The Analysis of Band Structure of Photonic Crystals

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Abstract

In this paper, a finite element is developed to calculate the band structures of one dimensional photonic crystals. The Maxwell's equation governing the propagation of electromagnetic waves, which combine with Bloch theory, the FEM transform the complex band diagram problems into a simple eigenvalue by solving the eigenvalue with respective to wave vector K by frequency. And then using the COMSOL for simulation.

Keywords: band structure, finite element method, Maxwell equation, eigenvalue, COMSOL.

1. Introduction

Photonic crystals [1] are a kind of artificial microstructure material formed by periodic arrangement of the medium. According to the periodic structural features in different directions of space, photonic crystals are divided into one-dimensional, two-dimensional and three-dimensional photonic crystals. When electromagnetic waves propagate in photonic crystal, due to the periodic arrangement of materials, Bragg diffraction [2] occurs and the electromagnetic wave is modulated to form an energy band structure. This energy band structure is called a photonic band structure. If the ratio of the dielectric constants of the constituent materials is large enough, a bandgap may exist in the photonic band structure, which is called Photonic Band Gap [3]. Ellipsoid, Brillouin, and Bloch state in solid state physics can all be used to describe photonic crystals.

As a starting point for the study of photonic crystal theory, band structure is the object of all calculations. It is one of the research focuses in the field of photonic crystals to study the band structure of photonic crystals. There are many ways to calculate the energy band structure, commonly used are the plane wave expansion method, the finite difference time domain method, the transfer matrix method, etc., but these methods have their own drawbacks and limitations. For example, the use of plane wave expansion method can only be limited to simple geometry. Time-domain finite-difference methods may not be useful for some practical engineering problems in some cases. It is therefore important to develop a solver that is fast and accurate in calculating the band structure.

In this paper, starting from Maxwell's equation [4], to derive the scalar equation of wave equation, and using the finite element method to get the eigenvalue matrix equation, finally, using the COMSOL [6] for simulation, COMSOL specify the scalar function and translate the scalar equation into weak form.

2. Numerical derivation of band structure of photonic crystals

The propagation of an electromagnetic wave through a periodic medium (such as the photonic crystals) is described by Maxwell's equations.

$$\nabla \times H = J + \frac{\partial \varepsilon E}{\partial t} \quad (1)$$

$$\nabla \times E = -\frac{\partial H}{\mu_0 \partial t} \quad (2)$$

$$\nabla \cdot \varepsilon E = \rho \quad (3)$$

$$\nabla \cdot H = 0 \quad (4)$$

where E and H are the electric and magnetic fields, ε is relative permittivity, J and ρ are the free charge and current densities. With this type of medium in mind, we can set ρ=0 and J=0.

For mathematical convenience, this allows us to write a harmonic mode as a spatial pattern times a complex exponential:

$$H(r,t) = H(r)e^{-i\omega t} \quad (5)$$

$$E(r,t) = E(r)e^{-i\omega t} \quad (6)$$

put (5) and (6) insert into Maxwell's equation, the wave equation can be expressed by the form of electric field:

$$\frac{1}{\varepsilon(r)}[\nabla \times \nabla \times E(r)] = \left(\frac{w}{c}\right)^2 E(r) \quad (7)$$

In TE case, there is no electric field component in the propagation.In this paper, assuming that Electromagnetic waves propagate along the z axis, as shown in Figure 1.

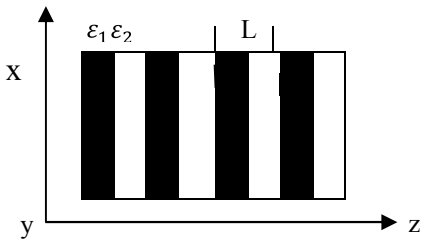

Fig.1.The Multilayer film,1D photonic crystals. Where $\varepsilon_1, \varepsilon_2$ are different dielectric constants, L is spatial period.

In the TE case, E($\vec{r}$)=(0, E, 0), (7) can be derived:

$$-\frac{1}{\varepsilon(r)}\nabla^2 E(\vec{r}) = \left(\frac{w}{c}\right)^2 E(\vec{r}) \quad (8)$$

According to the Bloch State:

$$E(\vec{r}) = \hat{y}E_o(z)e^{-i\vec{K}\cdot\vec{r}} \quad (9)$$

$$\vec{K}\cdot\vec{r} = K_z\hat{z}\cdot\vec{r} = K_z z$$

$$E(\vec{r}) = \hat{y}E_o(z)e^{-iK_z z} \quad (10)$$

Setting Φ replace $E_o(z)$, Φ =$E_o(z)$, and put (10) insert into (2), we can get the scalar function:

$$\frac{1}{\varepsilon(z)}\frac{\partial^2 \emptyset}{\partial z^2} - 2\frac{1}{\varepsilon(z)}iK_z\frac{\partial \emptyset}{\partial z} - \frac{1}{\varepsilon(z)}{K_z}^2\emptyset = \left(\frac{w}{c}\right)^2 \emptyset \quad (11)$$

3. FEM solution

The finite element method is a numerical analysis method that is very important for solving the photonic crystals problem. In FEM, it is first step to get the Weak form:

$$\int V_i[\frac{1}{\varepsilon(z)}\frac{\partial^2 \emptyset}{\partial z^2} - 2\frac{1}{\varepsilon(z)}iK_z\frac{\partial \emptyset}{\partial z} - \frac{1}{\varepsilon(z)}{K_z}^2\emptyset - \left(\frac{w}{c}\right)^2 \emptyset]dz=0 \quad (12)$$

