

To Calculate Band Gap in Photonic Crystal in 2D using Finite Difference Time Domain

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Abstract

The band gap for 2D PhC with different modes and different lattice structures using FDTD have been computed. Three PBGs between the first and the second bands, between the second and the third bands and between the fourth and fifth bands are concluded. Simulation results shows that for band structure computation is of 1D PhC using FDTD, it is found that some additional solutions appear, which are drop out from the general set. They are called spurious solutions. Such solutions appear due to space discretization and because of finite solution time interval and these could be eliminated manually.

Keywords: Eigen vector, Finite-difference time-domain, Helmholtz equation, Photonic Band Gap, Photonic Crystal

I. INTRODUCTION

The electronic energy band structure in semiconductors is well understood. An electron's momentum is modulated with the help of lattice of ions, yielding a gap of forbidden electronic energies without any influence of the electron's momentum. It is proposed that a periodic electromagnetic modulation created by a lattice composed of dielectric atoms could acquiesce a gap of forbidden photon (energies) irrespective of a photon's momentum.[1] Such a dielectric "crystal" have been dubbed a photonic band gap (PBG) structure, and its properties and applications are now being investigated. To create a photonic band gap, a numerous stringent criteria must be satisfied. The center frequency of the band gap is inversely associated to the lattice constant of the crystal. Additionally the analogy with solid state physics, a Brillouin zone (BZ) could be used to describe photonic propagation in electromagnetic reciprocal space. To create an omnidirectional photonic band gap, the model structure would have a spherical BZ and the face-centered cubic (fcc) BZ have the most spherical BZ, but even then its asphericity narrows the design space for PBG structures. The minimum dielectric contrast between "atoms" and interstitial space is essential for a PBG to open up in a given structure. As the width of the PBG increases as the contrast above that minimum increases. The "atom" size and the "atom" type and the "atom" shape also play significant roles in determining whether a gap will exist and how broad it would be [1]. In our work the (FDTD) is used for photonic crystal modeling. Generally, it involves intensive computations to implement is complicated and involves a huge number of statements in C or Fortran, similar to those given in the well-known MPB package[1]. In this paper, we present a simple and fast implementation method using MATLAB. Which AB provides many functions required for numerical analysis and graphics, also operations are optimized for matrix, so it is ideal for scientific analysis with little programming effort, especially those calculations involving intensive matrix operations.

II. THEORY OF FDTD

The FDTD is illustrated in several papers [4, 5]. Here, we summarize the theory very briefly. Maxwell's equations in a transparent, time-invariant, source free and non-permeable ($\mu = \mu_0$) space can be rewritten as Helmholtz's equation:

$$\nabla \times \frac{1}{\epsilon(r)} \nabla \times \vec{H}(r) = \frac{\omega^2}{c^2} \vec{H}(r) \quad (1)$$

With the transverse condition being:

$$\nabla \cdot \vec{H}(r) = 0 \quad (2)$$

In a photonic crystal, we assume infinite periodic medium, and using Bloch's theorem, a mode in a periodic structure can be expanded as a sum of infinite number of plane waves:

$$\vec{H}(r) = \sum_{\vec{G}_i, \lambda} h(\vec{G}_i, \lambda) \vec{e}_\lambda e^{i(\vec{k} + \vec{G}_i) \cdot \vec{r}} \quad (3)$$

is the wave vector in vacuum, \vec{G} is the reciprocal lattice vector. Using the Fourier transform, the dielectric function can be written as:

$$\varepsilon(r) = \sum_{\vec{G}_i} \varepsilon(\vec{G}_i) e^{i\vec{G}_i \cdot \vec{r}} \quad (4)$$

where G is any reciprocal lattice vector. Using equations (3) and (4), and applying the transverse condition, Helmholtz's equation can be transformed to an algebraic form [6]:

$$\sum_{G'} |k + G| |k + G'| \varepsilon^{-1}(G - G') \begin{bmatrix} \hat{e}_2 \hat{e}_2' & -\hat{e}_2 \hat{e}_1' \\ -\hat{e}_1 \hat{e}_2' & \hat{e}_1 \hat{e}_1' \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} = \frac{w^2}{c^2} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}. \quad (5)$$

This is a standard eigenvalue problem. If N plane waves are used, this will be $2N$ linear equations. Simplifications exist for 2D and 1D PBGs. For in-plane propagation in a 2D photonic crystal, equation (5) is decomposed into TE and TM modes:

$$\text{TM: } \sum_{G'} |\vec{k} + \vec{G}| |\vec{k} + \vec{G}'| \varepsilon^{-1}(\vec{G} - \vec{G}') h_1(\vec{G}') = \frac{\omega^2}{c^2} h_1(\vec{G}) \quad (6)$$

$$\text{TE: } \sum_{G'} (\vec{k} + \vec{G}) \cdot (\vec{k} + \vec{G}') \varepsilon^{-1}(\vec{G} - \vec{G}') h_2(\vec{G}') = \frac{\omega^2}{c^2} h_2(\vec{G}). \quad (7)$$

Each of them is a group of N linear equations if N plane waves are used, and the problem complexity is reduced half. For 1D normal incidence, TE and TM behave the same, so only one equation is needed. Off-plane 1D and 2D problems can be treated as 2D and 3D problems, respectively.

