Numerical and Analytical Comparison of Dispersion Relations of Weakly Modulated Fibonacci Sequence One-dimensional Photonic Crystals

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Numerical and Analytical Comparison of Dispersion Relations of Weakly Modulated Fibonacci Sequence One-dimensional Photonic Crystals

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Abstract. The photonic band and the equifrequency surface of the weakly modulated one-dimensional Fibonacci sequence photonic crystal have been calculated by the finite difference time domain method and the analytical method, respectively, where the analytical method is based on the transfer matrix method. The results show that the equifrequency surface of the photonic crystals calculated by numerical method may lead to a completely wrong conclusion. Therefore, in the study of weakly modulated photonic crystals, the study of analytical methods is very necessary.

1. Introduction

The concept of photonic crystals (PhCs) is proposed by E. Yablonovich and S. John in the late 1980. On the study of PhCs, how to calculate the dispersion relation of this kind of new artificial material, that is how to calculate the photonic bands (PBs) and the Equifrequency Surfaces (EFS) of PhCs, has always been one of the focus of scientists [1, 2]. So during these years, scientists have obtained a variety of mature methods for calculating the PBs and the EFS of PhCs, such as plane wave expansion method, time-domain finite difference (FDTD) method, finite element method, etc. [3, 4]. However, most of these methods are numerical methods. Although there are some advantage for the numerical method, but there are also inherent defects for them. One of the defects is that there is always artificial intervention in the numerical method. For example, there is a problem for judging the convergence of the equation solution in solving the eigenequation for the plane wave expansion method; and how to define the power spectrum peaks is a problem for the FDTD method. These artificial interventions maybe lead to errors on the final results in calculating the dispersion of the weakly modulated PhCs.

In this paper, the analytical calculation of physical quantities, such as PBs, EFS, wave vector and group velocity of one-dimensional (1D) Fibonacci sequence (FS) PhCs has been studied by the transfer matrix method (TMM) [5], and the results of the analytical and numerical calculation for the PBs and the EFS of the weakly modulated 1D FS PhCs have been studied comparatively.

2. Model and Formulas

In this paper, we use the same way in literature [6] to construct the cell of the order 2 1D FS PhCs, in which the layer A and B constituted by materials A and B are arranged in the order of ABAAB. Then, the 1D PhCs has been constructed by a repetition of blocks of the cell with infinite periods. When the layers A and B have the same thickness d, the lattice constant of the PhCs will be D=5d.

When the films arrange along z direction, the medium distribution of the 1D PhCs is uniform in x and y directions. We assume that the medium constituting the 1D PhCs is an isotropic homogeneous and lossless dielectric, and the monochromatic electromagnetic wave (EMW) with frequency ω is

transmitting in the x-z plane. Thus, the EMW will have a propagation factor β in the x direction, and it will satisfy

$$k_{iz} = \frac{\sqrt{4\pi^2 n_i^2 \tilde{\omega}^2 - \tilde{\beta}^2}}{D} \tag{1}$$

here, k_{iz} (i=1,2,⋯) is the component of the wave vector along z direction in the i-th layer medium; n_i is the refractive index of the i-th film; $\tilde{\omega} = \omega D/(2\pi c)$ is the normalized frequency; $\tilde{\beta} = \beta D$ is the normalized wave number along x direction, c is light speed in vacuum.

In addition, due to the periodicity of the films, the magnetic field of the TM_y mode (H_y,E_x,E_z) of the EMW between the n-1th period and the nth period in the order 2 1D FS PhCs can be connected by the transfer matrix[5], and the sum of the main diagonal elements of the transfer matrix for the TM_y mode can be written as

$$\begin{aligned} SUM_{2M} = {} & 2\cos(3k_{1z}d)\cos(2k_{2z}d) - \frac{k_{1z}^2\varepsilon_2^2 + k_{2z}^2\varepsilon_1^2}{k_{1z}k_{2z}\varepsilon_1\varepsilon_2}\sin(3k_{1z}d)\sin(2k_{2z}d) \\ & + \left(\frac{k_{1z}^2\varepsilon_2^2 - k_{2z}^2\varepsilon_1^2}{k_{1z}k_{2z}\varepsilon_1\varepsilon_2}\right)^2 \sin(2k_{1z}d)\sin(k_{1z}d)\sin^2(k_{2z}d) \end{aligned} \tag{2}$$

here, ε_i (i=1,2) is dielectric constant of materials A and B, respectively.

