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TRANSFER MATRIX METHOD FOR ONE-DIMENSIONAL PHOTONIC CRYSTALS

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Dedicated to Prof. K. Srinivasa Rao on his 75^{th} ***Birth Anniversary***

Abstract: Theory of photonic crystals includes an extensive study of electromagnetism and optics in conjunction with solid state physics. Many things have been known for over a century and I want to explore how the calculation on photonic crystal emanates from the theories of electromagnetic waves, basic material optics and some concepts from the field of solid state physics. The electromagnetic wave interacts at the interfaces of the building blocks in the photonic crystals. Maxwells equations can be used to predict the photonic behavior of light propagating in the structure in terms of Bloch functions, band structures and band gaps with the application of transfer matrix method.

Keywords and Phrases: Reflection and Transmission spectra, photonic crystals, transfer matrix method.

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1. Introduction

The band structure of photonic crystals (PCs) can be calculated in mainly three fashions: either by a Plane Wave (PW) method [1], with a Finite Difference Time Domain (FDTD) method [2] or with a Transfer Matrix Method (TMM) [3].

All of these methods calculate with high efficiency and accuracy and are in good agreement with experimental results. These methods are chosen according to the problem tackled. The PW method is a straight-forward method, which assumes a linear combination of plane waves as a solution for Maxwell's equation on a defined lattice. It is very easy to implement and obtain the band structure when the direction is specified. The codes give all the propagating/evanescent energies for that direction. A defect in the infinite photonic crystal will be treated using a supercell. Many results have been obtained with this method [4-5]. The limitation of the

method is linked to the memory storage that depends on the number of plane waves used for the expansion of the field, and this number escalates when the photonic crystal diverges from a periodic structure. The calculation of sophisticated defects is not possible by this method.

The FDTD method is used to calculate photonic band gap (PBG) and optical properties of photonic crystals with dispersive media of 2-D and 3-D photonic structures. It analyses the Maxwell's equations in time domain and the results are in good agreement with experimental measurements as found in [6-7]. Many works on photonic crystals have been reported using this method. To obtain the transmission spectrum of the crystal, an electromagnetic pulse is sent on the material and the output signal is recorded. Electromagnetic modes of a defect can be calculated as the transmission ratio of the material. A fast Fourier transform is applied to both incident and transmitted signals and the transmission spectrum is calculated. The FDTD method allows the simulation of finite or infinite crystals with inner or outer electromagnetic sources. In some cases, this method permits the simulation of an entire experimental setup with a photonic crystal. Results of this experiment are then analyzed. This is the most common technique to simulate a photonic crystal. The limitation of this method is the size of the memory to calculate a large crystal and the lack of an accurate electromagnetic model for some particular objects like thin wires for example. Another advantage of this method is the attractive capability to simulate nonlinear materials [2].

The band structure for dispersive materials in 1-D, 2-D and 3-D photonic structures is calculated by the Transfer Matrix Method (TMM)[3]. The TMM consists on writing the Maxwell's equations in the k-space and rewriting them on a mesh. It performs the operation with layer by layer calculations. Structures with defects can be dealt only by considering a super-cell. The band structures, reflectivity and transmission coefficients can be found by this method easily. Many researchers have used this method [8-9]. It has also proved very useful and accurate when comparisons with experimental structures are undertaken. But it is difficult to deal with the geometry different from cubic geometry by this method. Also, memory storage is the limitation of this method.

In this paper, TMM method is adopted for the calculations of photonic band gap structure and optical properties of one-dimensional photonic crystals.

2. Mathematical Formulation

The wave behaviour in one-dimensional periodic lattice can be described by using the transfer matrix method (TMM). This method is largely based on interfaces of the two layers [3, 10-15].

