Photonics Crystal

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1 Introduction of Photonic Crystal

A photonic crystal is a **periodic optical nanostructure** that affects the propagation of electromagnetic waves in much of the way that the periodic potential in a semiconductor affects the motion of electrons. The concept of photonic crystal was first proposed by Eli Yablonovitch and Sajeev John in 1987, from their separate work on the dielectric structure with more than one periodic dimension.

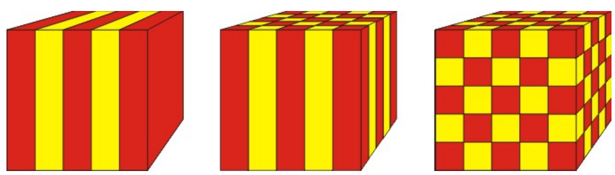


Figure 1: Comparison of 1-D, 2-D and 3-D photonic crystal structures.

2 Basic Theories of 1-D Photonic Crystal

2.1 The Bloch-Floquet Theorem

Theorem 1 (Bloch-Floquet Theorem)**.** *The wavefunction for a particle in a periodic potential field with period $\boldsymbol{a}$ can be writen in the form of*

$$\psi(\boldsymbol{r}) = \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{r}} u(\boldsymbol{r}) \tag{1}$$

where $u(\boldsymbol{r})$ has the same period $\boldsymbol{a}$.

The Bloch-Floquet theorem describes how the electrons moves in a periodic potential field. The eigenvalue equation writes in stationary state:

$$H\psi(\boldsymbol{r}) = -\frac{\hbar^2}{2m}\psi(\boldsymbol{r}) + V(\boldsymbol{r})\psi \tag{2}$$

where the potential field is a periodic function with the following property

$$V(\boldsymbol{r}) = V(\boldsymbol{r} + \boldsymbol{a}) \tag{3}$$

For electromagnetic waves propagating in a medium with periodic permittivity and permeability, the equation writes

$$\begin{aligned} \frac{1}{\epsilon(\boldsymbol{r})}\boldsymbol{\nabla} \times \frac{1}{\mu(\boldsymbol{r})}\boldsymbol{\nabla} \times \boldsymbol{E} = \frac{\omega^2}{c^2}\boldsymbol{E} \\ \frac{1}{\mu(\boldsymbol{r})}\boldsymbol{\nabla} \times \frac{1}{\epsilon(\boldsymbol{r})}\boldsymbol{\nabla} \times \boldsymbol{H} = \frac{\omega^2}{c^2}\boldsymbol{H} \end{aligned} \tag{4}$$

where the permittivity and the permeability respectively obey

$$\epsilon(\boldsymbol{r} + \boldsymbol{a}) = \epsilon(\boldsymbol{r}), \quad \mu(\boldsymbol{r} + \boldsymbol{a}) = \mu(\boldsymbol{r}) \tag{5}$$

Equation (4) can be rewrited as

$$L\psi(\boldsymbol{r}) = \lambda\psi(\boldsymbol{r}) \tag{6}$$

where L represents $\frac{1}{\epsilon(\boldsymbol{r})}\boldsymbol{\nabla} \times \frac{1}{\mu(\boldsymbol{r})}\boldsymbol{\nabla}\times$ or $\frac{1}{\mu(\boldsymbol{r})}\boldsymbol{\nabla} \times \frac{1}{\epsilon(\boldsymbol{r})}\boldsymbol{\nabla}\times$, and $\lambda = \frac{\omega^2}{c^2}$; $\psi(\boldsymbol{r})$ represents either $\boldsymbol{E}$ or $\boldsymbol{H}$. We now introduce the translation operator by

$$T_{\boldsymbol{R}}\psi(\boldsymbol{r}) = \psi(\boldsymbol{r} + \boldsymbol{R}) \tag{7}$$

Due to the periodicity of the permittivity and the permeability, it is easy to verify that

$$T_{\boldsymbol{R}}L = LT_{\boldsymbol{R}} \tag{8}$$

and

$$T_{\boldsymbol{R_1}}T_{\boldsymbol{R_2}} = T_{\boldsymbol{R_2}}T_{\boldsymbol{R_1}} = T_{\boldsymbol{R_1}+\boldsymbol{R_2}} \tag{9}$$

