domain to infinite crystal. We chose a Gaussian pulse modulating a carrier covering the interesting frequency range as the exciting source. In the FDTD process, the fields $E(r,t)$ and $H(r,t)$ were recorded as FDTD result for some sampling points in the calculation window. To obtain the field spectral intensities, Padé approximation[10,11] was used. The peak locations of the spectrum represent the desired mode frequencies f, and quality factors were obtained by $f/\Delta f$, where Δf is the 3-dB bandwidth of the intensity spectrum. We took the same process for each wave vector, and then we attained the dispersion relation.

The localized states introduced by defect were simulated with the computation domain contains 7×7 PCs unit cells and surrounded by perfectly matched layer (PML)[5]. The defects were introduced by altering the dielectric constant and radius of the center rod of the lattice. Each unit cell contains 50×50 discretization grid points. We set a single pulse whose frequency domain covers the PBG of this structure at a point left aside the lattice as the input. The outputs were recorded at four points right aside the lattice respectively (Fig. 4). We obtained the transmission spectra from the ratio of the output spectral intensity to the input spectral intensity. Since we are only interested in the frequencies of the localized states in PBG, the transmission obtained in our calculation is available. The results shown in Fig. 4 agree well with the results in Ref. [4]. So the simple point source is available in FDTD calculation for the transmission.

Since TE modes (whose magnetic field lies along the rods) and TM modes (whose electric field lies along the rods) are linearly independent, it is possible to study the behavior of each polarization separately. In this paper, only the TM modes are considered.

3 PBG in perfect PCs

Figure 1 shows the band diagram for the PCs with refractive index of rods $n=3.4$ and radius of rods $r=0.2a$. It can be seen that the TM mode has a PBG with big width centered at $f=0.35c/a$. And a narrow second PBG also arises in the higher frequency region considered. Two or three modes have the same eigenfrequency on the highly symmetric points such as Γ and M. This property is closely related to the symmetry of the crystal structure. There are, of course, not complete gaps since those eigenmodes of the TE polarization and those with off-plane wave vectors have eigenfrequencies in the above gaps. Therefore, the spontaneous emission of photons from atoms embedded in the PCs can be inhibited partially.

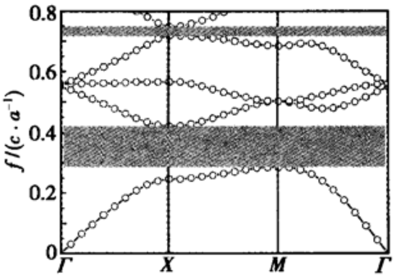

Fig. 1　Band diagram for a 2D PC which is a square array of circle dielectric rods surrounded by air with dielectric constant $n = 3.4$ and radius of dielectric rods $r = 0.2a$

We fixed the radius of dielectric rods and modified the refractive index n of dielectric rods to modulate the PBG. The low edge and up edge of each PBG versus the refractive index of rods are shown in Fig. 2. It can be seen that two PBGs arise in the frequency region we considered when $n \geqslant 3.0$. And the width of each PBG increases with the increasing contrast of dielectric constant between dielectric rods and air. The cavity quantum electrodynamics (QED) theory tells us that the mode with low frequency concentrates in high dielectric constant region and the mode with high frequency concentrates in low dielectric constant region[2]. So the increasing contrast between the rods and air results in the increasing of the difference between the

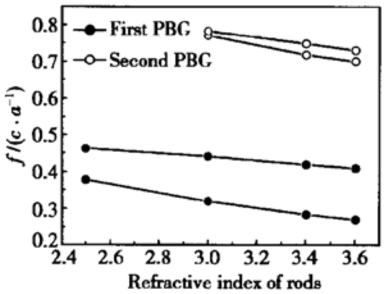

Fig. 2　Low edge and up edge of each PBG versus refractive index of rods in a 2D PC which is a square array of circle dielectric rods surrounded by air with $r = 0.2a$

two frequency bands, the gap is open larger. It is also observed that the mode frequencies decrease with the increasing contrast. Since the approximatively inverse ratio relation between refractive index n and frequency ω in wave equation, the large n must result in the low frequency and accordingly the location of PBG declines. This causes multi-PBG in the frequency domain considered.