Maxwell's electromagnetic equations are given as,

$$\overrightarrow{\nabla}.\overrightarrow{D} = \rho \tag{2.1}$$

$$\overrightarrow{\nabla}.\overrightarrow{B} = 0 \tag{2.2}$$

$$\overrightarrow{\nabla} \times \overrightarrow{E} = -\frac{\partial \overrightarrow{B}}{\partial t} \tag{2.3}$$

$$\overrightarrow{\nabla} \times \overrightarrow{H} = \overrightarrow{J} + \frac{\partial \overrightarrow{D}}{\partial t} \tag{2.4}$$

Here, $\overrightarrow{E}$ and $\overrightarrow{H}$ are the electric field vector and magnetic field vector respectively. These two field vectors describe the electromagnetic field. $\overrightarrow{D}$ (Electric displacement) and $\overrightarrow{B}$ (magnetic induction) are introduced to include the effect of the field on matter. The quantities ρ (electric charge density) and $\overrightarrow{J}$ (current density) may be considered as the sources of the fields $\overrightarrow{E}$ and $\overrightarrow{H}$. The electromagnetic field can be determined completely by these equations.

Maxwell's equations consist of 8 scalar equations that relate a total of 12 variables, 3 for each of the 4 vectors $\overrightarrow{E}, \overrightarrow{H}, \overrightarrow{D}$ and $\overrightarrow{B}$. They cannot be solved uniquely unless the relationship between $\overrightarrow{B}$ and $\overrightarrow{H}$ and that between $\overrightarrow{E}$ and $\overrightarrow{D}$ are known to obtain a unique determination of the field vectors. The material equations are,

$$\overrightarrow{D} = \varepsilon \overrightarrow{E} = \varepsilon_0 \overrightarrow{E} + \overrightarrow{P} \tag{2.5}$$

$$\overrightarrow{B} = \mu \overrightarrow{H} = \mu_0 \overrightarrow{H} + \overrightarrow{M} \tag{2.6}$$

where the constitutive parameters ε and μ are tensors of rank 2 and are known as the dielectric tensor (or permittivity tensor) and the permeability tensor, respectively, $\overrightarrow{P}$ and $\overrightarrow{M}$ are electric and magnetic polarization, respectively. The constant ε_0 is called the permittivity of a vacuum and has a value of 8.854×10^{-12} F/m. The constant μ_0 is known as the permeability of a vacuum. For the isotropic medium, both ε and μ tensors reduce to scalars. The quantities ε and μ are assumed to be independent of the field strengths. But for the sufficiently strong field, the dependence of these quantities on $\overrightarrow{E}$ and $\overrightarrow{H}$ must be considered.

For dielectric materials, electric polarization is linear ($\overrightarrow{P} = 0$), independent of and magnetic polarization is non-magnetic ($\overrightarrow{M} = 0$) and absorption of light is also mathematically neglected. The assumptions are applying for dielectric photonic crystal where ε is real valued. But for the metallic photonic crystal, I assume that

electric polarization is linearly dependent on $\overrightarrow{E}$ and non-magnetic and for negative index material structure, both electric polarization and magnetic polarizations are considered as dispersive materials ($\overrightarrow{P} \neq 0$ and $\overrightarrow{M} \neq 0$), linearly dependent on $\overrightarrow{E}$ and $\overrightarrow{H}$.

The electric field E and the magnetic field H can be written as product of a function of the position and a function depending only on the time as,

$$\overrightarrow{E}(r,t) = \overrightarrow{E}(r)e^{-i\omega t + i\overrightarrow{k}.\overrightarrow{r}} \quad \text{and} \quad \overrightarrow{H}(r,t) = \overrightarrow{H}(r)e^{-i\omega t + i\overrightarrow{k}.\overrightarrow{r}}$$

Hence, for the Maxwell's equation,

$$\frac{\partial}{\partial t} \leftrightarrow -i\omega \tag{2.7}$$

and

$$\frac{\partial}{\partial x} \leftrightarrow -ik \tag{2.8}$$

Equation (2.3) and (2.4) implies to,

$$\overrightarrow{\nabla} \times \overrightarrow{H} = -i\omega\varepsilon\overrightarrow{E} \tag{2.9}$$

$$\overrightarrow{\nabla} \times \overrightarrow{E} = +i\omega\mu\overrightarrow{H} \tag{2.10}$$