Equation (8) show that their exist simultaneous eigenstates for $T_{\boldsymbol{R}}$ and L. So that

$$\begin{cases} L\psi(\boldsymbol{r}) = \lambda\psi(\boldsymbol{r}) \\ T_{\boldsymbol{R}}\psi(\boldsymbol{r}) = c(\boldsymbol{R})\psi(\boldsymbol{r}) \end{cases} \tag{10}$$

According to (9) we obtain that

$$c(\boldsymbol{R_1} + \boldsymbol{R_2}) = c(\boldsymbol{R_2} + \boldsymbol{R_1}) = c(\boldsymbol{R_1})c(\boldsymbol{R_2}) \tag{11}$$

so that it can be chosen in terms of

$$c(\boldsymbol{R}) = \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{r}} \tag{12}$$

and the corresponding eigenstate

$$\psi(\boldsymbol{r}) = \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{r}}u(\boldsymbol{r}) \tag{13}$$

2.2 The Transfer-Matrix Method in Optics

The **transfer-matrix method** (also called $ABCD$ matrix) is a method used in optics to analyze the propagation of EM waves in **stratified medium**. The transfer-matrix relates the total field in the region on both sides of a optical structure. We consider a EM wave propagates along z direction and has only x and y components. For a dielectric perpendicular to the propagation direction with thickness d and impedance $\eta_d = \sqrt{\mu(\omega)/\epsilon(\omega)}$, the transfer matrix writes a $4\times$ matrix

$$\boldsymbol{T} = \begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{C} & \boldsymbol{D} \end{pmatrix} = \begin{pmatrix} \cos(kd)\boldsymbol{I} & -\mathrm{i}\sin(kd)\eta_d\boldsymbol{n} \\ \mathrm{i}\sin(kd)\eta_d^{-1}\boldsymbol{n} & \cos(kd)\boldsymbol{I} \end{pmatrix} \tag{14}$$

where $\boldsymbol{n}$ and $\boldsymbol{I}$ respectively are

$$\boldsymbol{n} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{15}$$

The electric field and the magnetic field are perpendicular to each other in the presence of electromagnetic waves. so that

$$\boldsymbol{H} = \boldsymbol{n}\boldsymbol{E}, \quad -\boldsymbol{E} = \boldsymbol{n}\boldsymbol{H} \tag{16}$$

where

$$\boldsymbol{E} = (E_x, E_y)^T, \quad \boldsymbol{H} = (H_x, H_y)^T \tag{17}$$

So it is easy to verify that

$$\begin{aligned} \boldsymbol{T}\begin{pmatrix} \boldsymbol{E}_2 \\ \boldsymbol{H}_2 \end{pmatrix} &= \begin{pmatrix} \cos(kd)\boldsymbol{I} & -\mathrm{i}\sin(kd)\eta_d\boldsymbol{n} \\ \mathrm{i}\sin(kd)\eta_d^{-1}\boldsymbol{n} & \cos(kd)\boldsymbol{I} \end{pmatrix}\begin{pmatrix} \boldsymbol{E}_2 \\ \boldsymbol{H}_2 \end{pmatrix} \\ &= \begin{pmatrix} (\cos(kd) + \mathrm{i}\sin(kd))\boldsymbol{E}_2 \\ (\cos(kd) + \mathrm{i}\sin(kd))\boldsymbol{H}_2 \end{pmatrix} \\ &= \begin{pmatrix} \mathrm{e}^{\mathrm{i}kd}\boldsymbol{E}_2 \\ \mathrm{e}^{\mathrm{i}kd}\boldsymbol{H}_2 \end{pmatrix} = \begin{pmatrix} \boldsymbol{E}_1 \\ \boldsymbol{H}_1 \end{pmatrix} \end{aligned} \tag{18}$$

An obvious consequence is that the transfer matrix is a **unimodular matrix** since the absorption of the waves is not considered.

