PWE ANALYSIS MODELING FOR BI-ANISOTROPIC PBG STRUCTURE

Long Gen ZHENG & Wen Xun ZHANG*
State Key Laboratory of Millimeter Waves, Southeast University
Nanjing, Jiangsu, 210096, China **(wxzhang@ieee.org)**

Introduction

Many literatures have been published on analysis, experiment and application of PBG structure since Yablonovitch [1] discovered that structure prohibits EM wave propagation for specific frequency bands. Many analytical methods have been developed, such as PWE (Plane Wave Expansion) [2-5] in frequency domain, FDTD [6] in time domain, and transfer matrix method [7], etc. Among them, PWE is suitable for a structure with infinite periods, whereas FDTD is the best for a structure with finite periods. For a PBG structure consisting of isotropic or anisotropic media, MIT Photonic-Bands package [5], based on the model of $\vec{H}$ wave-equation derived from Maxwell equations, is a source-opened powerful tool. On the contrary, there is no analytical tool available for PBG structures consisting of general complex medium, especially bi-isotropic and bi-anisotropic materials, hence their frequency responses of propagation characteristics are still unknown. The aim of this article is just to report our work on developing a simulating tool, based on PWE method, to analyze PBG structure consisting of general complex media. In addition, some simulated results for typical 2-D PBG structure consisting of chiral medium are given, which shows that the appropriate chirality can obviously enhance the width of band-gap.

Modeling

In a source free, inhomogeneous medium, Maxwell equations have the form:

$$\begin{cases} \nabla\times\vec{H} = j\omega\vec{D}, & \nabla\cdot\vec{D} = 0 \\ \nabla\times\vec{E} = -j\omega\vec{B}, & \nabla\cdot\vec{B} = 0 \end{cases} \tag{1}$$

with constitution of $\begin{pmatrix}\vec{D}\\ \vec{B}\end{pmatrix} = \begin{pmatrix}\varepsilon & 0\\ 0 & \mu\end{pmatrix}\begin{pmatrix}\vec{E}\\ \vec{H}\end{pmatrix}$ for isotropic medium,

and $\begin{pmatrix}\vec{D}\\ \vec{B}\end{pmatrix} = \begin{pmatrix}\vec{\varepsilon} & \vec{\xi}\\ \vec{\zeta} & \vec{\mu}\end{pmatrix}\begin{pmatrix}\vec{E}\\ \vec{H}\end{pmatrix}$ or $\begin{pmatrix}\vec{E}\\ \vec{H}\end{pmatrix} = \begin{pmatrix}\vec{\kappa} & \vec{\chi}\\ \vec{\gamma} & \vec{\nu}\end{pmatrix}\begin{pmatrix}\vec{D}\\ \vec{B}\end{pmatrix}$ for bi-anisotropic medium.

Eliminating $\vec{E}$ and $\vec{H}$ from Eq.(1) by using constitutional relations, we have

$$\nabla\times[\mathbf{M}]\cdot\begin{pmatrix}\vec{B}\\ \vec{D}\end{pmatrix} = j\omega\begin{pmatrix}\vec{B}\\ \vec{D}\end{pmatrix}, \qquad \text{with } [\mathbf{M}] = \begin{pmatrix}-\vec{\chi} & -\vec{\kappa}\\ \vec{\nu} & \vec{\gamma}\end{pmatrix} \tag{2}$$

In a PBG structure, the periodic medium parameters with lattice vectors $\vec{R}$ can be written as: [8,9]

---

* This work is supported by the National Natural Sciences Foundation of China [*No. 60071007*], and the China-Singapore Joint Project [*listed in the document No.2001-62*].

