Calculation of Band Structures Through the Finite-Difference Time-Domain Method

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This paper presents the band structure computation of photonic crystals using FDTD. The analysis of 2D and 3D non disperssive lattices was carried out and compared to the well known PWE solutions. Results show a good agreement between both methods.

***Index Terms*—Photonic crystals, bandgap, FDTD, PWEM.**

I. Introduction

A photonic crystal is a periodic lattice of dielectric materials with cell dimensionscorresponding to the wavelength of visible light. The periodicity and symmetry of thepatterned material manifests itself as a periodic change of its dielectric constant. Forvisible light the required dimensions are around 500 nm, about three orders ofmagnitude higher than the atomic spacing of an ordinary crystal. Thus, the behavior oflight in a photonic crystal can be well described by the Maxwell equations. Based onsolid-state physics analogy, similarity can be deduced between the behavior ofelectrons in ordinary crystal lattices and the propagation of electromagnetic fields in photonic crystals. In both cases, as a result of Bragg reflections there are certainfrequencies that cannot propagate in the lattice and gaps will appear in the frequencyspectrum. The interesting optical properties of photonic crystals are consequences ofthe existing photonic bands (Joannopouloset al., 1995; Sakoda, 2001; Poole and Owens,2003).The finite difference time domain (FDTD) method (Taflove, 1995; Sullivan, 2000;Ward and Pendry, 1998) is widely used to determine the photonic bands of thesestructures. Passing a light pulse of Gaussian distribution through the photonic crystaland analyzing the transmitted wave can explore the photonic bands. Since thedielectric constant in real optical materials is a function of frequency, this dispersionshould be considered in the process of determining the accurate band structure. In contrast to PWE method, the FDTD provides the possibility of the refractive index vriation during the computation process, which allows to take into account losses and nonlinearity when computing the band structure.

II. Problem Definition

Employing the dirac notation to provide an independent representation for the fields and inner products, the source-free Maxwell's equations for a linear dielectric $\epsilon = \epsilon(\vec{r})$ can be written in terms of only the magnetic field $|H\rangle$ [1]:

$$\vec{\nabla} \times \frac{1}{\epsilon}\vec{\nabla} \times |H\rangle = -\frac{1}{c^2}\frac{\partial^2}{\partial t^2}|H\rangle, \tag{1}$$

$$\vec{\nabla} \cdot |H\rangle = 0, \tag{2}$$

where c is the speed of light, the magnetic field is time-dependent ($e^{-j\omega t}$) with a defined frequency ω. Furthermore, supposing that the system is periodic, the Bloch's theorem for periodic eigenproblems affirms that the states cn be chosen to be of the form [2]:

$$|H\rangle = e^{j(\vec{k}\cdot\vec{r}-\omega t)}|H_{\vec{k}}\rangle, \tag{3}$$

where $\vec{k}$ is the *Bloch wavevector* and $|H_{\vec{k}}$ is a periodic field completly defined by its values in the unit cell. Then, the eigenproblem in the unit cell becomes:

$$\hat{A}_{\vec{k}}|H_{\vec{k}}\rangle = (w/c)^2|H_{\vec{k}}, \tag{4}$$

where $\hat{A}_{\vec{k}}$ is the positive semi-definite Hermitian operator:

$$\hat{A}_{\vec{k}} = (\vec{\nabla} + j\vec{k}) \times \frac{1}{\epsilon}(\vec{\nabla} + j\vec{k}) \times . \tag{5}$$

All theorems related to Hermitian eigenproblems apply. Since $|H_{\vec{k}}$ has a compact support the solutions are a discrete sequence of eigenfrequencies $\omega_n(\vec{k})$ forming continuous *bnd structure* (or *dispersion relation*) as a function of $\vec{k}$. Additionally, the modes at a given $\vec{k}$

$$\langle H^{(n)}_{\vec{k}}|H^{(m)}_{\vec{k}}\rangle = \delta_{n,m}, \tag{6}$$

where $\delta_{n,m}$ is the Kronecker delta.