In Fig. 3 we show the low edge and up edge of each PBG versus radius of dielectric rods with fixed dielectric constant contrast. We modified the filling factor by radius of dielectric rods to modulate the

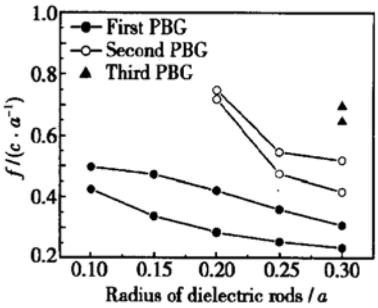

Fig. 3　Low edge and up edge of each PBG versus radius of rods in a 2D PC which is a square array of circle dielectric rods surrounded by air with $n = 3.4$

PBG in the same structure as mentioned above. It can be seen that the mode frequencies decrease with the increasing radius of dielectric rods resulting from the same mode "feels" a large equivalent dielectric constant on average, accordingly the location of PBG declines. This causes multi-PBG in the frequency domain considered, as can be see that two PBGs arise when $r \geqslant 0.2$, and three PBGs arise when $r \geqslant 0.3$. These are analogous to Fig. 2. So we can say the effect of increasing dielectric constant contrast is analogous to that of increasing radius of dielectric rods in some ways. This can be understood from the confinement of field. But the difference between them is apparent too. In Fig. 3 the width of first PBG does not increase with the increasing radius all the way. It decreases with the increasing radius when $r > 0.2a$. The width of second PBG increases with the increasing radius. When $r = 0.3a$ the width is larger than that of the first PBG. It is quite different from the Fig. 2 in which the width of second PBG is much narrower than the first one. What is more, the third PBG arises in the frequency region consider when $r = 0.3a$. So we can see the variation of band structure is more apparent than that of modulation the dielectric constant of dielectric rods.

4 Localized states in PCs with a point defect

We consider the same structure of PCs used in Fig. 1. This structure has a PBG for TM modes between the frequencies $f = 0.29c/a$ and $f = 0.42c/a$, where c is the speed of light in vacuum. In Refs. [4, 5] radius of defect is modified to modulate the defect states. Here we modify the refractive index $n_{\rm defect}$ of the center rod to introduce a defect in the PCs.

Figure 4 is the simulation model and transmission spectra obtained at each sampling point for a 2D PC which is a square array of circle dielectric rods surrounded by air ($n = 3.4$ and $r = 0.2a$) and

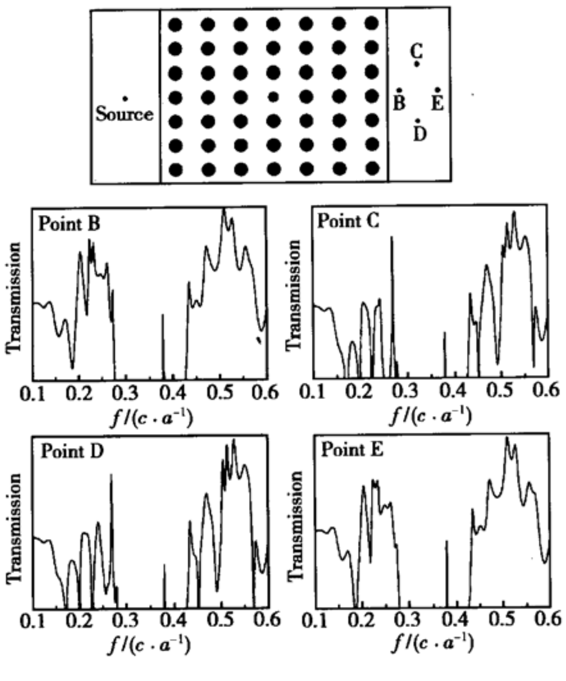

Fig. 4 Simulation model and transmission spectra obtained at each sampling point for a 2D PC which is a square array of circle dielectric rods surrounded by air ($n = 3.4$ and $r = 0.2a$) and the center rod is removed