0-7803-7846-6/03/$17.00 ©2003 IEEE

$$\begin{pmatrix} \vec{\varepsilon}(\vec{r}) & \vec{\xi}(\vec{r}) \\ \vec{\zeta}(\vec{r}) & \vec{\mu}(\vec{r}) \end{pmatrix} = \begin{pmatrix} \vec{\varepsilon}(\vec{r}+\vec{R}) & \vec{\xi}(\vec{r}+\vec{R}) \\ \vec{\zeta}(\vec{r}+\vec{R}) & \vec{\mu}(\vec{r}+\vec{R}) \end{pmatrix}; \begin{pmatrix} \vec{\kappa}(\vec{r}) & \vec{\chi}(\vec{r}) \\ \vec{\gamma}(\vec{r}) & \vec{\nu}(\vec{r}) \end{pmatrix} = \begin{pmatrix} \vec{\kappa}(\vec{r}+\vec{R}) & \vec{\chi}(\vec{r}+\vec{R}) \\ \vec{\gamma}(\vec{r}+\vec{R}) & \vec{\nu}(\vec{r}+\vec{R}) \end{pmatrix}. \tag{3}$$

By expressing the EM fields as Bloch waves, making Fourier expansion on the resulted periodic function, and further employing transversal characteristics of both $\vec{D}_{\vec{G}}$ and $\vec{B}_{\vec{G}}$ fields [always perpendicular to the wave vector $(\vec{G}+\vec{k})$], yields:

$$\begin{pmatrix} \vec{B} \\ \vec{D} \end{pmatrix} = e^{j\vec{k}\cdot\vec{r}} \sum_{\vec{G}} \begin{pmatrix} \vec{B} \\ \vec{D} \end{pmatrix}_{\vec{G}} e^{j\vec{G}\cdot\vec{r}} = \sum_{\vec{G}} \begin{pmatrix} \vec{B} \\ \vec{D} \end{pmatrix}_{\vec{G}} e^{j(\vec{G}+\vec{k})\vec{r}} = \sum_{\vec{G}} \left[\begin{pmatrix} B_{1G} \\ D_{1G} \end{pmatrix} \vec{e}_{1\vec{G}} + \begin{pmatrix} B_{2G} \\ D_{2G} \end{pmatrix} \vec{e}_{2\vec{G}} \right] e^{j(\vec{G}+\vec{k})\vec{r}} \tag{4}$$

where $\{\vec{G}\}$ are lattice-vectors in reciprocal lattice space, i.e. $\vec{k}$ -space, and $\vec{k}$ is in the first Brillouin zone of this space. The fields with subscript $\vec{G}$ are in the Fourier domain. Vector $(\vec{k}+\vec{G})$ is orthogonal to both $\vec{B}_{\vec{G}}$ and $\vec{D}_{\vec{G}}$. The unit-vectors $\vec{e}_{1\vec{G}}$, $\vec{e}_{2\vec{G}}$ and $\vec{e}_{3\vec{G}} = (\vec{k}+\vec{G}) / |\vec{k}+\vec{G}|$ span a $\vec{G}$ -specific orthogonal coordinates.

Substituting (4) into (2) yields an eigenvalue equation:

$$(\nabla + j\vec{k}) \times [\mathbf{M}(\vec{r})] \cdot \sum_{\vec{G}} [T]_{\vec{G},2x4} [F]_{\vec{G},4x1} e^{j\vec{G}\cdot\vec{r}} = j\omega \sum_{\vec{G}} [T]_{\vec{G},2x4} [F]_{\vec{G},4x1} e^{j\vec{G}\cdot\vec{r}} \tag{5}$$

where $[T]_{\vec{G},2x4}[F]_{\vec{G},4x1} = \begin{pmatrix} \vec{e}_{1\vec{G}} & \vec{e}_{2\vec{G}} & \vec{0} & \vec{0} \\ \vec{0} & \vec{0} & \vec{e}_{1\vec{G}} & \vec{e}_{2\vec{G}} \end{pmatrix} \begin{pmatrix} B_{1\vec{G}} \\ B_{2\vec{G}} \\ D_{1\vec{G}} \\ D_{2\vec{G}} \end{pmatrix} = \begin{pmatrix} B_{1\vec{G}} \\ D_{1\vec{G}} \end{pmatrix} \vec{e}_{1\vec{G}} + \begin{pmatrix} B_{2\vec{G}} \\ D_{2\vec{G}} \end{pmatrix} \vec{e}_{2\vec{G}}$.

This equation can be solved by using either matrix-based eigensolver or iterative eigensolver.