The electric field component is perpendicular to the plain of propagation for the TE-mode and the magnetic field component is perpendicular to the plain of propagation for the TM-mode. In the consequence of the equations (2.7) and (2.8), equation (2.1) becomes,

$$\overrightarrow{\nabla}.\overrightarrow{D} = (\overrightarrow{\nabla}\varepsilon.\overrightarrow{E} + \varepsilon\overrightarrow{\nabla}.\overrightarrow{E})e^{-i\omega t}$$

or

$$\overrightarrow{\nabla}.\overrightarrow{D} = \varepsilon\overrightarrow{\nabla}.\overrightarrow{E}e^{-i\omega t} \tag{2.11}$$

and equations (2.1) and (2.2) simplifying to,

$$\overrightarrow{\nabla}.\overrightarrow{E} = 0 \tag{2.12}$$

$$\overrightarrow{\nabla}.\overrightarrow{H} = 0 \tag{2.13}$$

and equation only for E can obtained by taking the cross product of equation (2.10) and combining it with equation (2.9),

$$\overrightarrow{\nabla} \times \overrightarrow{\nabla} \times \overrightarrow{E} = \omega^2\mu\varepsilon E \tag{2.14}$$

and using the identity for the vector operation $\overrightarrow{\nabla} \times \overrightarrow{\nabla} \times \overrightarrow{E} = \overrightarrow{\nabla}(\overrightarrow{\nabla}.\overrightarrow{E}) - \overrightarrow{\nabla}^2\overrightarrow{E}$, which lead to the equation for E as,

$$\overrightarrow{\nabla}^2\overrightarrow{E} + \frac{\omega^2}{c^2}\varepsilon_r\mu_r\overrightarrow{E} = 0 \tag{2.15}$$

and

$$\overrightarrow{\nabla}^2\overrightarrow{H} + \frac{\omega^2}{c^2}\varepsilon_r\mu_r\overrightarrow{H} = 0 \tag{2.16}$$

where $c^2 = \dfrac{1}{\varepsilon_0\mu_0}, \varepsilon_r = \dfrac{\varepsilon}{\varepsilon_0}, \mu_r = \dfrac{\mu}{\mu_0}$. This equation (2.15 or 2.16) is the Helmholtz equation and further in this paper, we omit the subscript r in ε_r and μ_r for the sake of simplicity. For non-magnetic materials, $\mu_r = 1$, the equation (2.9) and (2.10) becomes

$$\overrightarrow{\nabla} \times \overrightarrow{H} = -i\omega\varepsilon_r\varepsilon_0\overrightarrow{E} \tag{2.17}$$

$$\overrightarrow{\nabla} \times \overrightarrow{E} = +i\omega\mu_0\overrightarrow{H} \tag{2.18}$$

These equations can be decoupled by dividing the equation (2.17) by ε, and then taking the curl. After using equation (2.18), we can eliminate $\overrightarrow{E}$. The result is an equation entirely in $\overrightarrow{H}$.

$$\overrightarrow{\nabla} \times \frac{1}{\varepsilon_r}\overrightarrow{\nabla} \times \overrightarrow{H} = \omega^2\varepsilon_0\mu_0\overrightarrow{H} \quad \text{or} \quad \overrightarrow{\nabla} \times \frac{1}{\varepsilon_r}\overrightarrow{\nabla} \times \overrightarrow{H} = \frac{\omega^2}{c^2}\overrightarrow{H} \tag{2.19}$$

The equation (2.19) is known as the Master Equation for Photonic Band Gap materials or Photonic Crystals [14, 15].

Now, consider a periodic arrangement of a multilayer film, with refractive indices n_1 and n_2 and each having thicknesses d_1 and d_2 respectively. The solution for the master equation will be the superposition of plane waves traveling to the right and to the left. Say, the right going and left going plane waves have amplitudes A_1 and B_1, for layer with index n_1, respectively and for layer with index n_2, the right going and left going plane waves have amplitudes C_1 and D_1 respectively. Hence, for layer with index n_1 the solution of equation (2.15) is,

$$\overrightarrow{E}(x) = A_1e^{ik_{1x}x} + B_1e^{-ik_{1x}x} \tag{2.20}$$

$$\overrightarrow{E}(x) = C_1e^{ik_{2x}(x-d_1)} + D_1e^{-ik_{2x}(x-d_1)} \tag{2.21}$$

for the layer with index n_2. The parameter k_{1x} and k_{2x} will be called the wave number, and the definition is given by the equation;

$$k_{1x} = \frac{\omega}{c}n_1\cos\theta_1 \quad \text{and} \quad k_{2x} = \frac{\omega}{c}n_2\cos\theta_2 \tag{2.22}$$

where, θ_1 and θ_2 are the ray angles in the two mediums respectively.

