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Existing conditions of full bandgaps and absolute negative refraction in metallic-dielectric photonic crystal*

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This paper has theoretically studied the characteristic frequencies of band structures in two-dimensional metallic-dielectric photonic crystals. It is demonstrated that a large filling fraction benefits the existence of absolute photonic band gap, while a smaller filling fraction benefits an absolute negative refraction band. In addition, it also finds that the relation between the cut-off frequency of E-polarized wave and the filling fraction exceeding 10% is content with a linear increasing function, whose coefficients are exponential to the normalized lattice constant. These investigations have significant implications for tuning the operational frequencies to desired applications and manufacturing photonic crystals.

Keywords: metallic-dielectric photonic crystal, absolute photonic band gap, absolute negative refraction
PACC: 4270Q, 4225G

1. Introduction

Photonic crystals (PCs) have attracted much attention since the initial predictions of Yablonovitch[1] and John.[2] This active research area has been extended to metallic-dielectric PC (MDPC) theoretically and experimentally.[3−11] By a careful match between the geometry of the structure and the frequency-dependent material, owing to multiple Bragg scattering, the photonic band gaps (PBGs) in MDPCs can be enlarged effectively.[3] In the visible and near-infrared regions, by combinations of metallic and dielectric background materials with a proper filling fraction, one can realize the superlensing effect in the far-field region and sub-wavelength imaging in the near-field region[4] due to negative refraction.[5,6]

However, a large number of discussions about the forbidden gaps and negative refraction in MDPC focus on a certain polarization, E- or H-polarization. Only few studies[7,8] have concentrated on discussing the complete PBG and negative refraction in MDPC. Moreover, the existing conditions of the structural parameters for the complete PBG and negative refraction are not clear. Therefore, a detailed investigation of band structure in two-dimensional MDPC to find out the working frequency region for complete PBG and negative refraction is urgently needed.

In this paper, the evaluation of characteristic frequencies in two-dimensional MDPC arranged in the square lattice is studied. We find the existing conditions of the absolute PBG and absolute negative refraction band (NRB), and present an expression of the cut-off frequency of E-polarized wave with filling fraction and normalized lattice constant in a simple form.

2. Model description

We utilize the frequency-dependent dielectric functions for the metal cylinders that meet the Drude formula:

$$\varepsilon(\omega) = 1 - \frac{\omega_{\rm p}^2}{\omega(\omega + {\rm i}\tau^{-1})},$$

where $\omega_{\rm p}$ and τ are the plasma frequency and relaxation time of the conducting electrons respectively.

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The plasma frequency $\omega_{\rm p}$ has been tabulated by fitting the Drude dispersion model to experimental measurements.[12,13] For example, the plasma wavelengths $\lambda_{\rm p}$ $(= 2\pi c/\omega_{\rm p})$ are about 84.0 nm for aluminium and 137.9 nm for aluminium and silver, which fit the experimental data from 400 nm to 10 μm. Notice that for calculating the band structure of an infinite periodic system, it is quite common and reasonable to regard τ as infinite.[3] Actually, the band structure with infinite τ, the so-called dispersion relationship, is consistent with the optical response with finite τ. In this case, for simplification, we employ the multiple scattering methods[14,15] to calculate the band structure in the absence of dissipation ($\tau = \infty$).

3. Results and discussions

The geometry of MDPC structure, shown in the inset of Fig.1(a), is arranged in a square lattice. Here, r and a are the radius of the metal cylinders and the lattice constant respectively. It is noted that the frequency range of photonic band structure is much influenced by the background materials, which should be transparent in order not to absorb any electromagnetic wave and whose dielectric constant should be large enough. Gallium nitride ($\varepsilon = 6.25$) is a well-considered choice for this purpose. With specific filling fraction ($f_{\rm s} = 50\%$) and unitary normalized lattice constant (i.e. $a/\lambda_{\rm p} = 1$), the lower photonic bands of both polarizations are shown in Figs.1(a) and 1(b).