$$\det(T) = 1 \tag{19}$$

For periodic structure stacked by two kinds of dielectrics with periodic refractive index

$$n(z) = \begin{cases} n_1 = \sqrt{\epsilon_{r1}}, ma < z < ma + d_1 \\ n_2 = \sqrt{\epsilon_{r2}}, ma + d_1 < z < (m+1)a \end{cases} \tag{20}$$

it is easy to obtain the transfer matrix in the medium 1 and 2

$$\boldsymbol{T_1} = \begin{pmatrix} \cos(k_1 d_1)\boldsymbol{I} & -\mathrm{i}\sin(k_1 d_1)\eta_1\boldsymbol{n} \\ \mathrm{i}\sin(k_1 d_1)\eta_1^{-1}\boldsymbol{n} & \cos(k_1 d_1)\boldsymbol{I} \end{pmatrix} \tag{21}$$

$$\boldsymbol{T_2} = \begin{pmatrix} \cos(k_2 d_2)\boldsymbol{I} & -\mathrm{i}\sin(k_2 d_2)\eta_2 \boldsymbol{n} \\ \mathrm{i}\sin(k_2 d_2)\eta_2^{-1}\boldsymbol{n} & \cos(k_2 d_2)\boldsymbol{I} \end{pmatrix} \tag{22}$$

The total transfer matrix is the product of all the transfer matrices

$$\boldsymbol{T}_{\text{total}} = \boldsymbol{T}_1 \boldsymbol{T}_2 \boldsymbol{T}_1 \cdots \tag{23}$$

Thus the incident field and the output field can be related by the total transfer matrix, which writes in terms of

$$\begin{pmatrix} \boldsymbol{E}_{\text{in}} \\ \boldsymbol{H}_{\text{in}} \end{pmatrix} = \boldsymbol{T}_{\text{total}} \begin{pmatrix} \boldsymbol{E}_{\text{out}} \\ \boldsymbol{H}_{\text{out}} \end{pmatrix} \tag{24}$$

2.3 The Transfer Matrices of 1-D Photonic Crystal, Spectrum of Relfectance and Transmittance

We consider a TE wave with only x component of electric field and y component of magnetic field. So that the transfer matrix can be reduced to a 2×2 matrix

$$\boldsymbol{T} = \begin{pmatrix} \cos(kd) & \mathrm{i}\sin(kd)\eta_d \\ \mathrm{i}\sin(kd)\eta_d^{-1} & \cos(kd) \end{pmatrix} = \begin{pmatrix} \cos(\delta) & \mathrm{i}\sin(\delta)\eta_d \\ \mathrm{i}\sin(\delta)\eta_d^{-1} & \cos(\delta) \end{pmatrix} \tag{25}$$

where $\delta = \dfrac{2\pi}{\lambda} nd$ is the optical spacing of the substrate. In a single period, the transfer matrix can be written as the product of two matrix

$$\begin{aligned} \boldsymbol{T} &= \boldsymbol{T}_1 \boldsymbol{T}_2 \\ &= \begin{pmatrix} \cos(\delta_1) & \mathrm{i}\sin(\delta_1)\eta_1 \\ \mathrm{i}\sin(\delta_1)\eta_1^{-1} & \cos(\delta_1) \end{pmatrix} \begin{pmatrix} \cos(\delta_2) & \mathrm{i}\sin(\delta_2)\eta_2 \\ \mathrm{i}\sin(\delta_2)\eta_2^{-1} & \cos(\delta_2) \end{pmatrix} \\ &\begin{pmatrix} \cos\delta_1\cos\delta_2 - \dfrac{\eta_2}{\eta_1}\sin\delta_1\sin\delta_2 & \mathrm{i}(\dfrac{\sin\delta_1\cos\delta_2}{\eta_1} + \dfrac{\sin\delta_2\cos\delta_1}{\eta_2}) \\ \mathrm{i}(\sin\delta_1\cos\delta_2\eta_1 + \sin\delta_2\cos\delta_1\eta_2) & \cos\delta_1\cos\delta_2 - \dfrac{\eta_1}{\eta_2}\sin\delta_1\sin\delta_2 \end{pmatrix} \end{aligned} \tag{26}$$

If the structure consists of N period, then the total transfer matrix

$$\boldsymbol{T}_{\text{total}} = \boldsymbol{T}^N = (\boldsymbol{T}_1 \boldsymbol{T}_2)^N \tag{27}$$