(I) ***Matrix-based eigensolver:*** the media parameters need to be further expressed in Fourier series as

$$[\mathbf{M}(\vec{r})] = \sum_{\vec{G}} [M]_{\vec{G}} e^{j\vec{G}\cdot\vec{r}} \qquad \text{with} \quad [M]_{\vec{G}} = \int_V [\mathbf{M}(\vec{r})] e^{-j\vec{G}\cdot\vec{r}} dV. \tag{6}$$

where the integration is done on a spatial cell V formed by $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$. The eigenvalue equations for all $\vec{G}$ in spectral domain are expressed in matrix form:

$$\sum_{\vec{G}'} \left\{ [T]^T_{\vec{G},2x4} \cdot \left[(\vec{k}+\vec{G}) \times [M]_{\vec{G}-\vec{G}'} \right] \cdot [T]_{\vec{G},2x4} \right\} [F]_{\vec{G}',4x1} = \omega [F]_{\vec{G},4\mathrm{x}1} \tag{7}$$

with a non-Hermitian matrix {•}. It is ready to be solved by matrix-based eigensolver such as ZGEEV in LAPACK from www.netlib.org.

(II) ***Iterative eigensolver:*** it is not necessary to build explicit matrix form. The matrix information is obtained by operation as shown in Eq.(5), which can be done efficiently in the following steps: (by N terms truncation of Fourier expansion)

(1) Inflate the given $4\times1\times N$ column vector in Eq.(4) into a $6\times1\times N$ column vector.
(2) Do FFT from spectral coefficients to field strength at discrete points in a primitive cell of spatial domain.
(3) Make scalar product of field vector by dyadic parameters of media at these

points.

(4) Do Inverse FFT from resulted field strength at discrete points in a primitive cell to the spectral coefficients.

(5) Make curl operation on the resulted field expansion expression and deflate the resulted column vector.

All the above procedures are diagonal or equivalent operation

Since the scalar-product of field vector by dyadic parameters of media are taken place at discrete points in a primitive cell of spatial domain, the convergence behavior as well as the frequency accuracy will not be guaranteed due to the poor representation of actual geometry of the structure. An averaging operation of effective constitutive parameters for a grid across the interface is beneficial to minimize the errors. Based on the law of continuity of either normal flux-density (D_n & B_n) or tangential field strength (E_t & H_t), the different averaging schemes are adopted. Denote:

$$[\mathbf{P}(\vec{r})]=\begin{bmatrix}\vec{\vec{\varepsilon}}(\vec{r}) & \vec{\vec{\xi}}(\vec{r})\\ \vec{\vec{\zeta}}(\vec{r}) & \vec{\vec{\mu}}(\vec{r})\end{bmatrix},\qquad [\mathbf{P}_{eff}]=\begin{bmatrix}\vec{\vec{\varepsilon}}_{eff} & \vec{\vec{\xi}}_{eff}\\ \vec{\vec{\zeta}}_{eff} & \vec{\vec{\mu}}_{eff}\end{bmatrix},\qquad [I]=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix},$$

then the effective constitution matrices may be summarized as:

$$[\mathbf{P}_{eff}]=[\mathbf{P}_{\mathbf{n}eff}]\cdot[I]\vec{n}\vec{n}+[\mathbf{P}_{\mathbf{t}eff}]\cdot[I]\vec{t}\vec{t} \tag{8}$$

where $[\mathbf{P}_{\mathbf{n}eff}]=\left[\frac{1}{V}\int_V[\mathbf{P}(\vec{r})]^{-1}dV\right]^{-1}$, $[\mathbf{P}_{\mathbf{t}}]_{eff}=\frac{1}{V}\int_V[\mathbf{P}(\vec{r})]dV$ and $\vec{t}\vec{t}=\vec{\vec{I}}-\vec{n}\vec{n}$.

Example

The structure under consideration is an array of parallel cylindrical air-holes periodically arranged as triangular lattice in a chiral medium. The dyadic constitutive parameters of chiral medium can be written as: $\vec{\vec{\varepsilon}}=\varepsilon_0\varepsilon_r\vec{\vec{I}}$, $\vec{\vec{\mu}}=\mu_0\mu_r\vec{\vec{I}}$, $\vec{\vec{\xi}}=\left(-j\kappa_r c^{-1}\right)\vec{\vec{I}}$ and $\vec{\vec{\zeta}}=j\kappa_r c^{-1}\vec{\vec{I}}$, $c=\sqrt{\varepsilon_0\mu_0}$.