III. The Finite-Difference Time-Domain Approach

$$\vec{\boldsymbol{E}}(\vec{\boldsymbol{r}}) = \vec{\boldsymbol{A}}(\vec{\boldsymbol{r}})e^{j\vec{\boldsymbol{\beta}}\cdot\vec{\boldsymbol{r}}} \tag{7}$$

$$\vec{\boldsymbol{A}}(\vec{\boldsymbol{r}} + \vec{\boldsymbol{t}}_{pqr}) = \vec{\boldsymbol{A}}(\vec{\boldsymbol{r}}) \tag{8}$$

$$\epsilon(\vec{\boldsymbol{r}} + \vec{\boldsymbol{t}}_{pqr}) = \epsilon(\vec{\boldsymbol{r}}) \tag{9}$$

$$\vec{\boldsymbol{t}}_{pqr} = p\vec{\boldsymbol{t}}_1 + q\vec{\boldsymbol{t}}_2 + r\vec{\boldsymbol{t}}_3 \tag{10}$$

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A. Bloch Periodic Boundary Conditions

$$\vec{\boldsymbol{E}}(x \pm \Lambda_x) = \vec{\boldsymbol{E}}(x) e^{j \pm \beta_x \Lambda_x} \tag{11}$$
$$\vec{\boldsymbol{E}}(y \pm \Lambda_y) = \vec{\boldsymbol{E}}(y) e^{j \pm \beta_y \Lambda_y} \tag{12}$$
$$\vec{\boldsymbol{E}}(z \pm \Lambda_z) = \vec{\boldsymbol{E}}(z) e^{j \pm \beta_z \Lambda_z} \tag{13}$$
$$\vec{\boldsymbol{H}}(x \pm \Lambda_x) = \vec{\boldsymbol{H}}(x) e^{j \pm \beta_x \Lambda_x} \tag{14}$$
$$\vec{\boldsymbol{H}}(y \pm \Lambda_y) = \vec{\boldsymbol{H}}(y) e^{j \pm \beta_y \Lambda_y} \tag{15}$$
$$\vec{\boldsymbol{H}}(z \pm \Lambda_z) = \vec{\boldsymbol{H}}(z) e^{j \pm \beta_z \Lambda_z} \tag{16}$$

B. Initial Conditions

To compute the photonic bandgap diagram for a given PhC, the time-dependent response of its structure by a source that excites all modes should be found at any point of the computational domain. Therefore, several distinct poralized impressed current sources with wide spectrum gaussian waveforms should be randomly placed throughout the computational domain to ensure that all modes of interest are excited. Moreover, as there is no absorption due to perioic boundary conditions, radiation will indefinetely exist.

C. Structure Response Analysis

The spectral analysis of the time dependent response can be carried out by the Fourier transform. Although the accuracy of the method achieves its maximum with infinite computtion time, given finite resources, the computation time should still be considerably large. The eigen-states of the structure are found searching for local maximas at the response spectrum. A more detailed analysis should be made to assure that no spurious solutions are considered, which usually appear as inessential peaks the the spectrum.

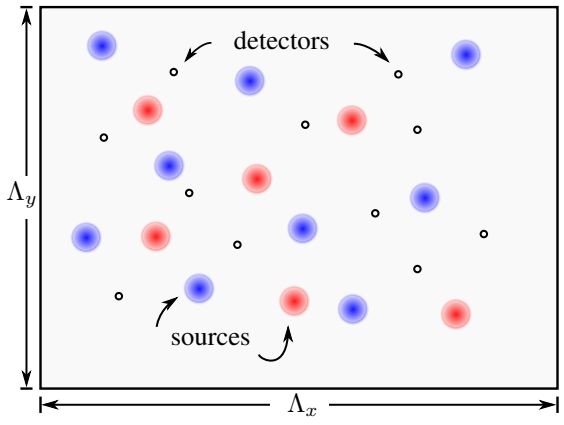

Fig. 1. Random distribution of sources and detectors.

IV. Results

FFT the record arrays to calculate the power spectral density recorded at each record point.

$$PSD_p(\omega) = \left| \mathcal{F} \left\{ \vec{\boldsymbol{E}}(t)|^p \right\} \right|^2 \tag{17}$$

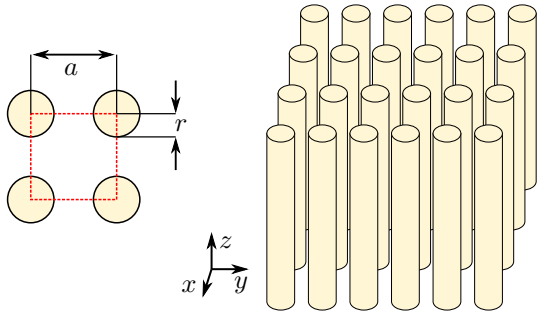

Fig. 2. A two-dimensional photonic crystal. This material is a square lattice of dielectric columns with radius r and dielectric constant ϵ. The material is homogeneous along the z direction, and periodic along x and y with lattice constant a. The left inset shows the square lattice from above with the unit cell framed in red.