So the incident field and the reflected and tranmitted field can be related by the total transfer matrix. Hence the reflectance and the transmittance coefficience can be solved by

$$\begin{aligned} r &= \frac{(T_{11} + T_{12}\eta_0)\eta_0 - T_{21} + T_{22}\eta_0}{(T_{11} + T_{12}\eta_0)\eta_0 + T_{21} + T_{22}\eta_0} \\ t &= \frac{2\eta_0}{(T_{11} + T_{12}\eta_0)\eta_0 + T_{21} + T_{22}\eta_0} \end{aligned} \tag{28}$$

$$R = r \cdot r^*, \quad T = t \cdot t^* \tag{29}$$

where η_0 is the wave impedance of the environment outside the photonic crystal. Commonly the environment can be regarded as vacuum. The above discussion is based on the case of **perpendicular incidence**. The formalism of **oblique incidence** can be similarly derived from adding an incident angle.

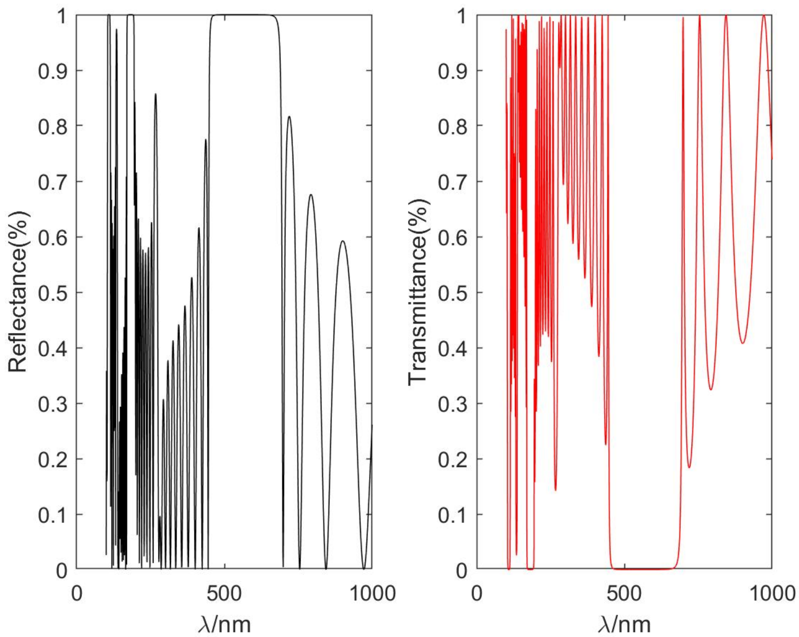


Figure 2: The reflectance and the transmittance. Parameters: $n_1 = 2.35, n_1 = 1.38, d_1 = 63.8\text{nm}, d_2 = 108.7\text{nm}, N = 10$.

2.4 Dispersion

According to Bloch-Floquet theorem and we obtain

$$\mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{a}} \begin{pmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{pmatrix} = \boldsymbol{T} \begin{pmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{pmatrix} \tag{30}$$

The prerequisite to obtain a nonzero solution for equation (30) is that the determinant of $\boldsymbol{T} - \mathrm{e}^{\mathrm{i}Ka}\boldsymbol{I}$ vanishes. Otherwise, a trivial zero solution means that the propagation is forbidden.

$$\begin{vmatrix} T_{11} - \mathrm{e}^{\mathrm{i}Ka} & T_{12} \\ T_{21} & T_{22} - \mathrm{e}^{\mathrm{i}Ka} \end{vmatrix} = 0 \tag{31}$$

where K can be solved by

$$K = \frac{1}{a} \arccos\Bigg(\cos(\delta_1)\cos(\delta_2) - \frac{1}{2}(\frac{\eta_1}{\eta_2} + \frac{\eta_1}{\eta_2}) \sin(\delta_1)\sin(\delta_2) \Bigg) \tag{32}$$

where

$$\delta_i = k_i d_i = d_i \sqrt{(\frac{n_i \omega}{c})^2 - k_y^2}, \quad i = 1, 2 \tag{33}$$