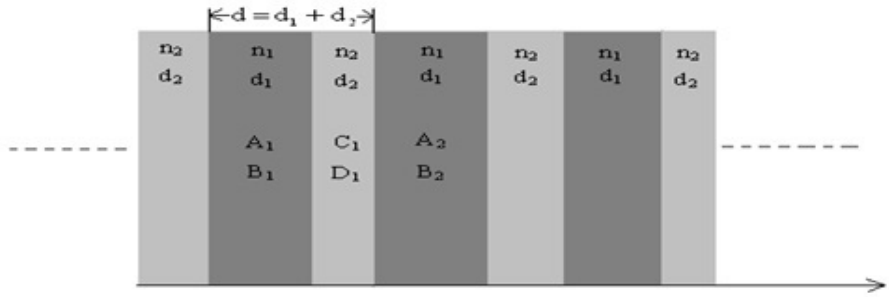

Figure 1 Schematic diagram of bilayer unit cells of refractive indices n_1 and n_2 with thicknesses d_1 and d_2 respectively.

At the interface between layers ($x = d_1$), the solution and its derivative should be continuous. This gives a relation between plane waves amplitude:

$$\begin{pmatrix} C_1 \\ D_1 \end{pmatrix} = M_{12} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \tag{2.23}$$

with

$$M_{12} = \begin{pmatrix} \frac{1}{2}\left(1 + \frac{k_{1x}}{k_{2x}}\right) e^{ik_{1x}d_1} & \frac{1}{2}\left(1 - \frac{k_{1x}}{k_{2x}}\right) e^{-ik_{1x}d_1} \\ \frac{1}{2}\left(1 - \frac{k_{1x}}{k_{2x}}\right) e^{ik_{1x}d_1} & \frac{1}{2}\left(1 + \frac{k_{1x}}{k_{2x}}\right) e^{-ik_{1x}d_1} \end{pmatrix} \tag{2.24}$$

and, also at $x = d$, the continuity of the plane waves at the interface between layers with indices n_2 and n_1 and its derivative gives

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = M_{21} \begin{pmatrix} C_1 \\ D_1 \end{pmatrix} \tag{2.25}$$

where the matrix M_{21} is the same as (2.24) but with interchanging the indices. From the two matrix equations (2.23) and (2.25), we have,

$$\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = M_{21}M_{12} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} A_2 \\ B_2 \end{pmatrix} = M_{i,j} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \tag{2.26}$$

where $M_{i,j} = M_{21}M_{12}$.
The matrix element of the matrix $M_{i,j}$ is given by,

$$M_{1,1} = e^{ik_{1x}d_1} \left[\cos(k_{2x}d_2) + \frac{1}{2}i\left(\gamma + \frac{1}{\gamma}\right)\sin(k_{2x}d_2)\right]$$

$$M_{1,2} = e^{-ik_{1x}d_1}\left[\cos(k_{2x}d_2) + \frac{1}{2}i\left(\frac{1}{\gamma} - \gamma\right)\sin(k_{2x}d_2)\right] \quad M_{2,1} = \overline{M_{1,2}}, \quad M_{2,2} = \overline{M_{1,1}},$$

where $k_{jx} = \dfrac{\omega}{c} n_j \cos\theta_j$ and $\gamma = \dfrac{k_{1x}}{k_{2x}}$ for TE mode, and $\gamma = \dfrac{k_{1x} \times n_2^2}{k_{2x} \times n_1^2}$ for TM mode.