Furthermore, since the medium composing the 1D FS PhCs periodically distribute along the z direction, the EMW transmitting along z direction should be the Bloch wave. Thus, on the condition $|SUM_{2M}|<2$, the Bloch wave number κ in z direction for the TM_y mode can be written as

$$\tilde{\kappa} = \kappa D = \cos^{-1}\left(\frac{SUM_{2M}}{2}\right) \tag{3}$$

here, $\tilde{\kappa}$ defined as the normalized Bloch wave number along z direction. And the group velocity of EMW in the 1D PhCs can be expressed as

$$\vec{v}_g = v_{xg}\hat{\vec{x}} + v_{zg}\hat{\vec{z}} = \left(\frac{\partial\omega}{\partial\beta}\right)_\kappa \hat{\vec{x}} + \left(\frac{\partial\omega}{\partial\kappa}\right)_\beta \hat{\vec{z}} \tag{4}$$

$$v_{xg} = \left(\frac{\partial\omega}{\partial\beta}\right)_\kappa = -2\pi c\frac{\left(\partial(SUM_{2M})/\partial\tilde{\beta}\right)_{\tilde{\omega},\tilde{\kappa}}}{\left(\partial(SUM_{2M})/\partial\tilde{\omega}\right)_{\tilde{\beta},\tilde{\kappa}}} \quad , \quad v_{zg} = \left(\frac{\partial\omega}{\partial\kappa}\right)_\beta = -\frac{4\pi c\sin(\kappa D_m)}{\left(\partial(SUM_{2M})/\partial\tilde{\omega}\right)_{\tilde{\beta},\tilde{\kappa}}} \tag{5}$$

Moreover, we can prove[7] that when the dot product (DP) between the unit wave vector and the unit group velocity is ±1, it indicates that the PhCs can be equivalent to isotropic right-handed (RH) or left-handed (LH) materials, respectively; when the DP is belong to the range (0, 1) or the range (-1, 0), it indicates that the PhCs can be equivalent to an anisotropic RH or LH material.

Thus, if let $\tilde{\beta} = 0$, the PBs of the order 2 1D FS PhCs can be analytically calculated by using equations (1) and (3); if let $\tilde{\beta}$ be in the range $\tilde{\beta} \in (-2\pi n_{\min}\tilde{\omega} \quad , \quad 2\pi n_{\min}\tilde{\omega})$, where n_{min} is the minimum refractive index in materials A and B, the EFS of the TM_y mode of the 1D PhCs can also be analytically calculated by the same formulas. Since $\tilde{\kappa}$ in formula (3) is the solution of the simple Brillouin zone, it should be expanded in calculating the EFS. And with the aid of the value of the dot product, we can further quantitatively determine whether the EFS is correct or not.

3. Numerical and Analytical Discussion

Using the FDTD method and the formulas above, we studied the TM_y mode dispersion relation of this kind of 1D PhCs model composed of aluminum (Al) and boron (B). The frequency range of the EMW

is [22.27, 24.31]nm, which is in the soft x-ray band. The relative dielectric constant of Al and B is 0.96316 and 0.82184, respectively [8]. It can be seen from the refractive indices of Al and B that this model is a weakly modulated 1D PhCs.

