Dispersion relation of 1-D photonic crystal paper

by Mark Finne

Dispersion Relation of 1-D Photonic Crystal

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Abstract— **Photonic crystal is a periodic dielectric material that affect the propagation of light. That produces a photonic bandgap. Photonic bandgap is a structure where a range of frequency cannot propagate through the structure. The charateristics can bee seen from the dispersion relation of the light propagate in the structure. In this paper, we use two different methods to simulate the dispersion relation; firstly we use a Plane wave method and secondly we use a transter matrix method. Both methods use a different approach to describe the periodic dielectric structures. In the simulation we try to compare both results and show them in graph of wavevector k vs frequency, with unit cell consisting GaAS as material of the dielectric and air as the gap. The width of GaAS is 0.8 micron and width of the air gap is 0.2 micron. We also rescaling both normalized frequency to be the similar. In the process we examine the normalised frequency values using both methods as well as the difference results appears on the calculations.**

Keywords— photonic crystal, plane wave method, transfer matrix method, GaAs, bandgap

I. INTRODUCTION

The electromagnetic waves that propagate through a medium other than vacuum will have their characteristics changed. Frequency, amplitude, wavelength, dispersion, will all changed depends on the medium where it propagate. Photonic crystal is the same, a periodic dielectric structure that affect the propagation of light so that on a range of specific frequency the light wont propagate through the medium.

The periodic dielectric function on photonic crystal have a same structure as crystalline atomic lattice that used in a semiconductors. On solid-state physics the crystal lattice affects the electrons that propagate through it, while at the photonic crystal it affects foton. These two same condition allow us to obtain the characteristics for dispersion relation of photonic crystal as same as on solid-state physics.

We will get the bandgap result in form of band diagram, that will represent the photonic bandgap on wavevector k vs normalized frequency graph. We use normalized frequency so that the solution wont depends on specific frequency range but will work on every frequency range.

In this paper we will only use two different simulation methods, plane wave method and transfer matrix method. Then comparing two different methods to simulate the dispersion relation. We obtain that the simulation results have a slight difference. For the comparison, we refer the transfer matrix method into plane wave method, which have more accurate results. Both of these methods use different approach to calculate the dielectric function for finding dispersion relation, thus resulting on different simulation results.

II. THEORY

A. Maxwell Equation in Dielectric Medium

On photonic crystal, the light wave propagates through a dielectric medium. The wave equation can be solved using macroscopic maxwell equation. Because the wave propagates through a periodicity that have a vector position, the structure does not vary with time and no free charges or currents. In this medium, we also assume that light propagates but there are no sources of light. So, in the maxwell equation we add additional parameter $\rho = 0$ and $J = 0$ and subtitute it into the equation.

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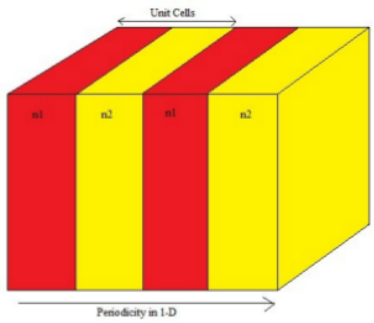

Fig. 1. The structure of one dimension photonic crystal

We then apply a harmonic modes to reduce the time dependant on calculation[1].

$$H(r,t) = H(r)e^{-i\omega t} \quad (1)$$

$$E(r,t) = E(r)e^{-i\omega t} \quad (2)$$

Subtitute the above equation into maxwell and we can obtain the master equation.

$$\nabla \times \left(\frac{1}{\varepsilon_{(r)}} \nabla \times H(r) \right) = \frac{\omega^2}{c^2} H(r) \quad (3)$$

B. Bloch Theorem

On solid-state physics, Bloch theorem was used to obtain the solution on semiconductor atomic crystal lattice. Bloch theorem says that the eigen-function inside an infinite periodic medium can be represented in the form of a plane wave multiplied by a periodic function with periodicity of the lattice[2].

$$H(r) = h(r)e^{ikr} \quad (4)$$

We can also obtain the solution for (3) using Bloch wave. Thus, the master equation became,

$$\frac{\partial^2}{\partial r^2} \frac{1}{\varepsilon(r)} h(r)e^{ikr} = \frac{\omega^2}{c^2} h(r)e^{ikr} \quad (5)$$

C. Plane Wave Method

To obtain the dispersion relation, plane wave method is using the fourier expansion to transfrom and calculate the dielectric function. The dielectric function is expressed with,

$$h(r) = h(r + R_i) \quad (5)$$

With R_i form the crystal lattice vector $R_i = l_1a_1 + l_2a_2 + l_3a_3$. And l_1, l_2, l_3 were integers, a_1, a_2, a_3 were primitive lattice vector. Thus, the periodic dielectric primitive lattice vector on dielectric function is transformed into reciprocal lattice vector using the fourier transform.