It can be seen that there exists a stop band of E-polarization extending from zero up to a cut-off frequency (denoted by $f_{\rm E0}$) for all symmetrical propagating directions. In addition, the forbidden bands can be opened up between $f_{\rm E2}$ ($f_{\rm H2}$) and $f_{\rm E3}(f_{\rm H3})$ which is denoted by bottom-left area. Moreover, it is known that the photonic band between $f_{\rm E1}(f_{\rm H1})$ and $f_{\rm E2}(f_{\rm H2})$ is the NRB which is denoted by bottom-right area due to the negative refraction phenomenon resulting in multiple Bragg scattering. Note that these characteristic frequencies determine the main shape of the photonic band structure and the operational frequency region. Therefore, it is important to understand the evolution of these characteristic frequencies when we change the normalized lattice constant and the filling fraction.

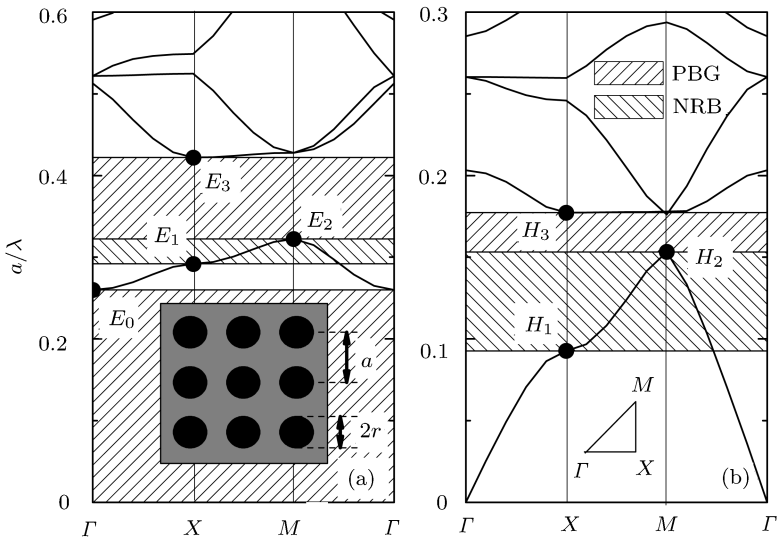


Fig.1. Photonic band structure of MDPC for (a) E- and (b) H-polarization with 50% filling fraction and unitary normalized lattice constant. The background material is GaN. E_i $(i = 0 - 3)$ and H_j $(j = 1 - 3)$ are the characteristic frequencies of E- and H-polarization, respectively. The inset graph is the schematic illustration of 2D MDPC. r and a are the radius of the metal pillars and the lattice constant, respectively. The bottom-left area is the PBG, while the bottom-right area is the NRB.

From the normalized parameters, one can simply design the positions of photonic band structures. If one intends to obtain the PBG in a certain frequency range, one can first choose the lattice constant according to the target photonic band with the desired frequency range. Then one can choose the normalized lattice constant and its relative radius according to the chosen metallic materials and the filling fraction, re-

spectively. For example, if the operating wavelength of PBG is desired to be 1 μm, since the normalized frequency is 0.36 (the star of Fig.2(b)), then the real and normalized lattice constant is 360 nm and 2.63 (in the case of silver), respectively. In addition, since the filling fraction is 30%, the radius of metallic cylinder is then about 111.2 nm. Therefore, in order to successfully and effectively guide the manufacturing process, it would be remarkably advantageous to design the size of the structure for the desired frequency region.