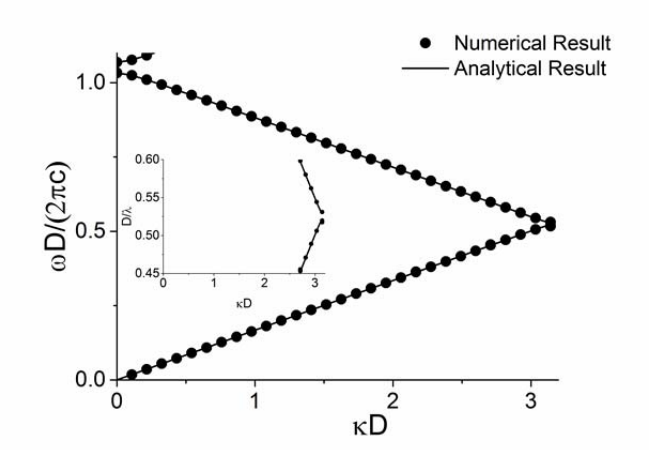

Figure 1. PBs of the order 2 1D FS PhCs

The PBs of the 1D FS PhCs is shown in figure 1. In figure 1, the horizontal and vertical coordinates are the normalized wave vector and the normalized frequency, respectively. The scatter and the solid line are the results obtained by the FDTD method and the analytical method, respectively. See the legend in figure 1. The inset of figure 1 is the PBs between the normalized frequency intervals [0.45, 0.55]. It can be seen from figure 1 that there is a small band gap between the first and second PBs, and the numerical results are in good agreement with the analytical results.

We further studied the EFS and the DP of the TM_y mode. The results are shown in figure 2 and figure 3.

Figure 2 shows the results of the first PBs, where figure 2(a) and 2(b) are the results of the EFS of the TM_y mode obtained by the FDTD and the analytical method, respectively, figure 2(c) is the analytical result of the DP between the unit wave vector and the unit group velocity changing with the wave vector angle at different frequencies. In figure 2(a) and 2(b), the horizontal and vertical axes are normalized wave vectors along z and x direction, respectively. In figure 2(c), the horizontal axis is the arctangent of the ratio of β to κ, its unit is degree; and the vertical axis is the value of dot product, its unit is s^{-1}.

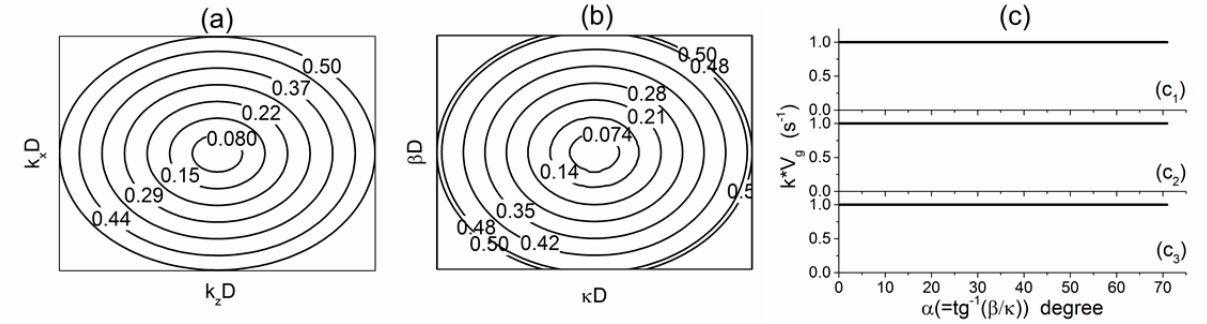

Figure 2. The results of the TM_y mode of the first PBs. (a) the FDTD results of the EFS. (b) the analytical results of the EFS. (c) the results of $\hat{\vec{k}} \bullet \hat{\vec{v}}_g$ changing with the wave vector angle, where (c_1), (c_2) and (c_3) show the results at the normalized frequency 0.1, 0.3 and 0.5, respectively.

It can be seen from figure 2(a) and 2(b) that the numerical results of EFS are in good agreement with the analytical results in the first PBs. Both the numerical results and the analytical results indicate that the order 2 FS 1D PhCs can be equivalent to an isotropic material with RH characteristics in the first PBs. This result is also confirmed by figure 2(c). In figure 2(c), the diagrams of (c_1), (c_2) and (c_3) are the results of the DP at the normalized frequency 0.1, 0.3, and 0.5, respectively. It can be seen from the three diagrams that the DP is always 1 in the first PBs, which indicates that the PhCs can be equivalent to a isotropic material with RH characteristics. Thus, we have the same conclusion by figure 2(a), 2(b) and 2(c).

