Classification of degenerate and non-degenerate modes of Photonic Crystals in FDTD analysis by group theory

Hiroaki Sakamoto\(^a\), Toru Uno, Takuji Arima, and Yujiro Kushiyama

Graduate School & Engineering, Tokyo University of Agriculture and Technology, Naka-cho, Koganei-shi, Tokyo, 184–8588, Japan
\(a\) 50012645211@st.tuat.ac.jp

Abstract: In recent years, Photonic Crystals (PCs) are widely applied in microwave engineering, antenna engineering and so on. Properties of PCs are often analyzed by the FDTD method. Propagation modes of PCs are one of the important properties. However, FDTD method cannot distinguish degenerate or non-degenerate mode due to its calculation procedure. This paper proposed a classification technique of the degenerate and non-degenerate mode in the FDTD analysis of PCs using a group theory.

Keywords: FDTD, periodic structures, degenerate, group theory

Classification: Antennas and Propagation

References

1 Introduction

In recent years, PCs are widely investigated in microwave engineering and antenna engineering [1, 2, 3, 4, 5]. PCs that exhibit novel characteristics that may not be found in nature are artificial periodic structures composed of dielectric, or magnetic, or metallic materials.

The analysis of propagation modes in periodic structures is often analyzed by the FDTD method. The FDTD method solves the Maxwell’s equations within the unit cell in time domain by applying a periodic boundary condition. In the FDTD method, the propagation modes are identified as the spectral peaks obtained from the Fourier transform of the electric fields in the time domain [6, 7]. However, the FDTD method cannot distinguish one mode between more than two modes like degenerate in the same frequency. On the other hand, a group theory [8] has been applied classification of propagation modes in PCs [9]. In this paper, the group theory is applied to distinguish degenerate and non-degenerate mode in the FDTD analysis of PCs.

2 Classification using group theory

In this section, classification method of PCs propagation modes in the FDTD analysis will be explained. The PCs are composed of symmetric structure. Therefore, electric fields in the structure also should be symmetric distribution. The classification method by group theory is using symmetric property. On the other hand, the purpose of this paper is to classify degeneration mode or non-degeneration mode from the FDTD electric field result. In the FDTD method, periodic structures as PCs are easily calculated by periodic boundary conditions in time domain. The FDTD calculation gives us time domain electric and magnetic fields. Field distributions in frequency domain are used to classify modes in group theory. Fortunately, field distributions in PCs in frequency domain can be obtained in FDTD analysis by Fourier's transform easily.

Next, classification method by group theory is explained. The PCs have a translational symmetry, therefore the electrical fields also have translational symmetry as eq.(1).

$$E(x + la, y + ma) = E(x, y)$$  \hspace{1cm} (1)

where $E$ is electric fields, $a$ is lattice distance, $l$ and $m$ are integers. Classification method by group theory uses electric fields in one unit structure. In classification method by the group theory, several groups are produced by using result of translational symmetry for electrical fields in PCs. We define the symmetry operation $\sigma_x$ that changes $x$ to $-x$, electrical fields in the structure are invariant under this operation as expressed in eq.(2).

$$\sigma_x[E(x, y)] = E(x, y)$$  \hspace{1cm} (2)

The fields are invariant under the symmetry operation $\sigma_y$ that changes $y$ to $-y$. 
Furthermore, there are $\sigma'_d$, which changes $(x, y)$ to $(y, x)$, and $\sigma''_d$, which changes $(x, y)$ to $(-y, -x)$. The fields are invariant when it is rotated by $\pi/2$, $\pi$, or $3\pi/2$ radian counterclockwise about the origin. These symmetry operations are denoted by $C_4$, $C_2 \equiv C^{24}_4$, and $C^{-1}_4 \equiv C^3_4$. $C_n$ generally means rotation by $2\pi/n$ radian. All these symmetry operations constitute the $C_4v$ point group [9]:

$$C_4v = \{E, C_4, C^{-1}_4, C_2, \sigma_v (= \sigma_x, \sigma_y), \sigma_d (= \sigma'_d, \sigma''_d)\}. \quad (3)$$

These symmetry operations in two dimensions can be represented by a $2 \times 2$ matrix.

$$\begin{align*}
\sigma_x & : \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} & \sigma_y & : \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
\sigma'_d & : \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & \sigma''_d & : \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \\
C_4 & : \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} & C^{-1}_4 & : \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \\
C_2 & : \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} & E & : \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\end{align*} \quad (4)$$