3 Basic Theories of 2-D Photonic Crystal

3.1 Reciprocal Lattice and Brillouin Zone

A 3-D Bravais lattice can be written in terms of

$$\boldsymbol{R} = n_1\boldsymbol{a_1} + n_2\boldsymbol{a_2} + n_3\boldsymbol{a_3}, \quad n_1, n_2, n_3 \in \mathbb{Z} \tag{34}$$

where $\boldsymbol{a_i}$ are the lattice constant along three different directions. $\{\boldsymbol{a_i}\}$ is a basis of the 3-D vector space of any vector inside the lattice. We now introduce its corresponding **reciprocal basis**, $\{\boldsymbol{b_i}\}$, by

$$\boldsymbol{b_i} \cdot \boldsymbol{a_j} = 2\pi\delta_{ij} \tag{35}$$

One obvious solution is

$$\boldsymbol{b_1} = 2\pi\frac{\boldsymbol{a_2} \times \boldsymbol{a_3}}{(\boldsymbol{a_1} \times \boldsymbol{a_2}) \cdot \boldsymbol{a_3}}, \ \boldsymbol{b_2} = 2\pi\frac{\boldsymbol{a_3} \times \boldsymbol{a_1}}{(\boldsymbol{a_1} \times \boldsymbol{a_2}) \cdot \boldsymbol{a_3}}, \ \boldsymbol{b_1} = 2\pi\frac{\boldsymbol{a_1} \times \boldsymbol{a_2}}{(\boldsymbol{a_1} \times \boldsymbol{a_2}) \cdot \boldsymbol{a_3}} \tag{36}$$

Mathematically, the reciprocal lattice space is the dual space of the Bravais lattice space. The reciprocal lattice is measured by the wave vector k. Thus every single vector in the reciprocal space can be written in the form of

$$\boldsymbol{G} = m_1\boldsymbol{b_1} + m_2\boldsymbol{b_2} + m_3\boldsymbol{b_3}, \quad m_1, m_2, m_3 \in \mathbb{Z} \tag{37}$$

For 2-D cases

$$\boldsymbol{R} = n_1\boldsymbol{a_1} + n_2\boldsymbol{a_2}, \quad n_1, n_2 \in \mathbb{Z} \tag{38}$$

we have

$$\boldsymbol{b_1} = 2\pi\frac{\boldsymbol{n}\boldsymbol{a_2}}{\boldsymbol{a_1} \cdot \boldsymbol{a_2}}, \quad \boldsymbol{b_2} = 2\pi\frac{\boldsymbol{n}\boldsymbol{a_1}}{\boldsymbol{a_2} \cdot \boldsymbol{a_1}} \tag{39}$$

where $\boldsymbol{n}$ is the matrix in (15), which represents a rotation of a vector by 90 degree.

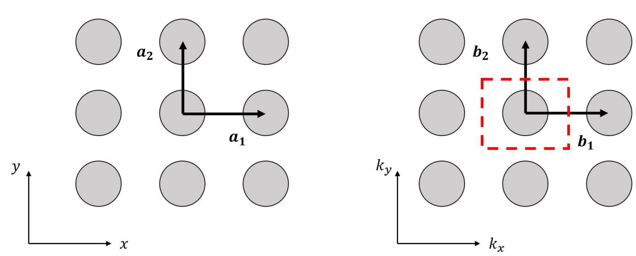


Figure 3: The Bravais lattice(left) and corresponding reciprocal lattice(right) of square lattice. The red frame indicates the first Brillouin zone.

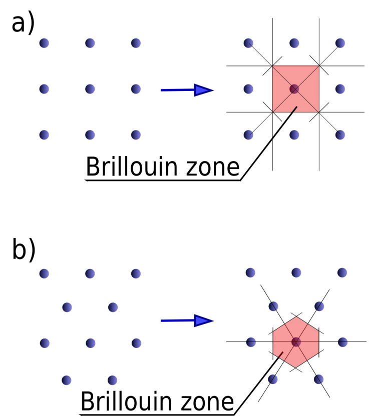


Figure 4: The diagram of the first Brillouin zone of a) square lattice and b) triangle lattice.