The further results of the TM_y mode of the second PBs are shown in figure 3. Figure 3(a) and 3(b) are also the EFS results obtained by the FDTD method and the formulas above, respectively. In figure 3(c), the diagrams of (c_1), (c_2) and (c_3) are the analytical results of the DP between the unit wave vector and the unit group velocity changing with the wave vector angle at the normalized frequency 0.628, 0.804 and 0.980, respectively. The horizontal and vertical axes of figure 3(a), 3(b) and 3(c) are same with those of figure 2(a), 2(b) and 2(c), respectively.

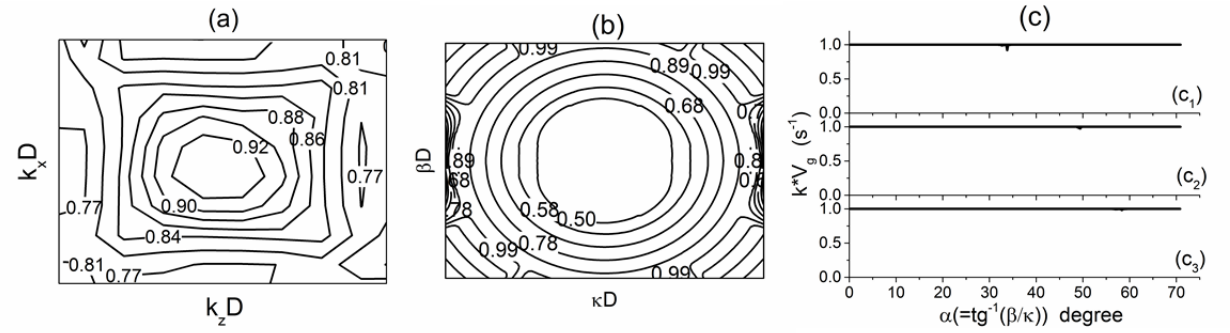

Figure 3. The results of the TM_y mode of the second PBs. (a) the FDTD results of the EFS. (b) the analytical results of the EFS. (c) the results of $\hat{\vec{k}} \bullet \hat{\vec{v}}_g$ changing with the wave vector angle, where (c_1), (c_2) and (c_3) show the results at the normalized frequency 0.628, 0.804 and 0.980, respectively.

It can be seen from figure 3(a), the numerical result shows that the order 2 FS 1D PhCs exhibits an approximately isotropic property with LH characteristics. But the analytical result coming from figure 3(b) shows that the 1D PhCs is still equivalent to an isotropic material with RH characteristics. Obviously, this result tell us that either figure 3(a) or figure 3(b) must be wrong. However, based on the further analysis about the result coming from figure 3(c), it can be found that the conclusion coming from figure 3(b) has been supported. It can be seen from the three diagrams of figure 3(c) that the DP is 1 in most of the angles for every frequency. There is only a very little fluctuation in a small angle in figure 3(c_1). The little fluctuation can also be confirmed by the EFS pattern of figure 3(b) in the low frequency. This phenomenon only means that the PhCs has a slight deviation from the isotropic property in the low frequency. But the results in figure 3(c) confirm generally that the PhCs still be approximately equivalent to an isotropic material with RH characteristics. Therefore, we have to say that the result of figure 3(a) is wrong.

4. Conclusion

The TMM is used to give the formulas for calculating the PBs, the EFS, the group velocity and the wave vector of the 1D FS PhCs. On this basis, the analytical results of the dispersion relation of the PhCs are compared with the numerical results obtained by the FDTD method. The result shows that both the numerical methods and the analytical method have the same accuracy in calculating the PBs of the weakly modulated PhCs. But the result also shows that when the numerical method is used to calculate the EFS of a weakly modulated PhCs, errors in numerical calculation for EFS easily tend to an erroneous result. At the same time, the calculation results for the physical properties of the chiral characteristics of the medium also support the above conclusions.

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