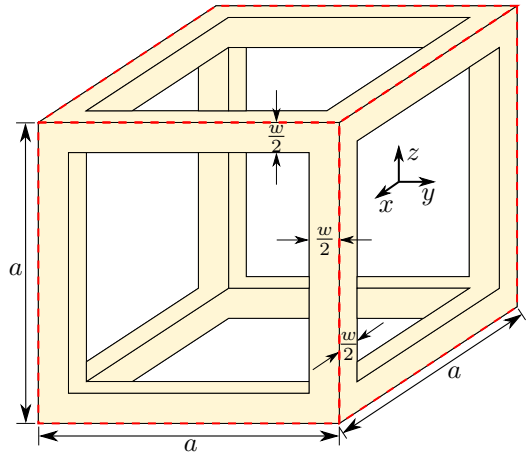

Fig. 3. A three-dimensional photonic crystal. The material is a cubic lattice of dielectric edges with width w and dielectric constant ϵ. The material is periodic along x, y and z with lattice constant a. The edges of the cubic unit cell is shown framed in red.

The power spectral densities from all detector points are added

$$PSD(\omega) = \sum_p PSD_p(\omega) \tag{18}$$

frequencies corresponding to Bloch modes are identified as sharp peaks in the overall PSD.

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V. Conclusion

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Appendix A
Proof of the First Zonklar Equation

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Appendix B

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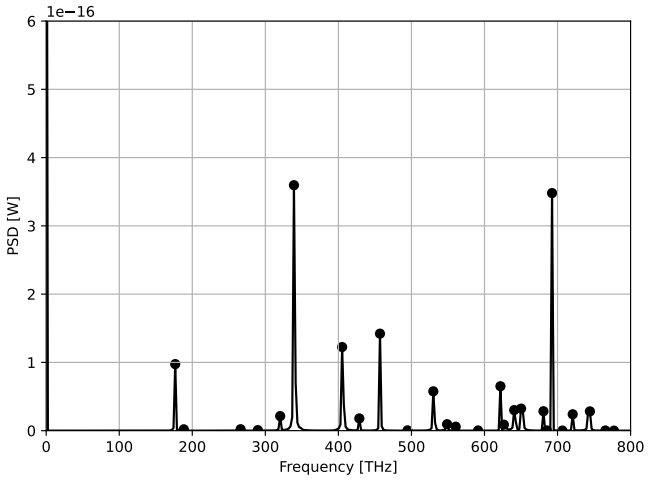

Fig. 4. Power spectral density and eigen-states peaks.

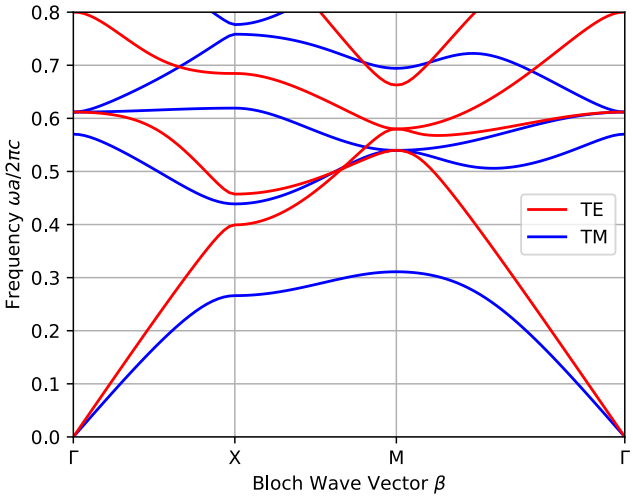

Fig. 5. The photonic band structure for a square array of dielectric columns with $r = 0.2a$. The blue bands represent TM modes and the red bands represent TE modes. The inset shows the Brillouin zone, with the irreducible zone shaded light blue. The results were calculated using PWEM where columns (ϵ_r = 8.9, as for alumina) are embedded in air (ϵ_r = 1).