$$\varepsilon(r) = \sum_G g(G)e^{iGr} \quad (6)$$

$$H(r) = \sum_G h_{k,n}(G)e^{i(k+G)r} \quad (7)$$

G is reciprocal lattice vector $G = h_1b_1 + h_2b_2 + h_3b_3$ where h_1, h_2, h_3 were integers, b_1, b_2, b_3 were primitive lattice vector. We subtitute (8) and (7) to (5). Then obtain,

$$\sum_{G^\phi} g^{-1}\left(G - G^\phi\right)\left(\left(k + G^\phi\right)\left(k + G\right)\right) h_{k,n}\left(G^\phi\right) = \frac{\omega^2}{c^2} h_{k,n}(G) \quad (8)$$

Further, we simplify (9) and transform it into matrix form. Hence,

$$\begin{bmatrix} m_{11} & m_{12} & \cdots & m_{1,2N} \\ m_{21} & m_{22} & \cdots & m_{2,2N} \\ \vdots & & \ddots & \vdots \\ m_{2N,1} & m_{2N,2} & \cdots & m_{2N,2N} \end{bmatrix} \begin{bmatrix} h_1(G_1) \\ \vdots \\ h_N(G_N) \\ h_2(G_1) \\ \vdots \\ h_N(G_N) \end{bmatrix} = \frac{\omega^2}{c^2} \begin{bmatrix} h_1(G_1) \\ \vdots \\ h_N(G_N) \\ h_2(G_1) \\ \vdots \\ h_N(G_N) \end{bmatrix} \quad (9)$$

We use (10) to find the dispersion relation with plane wave method. To transform above equation into code there is a general step, which is[3]:

- Given a K point to solve the associating frequency
- Find the reciprocal lattice and choose the G vector set
- Find each of the fourier transform coefficient $\varepsilon^{-1}(G - G')$
- Find the $k + G$ and the two unit vector sets
- Calculate the eigen value

D. Transfer Matrix Method

Transfer matrix is another method used to analyze the propagation of electromagnetic waves through a periodic medium. According to Maxwell, light that propagate in layered or periodic dielectric medium have different characteristics on each layer. With transfer matrix method, the field at the end of the layer can be derived from a simple matrix operation.

The layered dielectric medium can be seen as a matrix system that obtained from the sum of individual layer matrices. From the sum results we can obtain the reflectance and transmittance coefficient for the layered dielectric medium and transform it into dispersion relation. The method is then applied to electromagnetic waves with a specific frequency propagating through the layer at normal incidence angle.

To understand the transfer matrix method, we begin with the S-Matrix formalism,

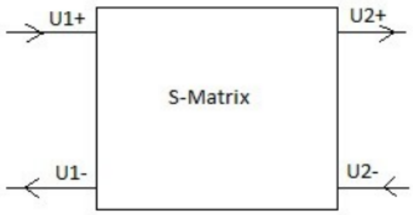

Fig. 2. S-matrix formalism for dielectric layer

From the picture above, we know that in the layered structure there is two different electromagnetic field that occured. The propagating/forward field and the reflected/backward field. The reflected field was a result from reflectance of the propagating field in the boundary between dielectric layer with different refractive index.

Thus, according to S-Matrix formalism, the field characteristics on the dielectric layer is,

$$U_2^+ = t_{12}U_1^+ + r_{21}U_2^+ \quad (10)$$

$$U_1^- = r_{12}U_1^+ + t_{21}U_2^+ \quad (11)$$

Where t_{12} and t_{21} is a transmittance field, while r_{12} and r_{21} is a reflectance field. The matrix form of the equation is,

$$\begin{bmatrix} U_2^+ \\ U_1^- \end{bmatrix} = \begin{bmatrix} t_{12} & r_{21} \\ r_{12} & t_{21} \end{bmatrix} \begin{bmatrix} U_2^+ \\ U_1^- \end{bmatrix} \quad (12)$$

We can further define the S-Matrix and its M-Matrix part using the transform relation between them. If there is no loss and the transmission coefficient t and reflection coefficient r in forward and backward are identical, we get

$$S = \begin{bmatrix} t & r \\ r & t \end{bmatrix} \quad (13)$$

$$M = \begin{bmatrix} 1/t^* & r/t \\ r^*/t^* & 1/t \end{bmatrix} \quad (14)$$

Where: $t/r = -(t/r)^*$, $|t|^2 + |r|^2 = 1$

We use the same S-Matrix above to reconstruct the dielectric function of photonic crystal into matrix form. To obtain these matrices, we use Bloch theorem to explain how the electromagnetic field in each layer was different.