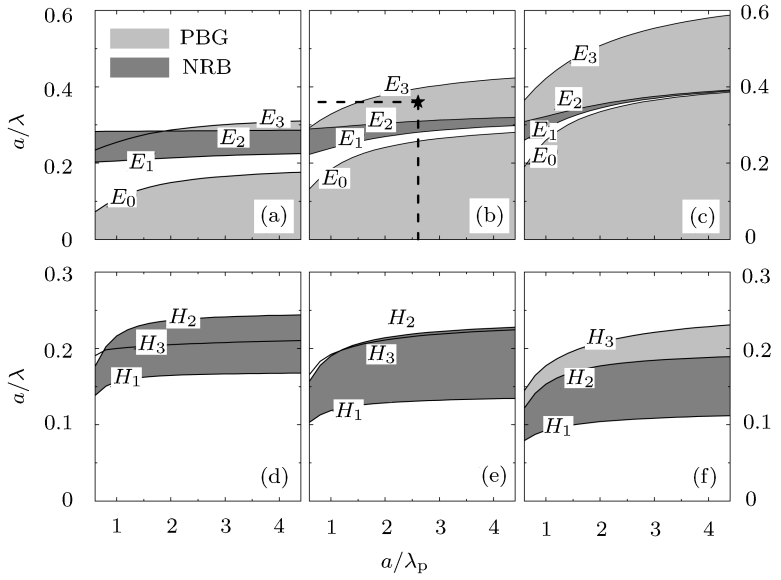


Fig.2. The E-polarized (a)–(c) and H-polarized (d)–(f) characteristic frequencies as function of the normalized lattice constant a/λ_p for the filling fraction $f_s = 10\%$ ((a), (d)), 30% ((b), (e)) and 50% ((c), (f)), respectively. The light grey area is the PBG, while the dark grey is the NRB. Star corresponds to an E-polarized PBG in silver–GaN MDPC. The operating wavelength is 1 μm and the parameters are $a = 360$ nm, $r = 111.2$ nm.

In order to check the evolution of characteristic frequencies, we have performed multiple scattering calculations on the MDPC with different pairs of structural parameters. Figure 2 shows the remaining characteristic frequencies, i.e. the PBGs and NRBs, with the normalized lattice constant in the large filling fraction case for E- and H-polarization. First, as shown in Figs.2(a)–2(c) and 2(f), the PBGs become narrow with the decrease of the normalized lattice constant. This is because in the small dimensional limit, the skin depth of metal is comparable to the radius of the cylinder. The electromagnetic wave may have almost penetrated into the metal cylinder entirely. Thus there is little Bragg multiple scattering, i.e. a narrow Bragg forbidden gap. Moreover, as shown in the Fig.2(a), there exists a narrow PBG of E-polarization in 10% filling fraction when the normalized lattice constant is larger than 2.0, whereas no PBG of H-polarization exists (see Fig.2(d)) in the same parameters since the characteristic frequencies f_{H2} and f_{H3} are still overlapping each other. Thus, only a broad PBG of E-polarization can be obtained in the visible region. For example, a 36%-wide gap-to-midgap ratio is achieved when the lattice constant is 300 nm and the radius of metallic cylinder is 120 nm. Furthermore, for E-polarization, the propagating frequencies are the increasing function of the normalized lattice constant as demonstrated by the simple waveguide model. On the contrary, the photonic band structure is depressed with the increasing normalized lattice constant as demonstrated by the Maxwell–Garnett approximation. This opposite variation of two polarizations is the advantage of obtaining the absolute PBG. By properly choosing the structural parameters, the absolute PBG in the near-infrared region can be obtained. The width of the absolute PBG is determined by the bandgap width of H-polarization, which is shown as a grey pattern in Fig.2(f).

As for the NRB structure, the evolution is quite different from the PBG. For E-polarization, the width of NRB decreases with the normalized lattice constant. Moreover, the NRB nearly vanishes while the normalized lattice constant is over 4.0 in large filling fraction which is shown in Fig.2(c). By contrast, for

H-polarization, the frequency range and the width of NRB increase dramatically in small normalized lattice constant case, while they are improved a little in large normalized lattice constant case. Figure 3 shows the equifrequency surface (EFS) of the Bloch wave vectors when the filling fraction is 55% and the normalized lattice constant is 1.25. The NRB range of E-polarization in this case is from 0.3299 to 0.3472 in the unit of a/λ, which corresponds to the visible spectrum $495-521$ nm. Furthermore, it is shown that the absolute NRB in the near-infrared region can be obtained in the case of 10% filling fraction. The width of NRB is determined by the E-polarization. That is to say, the absolute NRB can be realized in the small filling fraction case, whereas the absolute PBG is favour to the large filling fraction case as mentioned above.