For each specific k , the frequency w for the eigenmode is the eigenvalue of the above equations. Using N plane waves, we will get $2N$ (for TE & TM is N) discrete frequencies for each k -point. These frequencies are sorted ascendantly and labeled as 1 to $2N$. One band is formed by all the eigen-frequencies with the same order for all k -vectors in First Irreducible Brillouin zone (IBZ). We can calculate only the eigen-frequencies for those k -vectors along the edge of the IBZ, since those frequencies for the k -vectors falling inside the IBZ will fall inside the band.

The eigenvectors can be used to form the \vec{H} and \vec{D} field according to equation (3) and the relation:

$$\vec{D}(r) = \frac{-i}{k} \nabla \times \vec{H}(r) \quad (8)$$

where k is the magnitude of the vacuum wave vector.

III. IMPLEMENTATION

We illustrate the implementation in the case of 2D photonic crystals. The program for the computation of 2D PhC band structure is much more complex than the one for 1D PhC. There are more peculiarities such as definition of permittivity distribution inside unit cell. Therefore the program has various blocks and are discussed in detail. In first block is for the variables initialization. The parameters of the structure and the computation accuracy are defined. To PhC is define the lattice constant and the elements radius. The number of plane waves and the number of points in k -path determine the accuracy of the computation. In the second block, the permittivity distribution inside the unit cell is defined. The PhC with square lattice and circular elements so the definition is carried out by one loop. After the computation of second block is computed, we have three 2D arrays containing x -coordinate of each point, y -coordinate of each point and the permittivity values within these points. The third block sets up the k -path and the set of reciprocal lattice vectors. we considered the PhC with square lattice with side a , the Brillouin dimensions are equal to $2\pi/a$ in both k_x and k_y directions. The x and y components of the set is written to the corresponding array. In the fourth block, the Fourier expansion coefficients are computed for each value of G and G within the above selected set. The result is stored in 2D array. As in case of 1D PhC, the Fourier expansion coefficients are computed before the matrix differential operator formation since it does not depends on the wave vector. In the sixth block, the eigen-values of matrix differential operator are found at each value of wave vector within the k -path and stored to the array. The stored eigen-values are then plotted as function of the wave vectors taken from the k -path array. Plots for several lower eigen-values only since the PBGs are usually observed at low frequencies in strictly periodic 2D PhCs. The axes are then signed. The relative frequency $\omega a / 2\pi c$ lies on the vertical axis. Though the values on the horizontal axis differ from those of 1D band structure. Here, we set the wave vector values from the Brillouin zone symmetry points by using FDTD plots for the 2D PhC band structure is drawn.

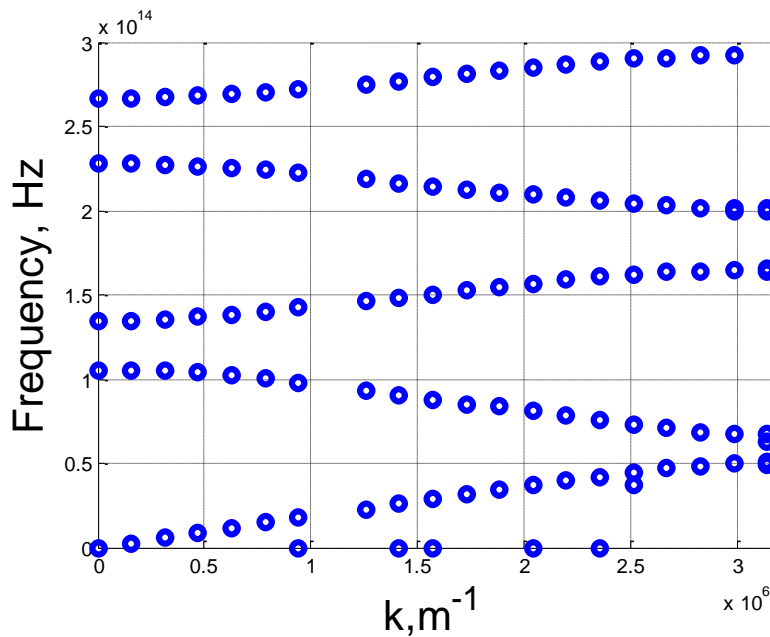


Fig. Band structure of 1D PhC obtained by FDTD technique

IV. CONCLUSION

The band gap for 2D PhC with different modes and different lattice structures using FDTD have been computed. It is concluded that there are three PBGs between the first and the second bands, between the second and the third bands and between the fourth and fifth bands. The values on the horizontal axis differ from those of 1D band structure.

It is observed from the simulation results for band structure computation is of 1D PhC using FDTD, it is found that some additional solutions appear, which are drop out from the general set. They are called spurious solutions. Such solutions appear due to space discretization and because of finite solution time interval. Such solutions may easily be eliminated even manually.

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