the center rod is removed. From Fig. 4 we can see an obvious peak at $f = 0.38c/a$ corresponding to the defect resonator in the low transmission band between $f = 0.28c/a$ and $f = 0.42c/a$ for each sampling point. So the defect states do not shift for different sample point, transmission obtained in the way used in this paper is available. The low transmission band is more obvious than that in Ref. [4] which results from the advantage of Padé approximation[10, 11] and the peak agree well with that in Ref. [4]. We also calculated the spectra intensity of the FDTD result of a sampling point located in the defect region. The peak agrees well with the counterpart in transmission spectra.

We calculated the localized states for the PCs contain defect rod with the same radius as other rods and different $n_{\rm defect}$. The mode frequencies and quality factors are shown in Fig. 5. It can be seen that the resonance frequencies increase when gradually reduce $n_{\rm defect}$. At the same time, since the field confined in the resonator decline with the deceasing

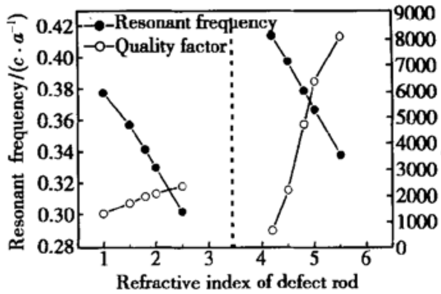

Fig. 5 Resonant frequencies and quality factors of localized states versus refractive index of defect for a 2D PC that is a square array of circle dielectric rods surrounded by air

$n_{\rm defect}$, the value of Q decreases. When gradually enlarge $n_{\rm defect}$, the resonance frequencies decrease. Synchronously, Q-factor increases resulting from the stronger confinement of light for the larger $n_{\rm defect}$. What should be noticed is that the modes correspond to $n_{\rm defect} > n_{\rm rod}$ and $n_{\rm defect} < n_{\rm rod}$ are not the same modes. When $n_{\rm defect} > n_{\rm rod}$ the field has a node in the radial direction. When $n_{\rm defect} < n_{\rm rod}$ the field has no node in the radial direction. From Ref. [4] and this paper, we can see that the localized states can be easily modulate by modifying the radius and dielectric constant of defect.

5 Conclusion

The effect of dielectric constant contrast and filling factor on PBG for perfect PCs and localized states in PCs with point defect are investigated. The results show the location, width and number of PBG and the frequency of defect states can be modulated by the two parameters. In our analysis, we consider that it is more efficient and convenient to modulate of filling factor than modulate dielectric constant contrast. We also find that different dielectric constant of defects can create different states in the gap: pull (push) a localized state down (up) from the upper (lower) band by increasing (decreasing) the dielectric constant of a single rod, and the quality factors change accordingly. The multi-PBG in PCs with proper parameter gives us more choice to control the spontaneous emission by PCs. The simple point source in FDTD simulation for transmission is testified to be efficient and available.

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介电常数对比和填充率对光子晶体中光子禁带和局域态的调节*

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摘要: 用有限时域差分法 (FDTD) 和Padé近似分析了二维光子晶体的能带结构和缺陷引起的局域态. 针对介电常数对比和填充率对完整光子晶体中光子禁带以及缺陷态的影响作了研究. 计算了不同缺陷的光子晶体模式的振荡频率和质量因子. 数值模拟的结果表明通过改变介电参数对比和填充率可以实现对光子禁带的位置、宽度、数目以及对缺陷态的调整.

关键词: 光子晶体; 光子禁带; 缺陷态; 有限时域差分法

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