The matrix $M_{i,j}$ is called as the transfer matrix of one unit of the periodic lattice. The matrix $M_{i,j}$ depends on the frequency ω, and it is unimodular (it is a square matrix with determinant equal to unity). Hence, for each ω, the matrix $M_{i,j}$ defines a unique mapping for amplitudes of the plane waves in layer n_1 into the amplitude of the next layer with index n_2.

Similarly, the wave vector for negative index materials is slightly different from the dielectric materials. The wave vector is given as $k_{jx} = \dfrac{\omega}{c} n_j \cos\theta_j$, where refractive index, $n_j(x) = \sqrt{\varepsilon_j(x)}\sqrt{\mu_j(x)}$, and impedance, $Z_{jx} = \dfrac{\sqrt{\mu_j(x)}}{\sqrt{\varepsilon_j(x)}} / \cos\theta_j$. Here j=1, 2 for the thicknesses d_1 and d_2 respectively. Then the matrix element of $M_{i,j}$ is given by

$$M_{1,1} = e^{ik_{1x}d_1}\left[\cos(k_{2x}d_2) + \frac{1}{2}i\left(\frac{Z_{2x}}{Z_{1x}} + \frac{Z_{1x}}{Z_{2x}}\right)\sin(k_{2x}d_2)\right]$$

$$M_{1,2} = e^{-ik_{1x}d_1}\left[\cos(k_{2x}d_2) + \frac{1}{2}i\left(\frac{Z_{1x}}{Z_{2x}} - \frac{Z_{2x}}{Z_{1x}}\right)\sin(k_{2x}d_2)\right]$$

$M_{2,1} = \overline{M}_{1,2}, M_{2,2} = \overline{M}_{1,1}$

where $k_{jx} = \dfrac{\omega}{c}\sqrt{\varepsilon_j(x)}\sqrt{\mu_j(x)}\cos\theta_j$ and $Z_{jx} = \dfrac{\sqrt{\mu_j(x)}}{\sqrt{\varepsilon_j(x)}} / \cos\theta_j$ with $j = 1, 2$.

For an infinite lattice extending on the whole x-axis, the solution of the Helmholtz equation (2.19) can be written in terms of Bloch waves [11-14] as,

$$\overrightarrow{E}(x, K) = U_K(x)e^{iK(\omega)x} \tag{2.27}$$

where, $U_K(x)$ is a complex valued periodic function with the period of the lattices $(d = d_1 + d_2)$, $U_K(x) = U_K(x + d)$. The parameter $K(\omega)$ is called the Bloch wave number or Dispersion Relation, where for a periodic lattice with indices n_1 and n_2, there is an explicit expression for $K(\omega)$ as follows;

$$K(\omega) = \frac{1}{d}\cos^{-1}\left(\frac{1}{2}Tr[M_{i,j}]\right) \tag{2.28}$$

with $M_{i,j}$ given as above.

After simplifying (2.28), one can obtain as,

$$K(\omega) = \frac{1}{d}\cos^{-1}\left[\cos(k_{1x}d_1) \times \cos(k_{2x}d_2) - \frac{1}{2}\left(\gamma + \frac{1}{\gamma}\right) \times \sin(k_{1x}d_1) \times \sin(k_{2x}d_2)\right] \tag{2.29}$$

where $\gamma = \dfrac{k_{1x}}{k_{2x}}$ for TE mode, and $\gamma = \dfrac{k_{1x} \times n_2^2}{k_{2x} \times n_1^2}$ for TM mode and $k_{jx} = \dfrac{\omega}{c} n_j \cos\theta_j$ with $j = 1, 2$. For negative index materials (NIM), the dispersion relation $K(\omega)$ is given by,

$$K(\omega) = \frac{1}{d}\cos^{-1}\left[\cos(k_{1x}d_1)\cos(k_{2x}d_2) - \frac{1}{2}\left(\frac{Z_{1x}}{Z_{2x}} + \frac{Z_{2x}}{Z_{1x}}\right)\sin(k_{1x}d_1)\sin(k_{2x}d_2)\right]$$

The equation (2.29) is known as dispersion relation of the periodic lattice with refractive indices n_1 and n_2 and thicknesses d_1 and d_2 respectively.