Giving constitutive parameters $\varepsilon_r=13$, $\mu_r=1$; and sizes $|\vec{a}_1|=|\vec{a}_2|=a$ and $r=0.48a$.

When isotropic medium ($\kappa_r=0$) is used as host, it possesses a complete (for all directions and any polarization) band-gap, its bandwidth is about 18.34% (from MPB-code).

When chiral medium ($\kappa_r\neq 0$) is employed as host, the width of the band gap will be increased significantly. Table 1 & 2 show the results by using Matrix-based eigensolver and Iterative eigensolver, respectively. The former took about 6 hours, but the latter only 5 minutes to calculate multi-frequency $\{f\}$ for one value of wave-vector $\vec{k}$. Corresponding to an appropriate κ_r value, a maximal band-gap (about twice of that from isotropic host) is reached.

Conclusion

Two essential improvements on the plane wave expansion method are proposed: (1) Modeling *DB*-eigenvalue equations (replacing the H-eigenvalue equation). (2) Integrating an iterative eigensolver (replacing the matrix-based eigensolver). Two contributions are presented: (1) the modeling and eigensolver presented in this paper can be used to treat complicate structure with bi-anisotropic medium. (2) The computation process of PBG consisting of complex medium is fastened (with ~70 times of speed improvement). (3) A wideband PBG consisting of chiral medium is predicted (with double bandwidth of that of isotropic dielectric).

Based on *DB*-equations										
κ_r	1e-9	1e-5	0.1	1.0	2.0	2.5	2.75	3.0	3.3	3.6
Bandwidth (%)	17.70	17.70	17.73	21.13	29.95	35.36	35.98	35.33	30.97	19.43

Table 1. The bandwidth of PBG at different chirality (matrix-based eigensolver)

Based on *DB*-equations and iterative eigensolver										
κ_r	1e-9	1e-5	0.1	1.0	2.0	2.5	2.75	3.0	3.3	3.6
Bandwidth (%)	18.84	18.84	18.89	23.34	30.10	31.86	32.64	32.54	30.87	--

Table 2. The bandwidth of PBG at different chirality (iterative eigensolver)

References

[1] E. Yablonovitch and T.J. Gmitter, “Photonic Band Structure: The Face- Centered-Cubic case,” Phys. Rev. Lett. 63, pp.1950 (1989).

[2] R.D. Meade, A.M. Rappe, K.D. Brommer, J.D. Joannopoulos, and O.L. Alerhand, “Accurate theoretical analysis of photonic band-gap materials,” Phys. Rev. B vol.48, pp.8434-8437 (1993). Erratum: S.G. Johnson, ibid vol.55, pp.15942 (1997).

[3] S.G. Johnson and J.D. Joannopoulos, "Block-iterative frequency-domain methods for Maxwell's equations in a planewave basis," Optics Express 8, no.3, pp.173-190 (2001).

[4] J.D. Joannopoulos, R.D. Meade, and J.N. Winn, *Photonic Crystals: Molding the Flow of Light*, Princeton (1995).

[5] S.G. Johnson and J.D. Joannopoulos, The MIT Photonic-Bands Package, http://ab-initio.mit.edu/mpb/.

[6] J.D. Shumpert, W.J. Chappell, and L.P.B. Katehi, “Parallel-Plate Mode Reduction in Conductor-Backed Slots Using Electromagnetic Bandgap Substrates,” IEEE Trans. on MTT, Vol.47, No.11, pp.2099-2104 (1999).

[7] J.B. Pendry, “Photonic band structures”, Jour. of Modern Optics, Vol.41, No.2, pp.209-229. (1994).

[8] J.A. Kong, *Electromagnetic Wave Theory*, EMW Publishing, Cambridge, Massachusetts, USA, (2000).

[9] N.W. Ashcroft, N.D. Mermin, *Solid State Physics*, Holt-Saunders International Editions, Chapter 8. (1976)