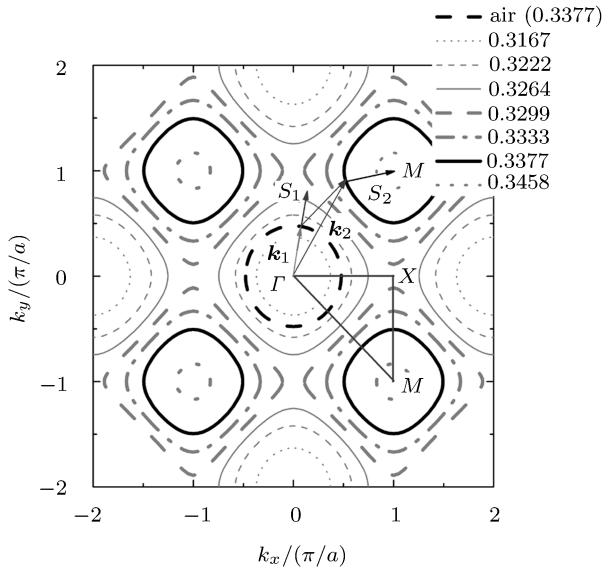


Fig.3. The EFS diagram of E-polarization for $f_s = 55\%$ and $a/\lambda_p = 1.25$. Thin (Thick) grey circles stand for EFS round $\Gamma(M)$ point in PC. Dashed (solid) black circles stand for EFS in vacuum (PC) at $a/\lambda = 0.3377$ with $n = -1$. For an incident plane wave with wave vector $\boldsymbol{k}_1$ and energy flow of S_1 in vacuum, a Bloch wave with wave vector $\boldsymbol{k}_2$ energy flow of S_2 can be excited in PCs.

Figure 4 shows the normalized cut-off frequency with different filling fraction f_s given the normalized lattice constant. It can be seen that the normalized cut-off frequency is almost linearly increasing to the filling fraction that is larger than 10%. By non-linear fitting method, a simple equation with the linear form can be obtained:

$$a/\lambda_{cut} = A + Bf_s,$$

where $A = 0.121 - 0.148\exp(-a/\lambda_p)$ and $B = 0.528 - 0.398\exp(-a/\lambda_p)$. It can be found that the coefficients A and B are exponential functions of the normalized lattice constant. This means that the cut-off frequency tends to an extreme value with the increase of the normalized lattice constant. From such quantitative relationship for the cut-off frequency over the filling fraction, one can easily determine the positions of the cut-off band gap to a target value by choosing the real lattice constant and the radius of metallic cylinder. In fact, the cut-off frequency can be regarded as the effective plasma frequency. The forbidden band below the cut-off frequency corresponds to the negative permittivity value that is very similar to the bulk metal. By simple calculation, the frequency range shown in Fig.3 is just in the near-infrared region. Therefore, if one can obtain the negative permeability[16,17] simultaneously in the visible and near-infrared region, the quantitative relationship may be useful to design the double negative metamaterials which have only been verified in the microwave region.[18] Note that the present expression is just valid when the filling fraction is over 10%. The dimensional size is too small to employ the bulk dielectric constant of materials when the filling fraction is less than 10%. As a result, the cut-off frequency would follow a distinct discipline. This is beyond the scope of our discussion here and will be further investigated in future research paper.

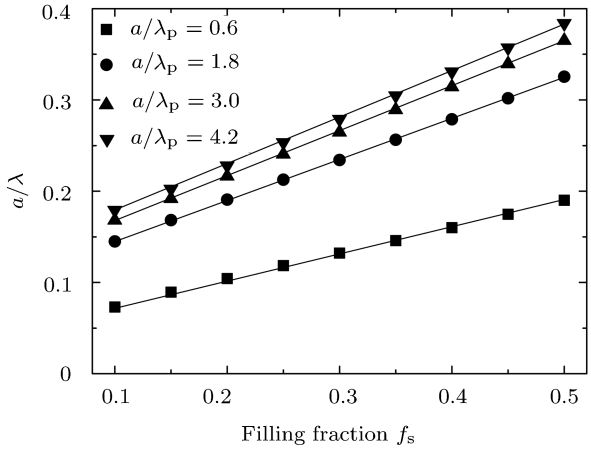


Fig.4. The cut-off frequencies as function of the filling fraction. The normalized lattice constant equals to 0.6 (•), 1.8 (■), 3.0 (▲) and 4.2 (▼), respectively. The solid lines show the linear relationship.

4. Conclusion

In conclusion, the characteristic frequencies of dispersion relations for two-dimensional metallic-dielectric photonic crystals in the square lattice have

been investigated in detail by multiple scattering methods. By analysing the physical mechanism and properly choosing the structural parameters, a broad E-polarization PBG, as well as the NRB, has been achieved in the visible region. Moreover, absolute PBG can be obtained in large filling fraction case, while absolute NRB can be realized in small filling fraction case. Furthermore, we have found that the cut-off frequency linearly increases in the filling fraction exceeded 10%. The coefficients of the linear function are exponential to the normalized lattice constant. This quantitative relationship is important for our manufacturing process and many other applications.

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