3.2 The Plane Wave Expansion Method

We have known from the Bloch-Floquet theorem that any light state can be written in the form of

$$\psi(\boldsymbol{K}, \boldsymbol{r}) = \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{r}} u(\boldsymbol{r}) \tag{40}$$

where the periodic function can be expanded in the reciprocal space

$$u(\boldsymbol{r}) = \sum_m u_m(\boldsymbol{K}) \mathrm{e}^{\mathrm{i}\boldsymbol{G}_m\cdot\boldsymbol{r}} \tag{41}$$

In anology, the inverse permittivity and permeability can also be expanded in the reciprocal space

$$\frac{1}{\epsilon(\boldsymbol{r})} = \sum_m \theta_m \mathrm{e}^{\mathrm{i}\boldsymbol{G}_m\cdot\boldsymbol{r}}, \quad m \in \mathbb{Z}^3 \tag{42}$$

$$\frac{1}{\mu(\boldsymbol{r})} = \sum_m \eta_m \mathrm{e}^{\mathrm{i}\boldsymbol{G}_m\cdot\boldsymbol{r}}, \quad m \in \mathbb{Z}^3 \tag{43}$$

In our consideration, the wave propagates in xy plane. We introduce two special cases: TE mode and TM mode. For TE mode, the electric field has no z component and the magnetic field has only z component. For TM mode, the magnetic field has no z component and the electric field has only z component. So that we only need to solve one master component in either case.

$$\text{TM mode:} \quad E_z = \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{r}} \sum_m A_m \mathrm{e}^{\mathrm{i}\boldsymbol{G}_m\cdot\boldsymbol{r}} = \sum_m A_m \mathrm{e}^{\mathrm{i}(\boldsymbol{G}_m+\boldsymbol{K})\cdot\boldsymbol{r}} \tag{44}$$

$$\text{TE mode:} \quad H_z = \mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{r}} \sum_m B_m \mathrm{e}^{\mathrm{i}\boldsymbol{G}_m\cdot\boldsymbol{r}} = \sum_m B_m \mathrm{e}^{\mathrm{i}(\boldsymbol{G}_m+\boldsymbol{K})\cdot\boldsymbol{r}} \tag{45}$$

To simplify our discussion, we let $\mu(\boldsymbol{r}) = 1$, which is true in the majority of medium. So equation (4) for TE mode turns into

$$\boldsymbol{\nabla} \times \frac{1}{\epsilon(\boldsymbol{r})} \boldsymbol{\nabla} \times \boldsymbol{H} = \frac{\omega^2}{c^2} \boldsymbol{H} \tag{46}$$

Notice that

$$\boldsymbol{\nabla} \times (\phi \boldsymbol{A}) = \boldsymbol{\nabla} \phi \times \boldsymbol{A} + \phi \boldsymbol{\nabla} \times \boldsymbol{A} \tag{47}$$

$$\boldsymbol{\nabla} \times \mathrm{e}^{\mathrm{i}\boldsymbol{S}\cdot\boldsymbol{r}} = \mathrm{i}\boldsymbol{S} \times \mathrm{e}^{\mathrm{i}\boldsymbol{S}\cdot\boldsymbol{r}}, \quad \boldsymbol{\nabla} \mathrm{e}^{\mathrm{i}\boldsymbol{S}\cdot\boldsymbol{r}} = \mathrm{i}\boldsymbol{S}\mathrm{e}^{\mathrm{i}\boldsymbol{S}\cdot\boldsymbol{r}} \tag{48}$$

So

$$\begin{aligned}
&\boldsymbol{\nabla} \times \frac{1}{\epsilon(\boldsymbol{r})} \boldsymbol{\nabla} \times \boldsymbol{H} \\
&= \boldsymbol{\nabla} \times \frac{1}{\epsilon(\boldsymbol{r})} \boldsymbol{\nabla} \times \left(\sum_m B_m \hat{\boldsymbol{e}_{\boldsymbol{z}}} \mathrm{e}^{\mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K})\cdot\boldsymbol{r}} \right) \\
&= \boldsymbol{\nabla} \times \frac{1}{\epsilon(\boldsymbol{r})} (\sum_m B_m \boldsymbol{\nabla} \mathrm{e}^{\mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K})\cdot\boldsymbol{r}} \times \hat{\boldsymbol{e}_{\boldsymbol{z}}}) \\
&= \boldsymbol{\nabla} \times \frac{1}{\epsilon(\boldsymbol{r})} \sum_m B_m \mathrm{e}^{\mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K})\cdot\boldsymbol{r}} \mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K}) \times \hat{\boldsymbol{e}_{\boldsymbol{z}}} \\
&= \boldsymbol{\nabla} \times \sum_n \sum_m \theta_n \mathrm{e}^{\mathrm{i}\boldsymbol{G}_n\cdot\boldsymbol{r}} B_m \mathrm{e}^{\mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K})\cdot\boldsymbol{r}} \mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K}) \times \hat{\boldsymbol{e}_{\boldsymbol{z}}} \\
&= \sum_n \sum_m \theta_n B_m \boldsymbol{\nabla} \times \left(\mathrm{e}^{\mathrm{i}(\boldsymbol{G}_{m+n} + \boldsymbol{K})\cdot\boldsymbol{r}} \mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K}) \times \hat{\boldsymbol{e}_{\boldsymbol{z}}} \right)
\end{aligned} \tag{49}$$