According to Bloch theorem, the electromagnetic field in each layer is a function plane wave times the periodicity. So we get the matrix,

$$\begin{bmatrix} U_{m+1}^+ \\ U_{m+1}^- \end{bmatrix} = M_0 \begin{bmatrix} U_m^+ \\ U_m^- \end{bmatrix} = e^{-ikr} \begin{bmatrix} U_m^+ \\ U_m^- \end{bmatrix} \quad (15)$$

Equation (17) can be reduced to,

$$\left| M_0 - e^{-ikr} \cdot I \right| = 0 \quad (16)$$

Where I is the identity matrix and M_0 is the matrix M. As stated before, the end product of transfer matrix is the dispersion relation. We then find the determinant from (18) to obtain the propagation characteristics. We obtain half of the dispersion relation,

$$e^{-ikr} = \left(\frac{1}{t^*} + \frac{1}{t} \right) \pm \sqrt{ \left(\frac{1}{t^*} + \frac{1}{t} \right)^2 - 4 \frac{1 - r^* r}{t^* t} } \quad (17)$$

$$cos(kr) = Re\left\{ \frac{1}{t} \right\} \quad (18)$$

We need to find the value of $1/t$ to complete the dispersion relation. In the figure below, the light first propagate through medium 1, then traveling across the boundary between medium 1 and 2, then propagate in medium 2, and back from medium 2 to medium 1 again.

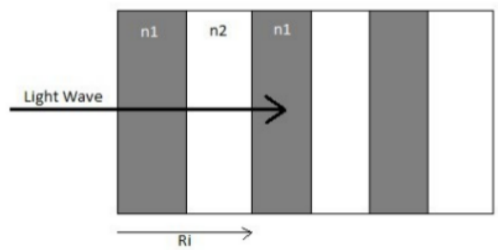

Fig. 3. Light propagation through layered structure

Light that propagate through the medium will change depends on the periodicity. So in matrix form, the dispersion relation for the structure obtained with multiplying all of the propagation matrices. That is,

$$M = M_{21} M_2 M_{12} M_1 \quad (19)$$

$$M_{12} = \frac{1}{2n_2} \begin{bmatrix} n_2 + n_1 & n_2 - n_1 \\ n_2 - n_1 & n_2 + n_1 \end{bmatrix} \quad (20)$$

$$M_{21} = \frac{1}{2n_1} \begin{bmatrix} n_1 + n_2 & n_1 - n_2 \\ n_1 - n_2 & n_1 + n_2 \end{bmatrix} \quad (21)$$

Where M_1 is the propagation matrix for medium 1, M_2 is the propagation matrix for medium 2, and M_{12}, M_{21} is the propagation matrix between two layer.

Using (21)(22)(23), we get the value of $1/t$. We then subtitute it with wavevector k and the periodicity d for both dielectric medium. Then our complete dispersion relation using transfer matrix method is,

$$cos(k.r) = cos(k_1 d_1 + k_2 d_2) - \frac{(k_1 - k_2)^2}{2k_1 k_2} sin(k_1 d_1) sin(k_1 d_2) \quad (22)$$

This equation is the equation of dispersion relation that obtained from multiplication of the matrices in the structure using transfer matrix method. Here the wavevector is,

$$k_n = \frac{\omega}{c_n} \tag{23}$$

And n is the medium number. We subtitute the value of k_1 and k_2 in (22) with (23), so we get the relations between k and ω,

$$\cos(k.d) = \cos\left(\frac{\omega d_1}{c_1} + \frac{\omega d_2}{c_2}\right) - \frac{(\omega/c_1 - \omega/c_2)^2}{2(\omega/c_1)(\omega/c_2)}\sin\left(\frac{\omega d_1}{c_1}\right)\sin\left(\frac{\omega d_2}{c_2}\right) \tag{24}$$

Equation (24) can further be simplified using a normalized frequency to eliminate the differences in value of light speed in the medium 1 and 2,

$$\omega_{norm} = \frac{\omega}{c_{(1,2)}} = \frac{\omega n_{(1,2)}}{c_0} \tag{25}$$

Where $n_{(1,2)}$ is the refractive index of medium 1 and 2, respectively. Subtitute the value of $\omega/c_{(1,2)}$ in equation (24) with (25). Hence, after simplification it become,

$$\cos(k.d) = \cos\left(\frac{\omega}{c_0}(n_1 d_1 + n_2 d_2)\right) - \frac{(n_1 - n_2)^2}{2 n_1 n_2}\sin\left(\frac{\omega n_1}{c_1} d_1\right)\sin\left(\frac{\omega n_2}{c_2} d_2\right) \tag{26}$$

Equation (26) is the final equation of dispersion relation with transfer matrix method.

III. Simulation Result and Discussion

A. *Dispersion Relation in Uniform and Nonuniform Medium*

For the simulation, the material used is GaAs with refractive index = 3.39866 and air gap. The width of the unit cell is 1 micron. Width of the GaAs = 0.8 micron, air gap = 0.2 micron.