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REFERENCES

[1] J. D. Joannopoulos, Pierre R. Villeneuve, and Shanhui Fan. Photonic crystals: putting a new twist on light. *Nature*, 386(6621):143–149, March 1997.

[2] Neil W. Ashcroft and N. David Mermin. *Solid state physics*. Holt, Rinehart and Winston, New York, 1976.

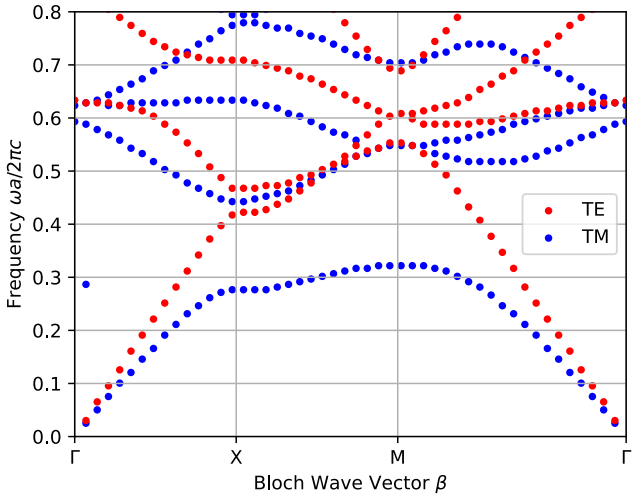

Fig. 6. The photonic band structure for a square array of dielectric columns with $r = 0.2a$. The blue bands represent TM modes and the red bands represent TE modes. The inset shows the Brillouin zone, with the irreducible zone shaded light blue. The results were calculated using FDTD where columns (ϵ_r = 8.9, as for alumina) are embedded in air (ϵ_r = 1).

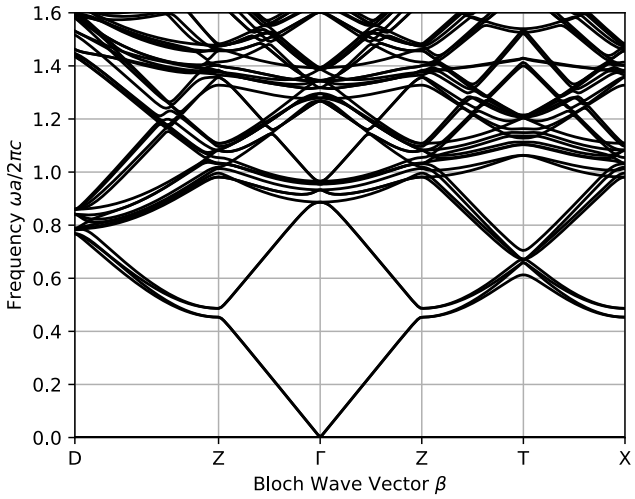

Fig. 7. The photonic band structure for the lowest-frequency electromagnetic modes of a simple cubic lattice with dielectric edges (w=0.2a,ϵ_r = 2.43) in air. Note the absence of a complete photonic band gap.

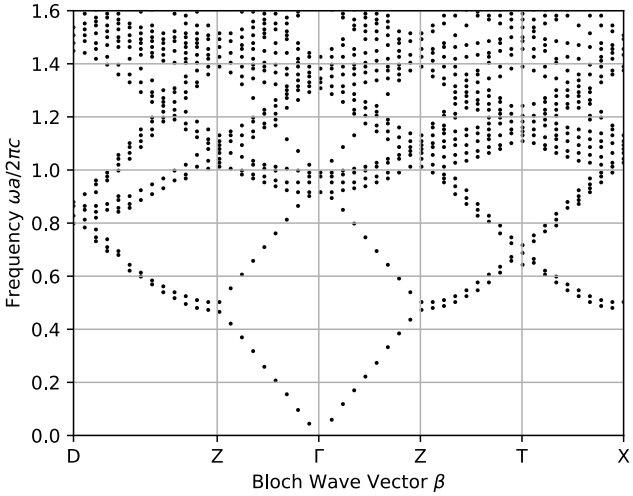

Fig. 8. FDTD 3D Graph