We now change the subscript $m + n$ to m and m to n, so that

$$\begin{aligned}
&\boldsymbol{\nabla} \times \frac{1}{\epsilon(\boldsymbol{r})} \boldsymbol{\nabla} \times \boldsymbol{H} \\
&= \sum_n \sum_m \theta_{m-n} B_n \boldsymbol{\nabla} \times \left(\mathrm{e}^{\mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K})\cdot\boldsymbol{r}} \mathrm{i}(\boldsymbol{G}_n + \boldsymbol{K}) \times \hat{\boldsymbol{e}_{\boldsymbol{z}}} \right) \\
&= \sum_n \sum_m \theta_{m-n} B_n \mathrm{e}^{\mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K})\cdot\boldsymbol{r}} \mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K}) \times (\mathrm{i}(\boldsymbol{G}_n + \boldsymbol{K}) \times \hat{\boldsymbol{e}_{\boldsymbol{z}}}) \\
&= \sum_n \sum_m \theta_{m-n} B_n \mathrm{e}^{\mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K})\cdot\boldsymbol{r}} (\boldsymbol{G}_m + \boldsymbol{K}) \cdot (\boldsymbol{G}_n + \boldsymbol{K}) \hat{\boldsymbol{e}_{\boldsymbol{z}}}
\end{aligned} \tag{50}$$

The right side of equation (46) turns into

$$\frac{\omega^2}{c^2} \sum_m B_m \mathrm{e}^{\mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K})\cdot\boldsymbol{r}} \hat{\boldsymbol{e}_{\boldsymbol{z}}} \tag{51}$$

Select the upper limit G for both n and m, then equation (46) turns into

$$\begin{aligned}
&\sum_{n=1}^{G} \sum_{m=1}^{G} \theta_{m-n} B_n \mathrm{e}^{\mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K})\cdot\boldsymbol{r}} (\boldsymbol{G}_m + \boldsymbol{K}) \cdot (\boldsymbol{G}_n + \boldsymbol{K}) \hat{\boldsymbol{e}_{\boldsymbol{z}}} \\
&= \frac{\omega^2}{c^2} \sum_{m=1}^{G} B_m \mathrm{e}^{\mathrm{i}(\boldsymbol{G}_m + \boldsymbol{K})\cdot\boldsymbol{r}} \hat{\boldsymbol{e}_{\boldsymbol{z}}}
\end{aligned} \tag{52}$$

Equation (52) can be written as a matrix equation

$$\Lambda(\boldsymbol{K})\begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_G \end{pmatrix} = \frac{\omega^2}{c^2}\begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_G \end{pmatrix} \tag{53}$$

The matrix elements of Λ are

$$\Lambda_{mn}(\boldsymbol{K}) = \theta_{m-n}(\boldsymbol{G}_m + \boldsymbol{K}) \cdot (\boldsymbol{G}_n + \boldsymbol{K}) \tag{54}$$

3.3 Expansion of Inverse Permittivity $1/\epsilon(\boldsymbol{r})$

Our goal is to solve the matrix equation (53). To clarify the matrix elements of Λ, we have to first know θ_m. So an important work is to give the Fourier expansion of inverse permittivity $1/\epsilon(\boldsymbol{r})$. We already know that

$$\frac{1}{\epsilon(\boldsymbol{r})} = \begin{cases} \frac{1}{\epsilon_a}, & \boldsymbol{r} \in \boldsymbol{R} \\ \frac{1}{\epsilon_b}, & \text{otherwise} \end{cases} \tag{55}$$