Then, the $C_4v$ has five categories based on combination of trace of $R$ where $R$ is symmetry operation such as eq.(4). These categories are called as irreducible representation. One of which is one-dimensional irreducible representations as $A_1$, $A_2$, $B_1$, $B_2$. In one-dimensional irreducible representation, the result of trace is $\text{Tr}(R) = -1$ or 1 and we can categorize to $A_1$-$B_2$ by combination of $\text{Tr}(R)$. Another type of irreducible representation is two-dimensional irreducible representation $E$ which is $\text{Tr}(R) = -2$, 0, or 2. This category $E$ is degeneration mode, because, degenerate mode has two propagation modes in one fields, we denote $f_E^{(1)}$ and $f_E^{(2)}$ respectively, then symmetry operation $R$ is indicated as

$$\begin{align*}
Rf_E^{(1)}(\mathbf{r}) & = A_{11}f_E^{(1)}(\mathbf{r}) + A_{12}f_E^{(2)}(\mathbf{r}) \\
Rf_E^{(2)}(\mathbf{r}) & = A_{21}f_E^{(1)}(\mathbf{r}) + A_{22}f_E^{(2)}(\mathbf{r}).
\end{align*} \quad (5)$$

We transform this equation as

$$R \begin{pmatrix} f_E^{(1)}(\mathbf{r}) \\ f_E^{(2)}(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} f_E^{(1)}(\mathbf{r}) \\ f_E^{(2)}(\mathbf{r}) \end{pmatrix} \quad (6)$$

Therefore, $R$ is recognized as eq.(4) in two dimensional irreducible representation. In one-dimensional irreducible representation, $R$ is just constant [9].

Next, we will explain classification method by group theory. Fig. 1 (b) shows its first Brillouin zone. The $\Gamma$, $X$, $M$ points in Fig. 1 (b) denote $(0, 0)$, $(\pm \pi/a, 0)$, $(\pm \pi/a, \pm \pi/a)$, respectively. In the group theory, symmetric property of electric fields are used to make group. The procedure of making group is indicated as follows. First, electric field distributions in frequency domain are calculated by FDTD method at $\Gamma$ and $M$ point. Because, degenerations
are occurred at these points [9] and these points are satisfied with all invariant symmetry operations for wave number space. Next, character table is used to classify category of transformed electric fields. Table I shows that character table for the $C_{4v}$ point group. In this table, “E” at bottom of first column is two-dimensional irreducible representation. Therefore, R is same as eq.(4). Here, “−2”, “0”, or “2” means $\text{Tr}(R)$. $A_1$~$B_2$ are one-dimensional representation. Therefore, $\text{Tr}(R) = −1$ or $1$ [9]. After making character table, translated electric fields are compared with original electric fields. Then, “1” or “2” means that the translated electric fields are invariant under symmetry operation. “−1” or “−2” means that plus and minus of the electric field reverses under symmetry operation R. Furthermore, “0” means that the electric field is not invariant or plus and minus of the electric field doesn’t reverse under symmetry operation. Finally, table of translated fields can be produced. The fields can be classified by comparing Table I and the produced table. For example, if the electric field is invariant under all symmetry operations, the electric field is regarded as $A_1$ mode.

### 3 Analysis result

In this section, an effectiveness of classification method by group theory in the FDTD analysis are indicated. The analysis model is shown in Fig. 1 (a) and we analyze in TM mode case. Fig. 2 (a), (b) shows the electric field distributions of the model that are observed at $\omega a/2\pi c = 0.556$ at the M point.
Fig. 2. Distribution of the electric fields of the E mode
that medium is dielectric and the ratio of the lattice constant to the radius of the cylinder is (a) 1 : 0.2 and (b) 1 : 0.4, and medium is metal and the ratio of the lattice constant to the radius of the cylinder is (c) 1 : 0.2 and (d) 1 : 0.4. (e) Dispersion relation and classified mode in (a) case.

and $\omega a/2\pi c = 0.389$ at the $\Gamma$ point of the model, respectively. The dielectric constants of the cylinders and the background are 8.9 and 1.0, and the ratio of the lattice constant to the radius of the cylinder is 1 : 0.2 and 1 : 0.4, respectively. If we classify these distributions of electric field by reference to Table I, we can readily see that they are E mode. Fig. 2(c), (d) shows the
distribution of the electric fields that are observed at $\omega a/2\pi c = 0.853$ at the M point and $\omega a/2\pi c = 1.655$ at the $\Gamma$ point when medium is PEC, the ratio of the lattice constant to the radius of the cylinder is 1 : 0.2 and 1 : 0.4, respectively. In the same way, we can readily see that they are E mode.

Fig. 2 (e) shows the classified modes and the dispersion relation at the $\Gamma$ and M point that is dielectric constants of the cylinders and the background are 8.9 and 1.0, and the ratio of the lattice constant to the radius of the cylinder is 1 : 0.2. Here, the points are the FDTD method and the lines are the plane wave expansion method. We can see that E mode calculated by the FDTD method conforms to degenerate calculated by the plane wave expansion method. In the case of the cylinders that medium is PEC, we can also classify degenerate mode as E mode. Hereby, regardless of kind or size of medium, we could see to classify degenerate or non-degenerate mode by using group theory.

4 Conclusion

In this paper, we applied the group theory to the FDTD analysis, in order to classify degenerate and non-degenerate mode. As a result, the effectiveness have been confirmed by classification two different models.