V_i: $test\ function$

division points:

$$\int\{\frac{1}{\varepsilon(z)}\frac{dV_i}{dz}\frac{d\emptyset}{dz} - 2\frac{1}{\varepsilon(z)}iK_z V_i\frac{d\emptyset}{dz} - [\frac{1}{\varepsilon(z)}{K_z}^2\emptyset + \left(\frac{w}{c}\right)^2 \emptyset]\}dz =0 \quad (13)$$

3.1. *Discrete the area and constructs interpolation function*

In this part, we will choose the second order element. This can achieve higher accuracy without increasing the number of nodes. Every node has three nodes, in every element, unknown function can be approximated as second order function:

$$\emptyset^e(x) = a^e + b^e x + c^e x^2 \quad (14)$$

$$\begin{cases} {\emptyset_1}^e = a^e + b^e x_1^e + c^e (x_1^e)^2 \\ {\emptyset_2}^e = a^e + b^e x_2^e + c^e (x_2^e)^2 \\ {\emptyset_3}^e = a^e + b^e x_3^e + c^e (x_3^e)^2 \end{cases}$$

solve the a^e, b^e, c^e, put them insert into (14), we can get:

$$\Longrightarrow \emptyset^e(x) = \sum_{j=1}^{3} N_j^e(x)\emptyset_j^e \quad (15)$$

e: element i, j: local node

e:1,2,3,4…m

i, j: 1,2,3

The interpolation function is given by:

$$N_1^e = \frac{(x - x_2^e)(x - x_3^e)}{(x_1^e - x_2^e)(x_1^e - x_3^e)}$$
$$N_2^e = \frac{(x - x_1^e)(x - x_3^e)}{(x_2^e - x_1^e)(x_2^e - x_3^e)}$$
$$N_3^e = \frac{(x - x_1^e)(x - x_2^e)}{(x_3^e - x_1^e)(x_3^e - x_2^e)}$$

put (15) insert into (13):

$$\sum_{j=1}^{3} \emptyset_j^e \int_{z_1^e}^{z_3^e} \{\frac{1}{\varepsilon(z)} \frac{dV_i^e}{dz} \frac{dN_j^e}{dz} - 2iK_z \frac{1}{\varepsilon(z)} \frac{dN_j^e}{dz} V_i^e - [\frac{1}{\varepsilon(z)} K_z{}^2 + \left(\frac{w}{c}\right)^2] N_j^e V_i^e\} dz = 0 \quad (16)$$

sort out above equation, we can get eigenvalue matrix equation

$$\sum_{j=1}^{3} \emptyset_j^e \left(\frac{w}{c}\right)^2 \int_{z_1^e}^{z_3^e} N_j^e V_i^e dz = \sum_{j=1}^{3} \emptyset_j^e \int_{z_1^e}^{z_3^e} [\frac{1}{\varepsilon(z)} \frac{dV_i^e}{dz} \frac{dN_j^e}{dz} - 2iK_z \frac{1}{\varepsilon(z)} \frac{dN_j^e}{dz} V_i^e \quad (17)$$

4. Simulation by COMSOL

COMSOL is a finite element solution software for solving multiphysics. It can be used to numerically solve the complex physical problems that are mutually coupled by incorporating a variety of physics equations and corresponding solvers. It is very important tool in physics research. Itself is a finite element solver that can be set to solve the equations needed for the weak form, and then solved. However, not all problems can be solved by the built-in weak form module. At this time, it is helpful to know the weak form equation and its finite element algorithm to solve practical physical problems. By setting the material factor, selected Floquet periodic condition, using study to compute the frequency of any wave vector k.

Dielectric materials are alternately arranged, dielectric constant ε_1=13, dielectric constant $\varepsilon_2 = 1$.

When solving eigenvalues, we give the dependent variable as frequency. Within the frequency range of interest, the eigenvector K, and the value of wave vector K is limited to the simplest Brillouin zone. using weak form of COMSOL, we can carry out the band calculation

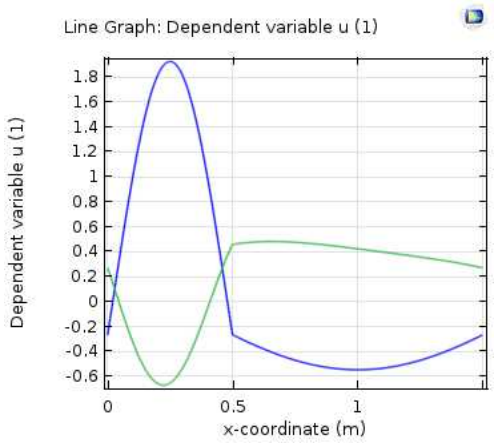

Fig. 2. The band structure of a multilayer film for E-field for mode.

for complex photonic crystals. weak form equations are the usual approaches to general finite element calculations

5. Conclusion

Discussed the basic characteristics of photonic crystals, and introduced weak form and eigenvalue matrix equation of one-dimensional photonic crystals from Maxwell's equations. Using COMSOL Multiphysics to compute band structure of 1D photonic crystals.

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