We show that the bandgap occured when the structure is nonuniform and compare it with uniform structure. In figure (2) we use transfer matrix method to calculate results. The red lines are dispersion relation when the structure is uniform, and the blue lines are dispersion relation when the structure is nonuniform.

The size of the bandgap increased when the difference between refractive index value of n1 and n2 is increased.

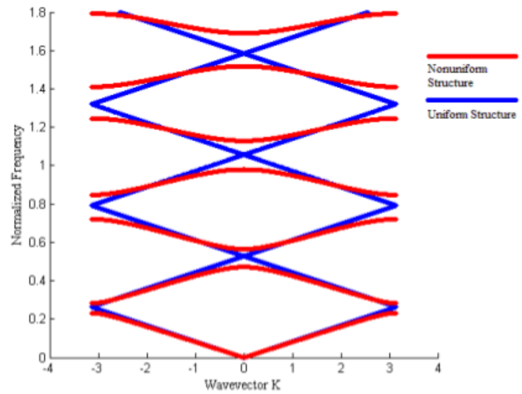

Fig. 4. Dispersion relation for uniform and nonuniform medium

B. *Comparison of Dispersion Relation with Plane Wave Method and Transfer Matrix Method*

With same simulation parameters, we then compute the dispersion relation using plane wave method and the transfer matrix method. To compare the above results, we need to equalize the value of normalized frequency.

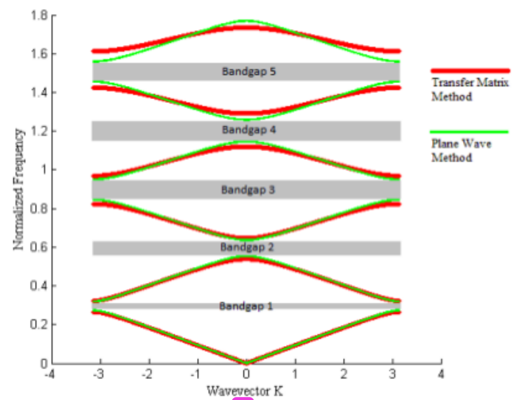

Fig. 5. Dispersion relation with plane wave method and transfer matrix method

From fig. 5, we obtain the value of normalized frequency that occured in all photonic bandgap. We calculate every value of beginning normalized frequency in bandgap 1 to 5. The result then displayed below.

TABLE I. Beginning Normalized Frequency for Each Bandgap

Bandgap Number	***Beginning Normalized Frequency***	
	Transfer Matrix Method	**Plane Wave Method**
1	0.2654	0.2726

Bandgap Number	*Beginning Normalized Frequency*	
	Transfer Matrix Method	**Plane Wave Method**
2	0.5391	0.5527
3	0.8243	0.8438
4	1.12	1.145
5	1.424	1.454

The error result between the two methods is increased as the number of bandgap increased. The number of bandgap means that in the normalised frequency, the bandgap that occur above normalized value 1 will have an increasing error. If we further compute the solution above normalized frequency 2, the error value will be huge. This is because the methods just compute the solution in normalised frequency. Thus, the bandgap solution is credible only between 0 to 1 normalized frequency. In this range, the result between two methods is almost the same, with just 0.0072 in length of error differences.

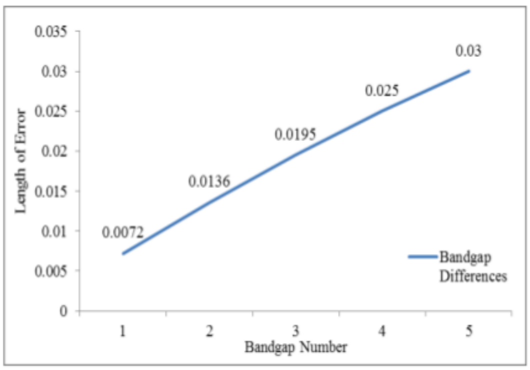

Fig. 6. The error results in two different methods

IV. Conclusion

From the simulation results and discussion, it can be concluded that the plane wave and transfer matrix method can be used to compute the dispersion relation in photonic crystal. Simulating the dispersion relation will show the photonic bandgap that occur when the dielectric structure is nonuniform and periodic. It is different according to the periodicity of the structure. For the uniform dielectric structure, we can see that there is no photonic bandgap phenomena, all frequencies of light will propagate through the structure. In the comparison between two methods, the error of normalized frequency that occured in the beginning of photonic bandgaps increased when the photonic bandgap range is higher. The value of error increased because in the bandgap computation we only compute the normalised frequency, which have credible value only in range 0 to 1. The bandgap that occur above the credible value will have increased into huge number of length of error.

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