The behavior of Bloch wave is characterized by this Bloch wave number or dispersion relation. Generally, the behaviour of Bloch wave can be divided into three cases:

- 1. For real $K(\omega)$, which lies in the first Brilluion zone $[0, \pi/d]$, $E(x, K)$ is a periodic and travelling wave function. In this case, it is said that ω is outside the band gap.
- 2. For imaginary $K(\omega)$, defined by, $K(\omega) = \pi/d + ip(\omega)$, $E(x, K)$ is a standing wave function, a product of two periodic functions with an exponential increasing and a decreasing function, depending on the sign of $\rho(\omega)$. In this case, ω is inside the band gap.
- 3. For $K(\omega) = \pi/d, E(x, K)$ is a periodic function of period 2^{nd} with special properties that it is a d-shift skew symmetric, $E(x + d, K) = -E(x, K)$.

3. Applications

This method applies for the one-dimensional photonic crystal structure with different materials constituents. The reflection and transmission coefficients of the electromagnetic wave at the dielectric interfaces between the layers can be calculated by using this.

In the area of optics and photonics, one often deals with situation in which surface charge density and the surface current density both vanish. It follows that, in such case, the tangential components of $\overrightarrow{E}$ and $\overrightarrow{H}$ and the normal component of $\overrightarrow{D}$ and $\overrightarrow{H}$ are continuous across the interface separating two media. These boundary conditions are important in solving many wave propagation problems in optics such as wave propagation in layered media and as guided wave optics.

References

[1] J. B. Pendry, Calculating photonic band structure, J. Phys. Cond. Mat. 8, 10851108, 1996.

[2] A. Taflove, Computational electrodynamics, The Finite-Difference Time - Domain Method, (Artech House, Boston, London, 1995).

[3] J. B. Pendry and A. MacKinnon, Calculation of photon dispersion relations, Phys. Rev. Lett. 69, 27722775, 1992.

[4] Special issues on photonic crystals, J. Mod. Opt., 41, 1994; J. Opt. Soc. Am. B, 10, 1993.

[5] Z. Y. Li, L.-L. Lin, and Z.-Q. Zhang, Spontaneous Emission from Photonic Crystals: Full Vectorial Calculations, Phys. Rev. Lett. 84, 43414344, 2000.

[6] S. Fan, P. R. Villeneuve, J. D. Joannopoulos, and E. F. Schubert, High Extraction Efficiency of Spontaneous Emission from Slabs of Photonic Crystals, Phys. Rev. Lett. 78, 32943297, 1997.

[7] C. T. Chan, Q. L. Yu, and K. M. Ho, Order-N spectral method for electromagnetic waves, Phys. Rev. B. 51, 16635-16642, 1995.

[8] J. B. Pendry, and L. Martin-Moreno, Energy loss by charged particles in complex media, Phys. Rev. B. 50, 50625073, 1994.

[9] F. Gadot, A. Chelnokov, A. De Lustrac, P. Crozat, and J.M. Lourtioz, D. Cassagne and C. Jouanin, Experimental demonstration of complete photonic band gap in graphite structure, Appl. Phys. Lett. 71, 17801782, 1997.

[10] K. Sakoda, Optical Properties of Photonic Crystal, (Springer-Verlag Berlin Heidelberg New York, 2001).

[11] P. Yeh, Optics in Layered Media, (John Willey and Sons, New York, 1988).

[12] A. Sopaheluwakan, Thesis on Defect States and Defect modes in 1D photonic crystals, (Univ. of Twente, Nitherland, December, 2003); A. Rung, Thesis on Numerical studies of energy gaps in photonic crystals, (Uppsala Univ., 2005).

[13] M. Born and E. Wolf, Principles of Optics, (Pergamon Press, Oxford, 1964, 2nd Edition).

[14] S. G. Johnson, Photonic Crystal: From Theory to Practice, (Chapter 1, 2001).

[15] K. Yasumoto, Electromagnetic theory and applications for photonic crystals, (Tailor & Francis Press, 2005).