So the inverse permittivity can be written in the form of

$$\frac{1}{\epsilon(\boldsymbol{r})} = \frac{1}{\epsilon_b} + (\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b})\boldsymbol{S}(\boldsymbol{r}) \tag{56}$$

where

$$S(\boldsymbol{r}) = \begin{cases} 1, & \boldsymbol{r} \in \boldsymbol{R} \\ 0, & \text{otherwise} \end{cases} \tag{57}$$

So

$$\begin{aligned} \theta(\boldsymbol{G}) &= \frac{1}{A_c}\int \mathrm{e}^{-\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{r}}\frac{1}{\epsilon(\boldsymbol{r})}\mathrm{d}\boldsymbol{r}^2 \\ &= \frac{1}{A_c}\int \mathrm{e}^{-\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{r}}\frac{1}{\epsilon_b}\mathrm{d}\boldsymbol{r}^2 + \frac{1}{A_c}\int \mathrm{e}^{-\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{r}}\mathrm{d}\boldsymbol{r}^2(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b})\boldsymbol{S}(\boldsymbol{r}) \\ &= \frac{1}{\epsilon_b}\delta(\boldsymbol{G} - 0) + (\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b})\frac{1}{A_c}\int_R \mathrm{e}^{-\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{r}}\mathrm{d}\boldsymbol{r}^2 \end{aligned} \tag{58}$$

The integral in the second term can be transformed to the first Bessel function, if $\boldsymbol{G} \neq 0$

$$\begin{aligned} \int_R \mathrm{e}^{-\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{r}}\mathrm{d}\boldsymbol{r}^2 &= \int \mathrm{d}\theta \int_0^R \mathrm{e}^{-\mathrm{i}|\boldsymbol{G}|\boldsymbol{r}\sin\theta} r\mathrm{d}r \\ &= 2\pi\int_0^R J_0(|\boldsymbol{G}|r)r\mathrm{d}r \\ &= 2\pi R^2\frac{J_1(|\boldsymbol{G}|R)}{|\boldsymbol{G}|R} \end{aligned} \tag{59}$$

So

$$\theta(\boldsymbol{G}) = \begin{cases} \frac{1}{\epsilon_b} + (\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b})f, & \boldsymbol{G} = 0 \\ 2(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b})f\frac{J_1(|\boldsymbol{G}|R)}{|\boldsymbol{G}|R}, & \text{otherwise} \end{cases} \tag{60}$$

where

$$f = \frac{\pi R^2}{A_c} \tag{61}$$

is the filling factor in the first Brillouin zone. For example, $f = \pi R^2/a^2$ for square lattice and $f = \pi R^2/(\sqrt{3}/2a^2)$ for triangle lattice. If we rewrite equation (60) into a matrix equation

$$\theta_m = \begin{cases} \frac{1}{\epsilon_b} + (\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b})f, & \boldsymbol{G} = 0 \\ 2(\frac{1}{\epsilon_a} - \frac{1}{\epsilon_b})f\frac{J_1(G_m R)}{G_m R}, & \text{otherwise} \end{cases} \tag{62}$$

3.4 Dispersion

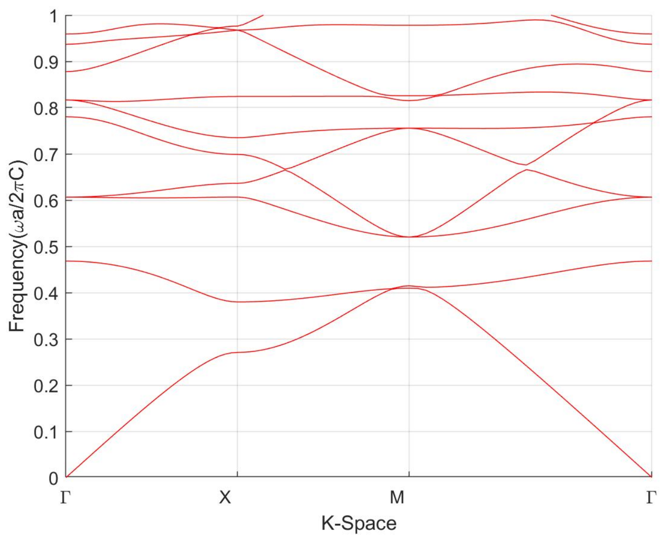
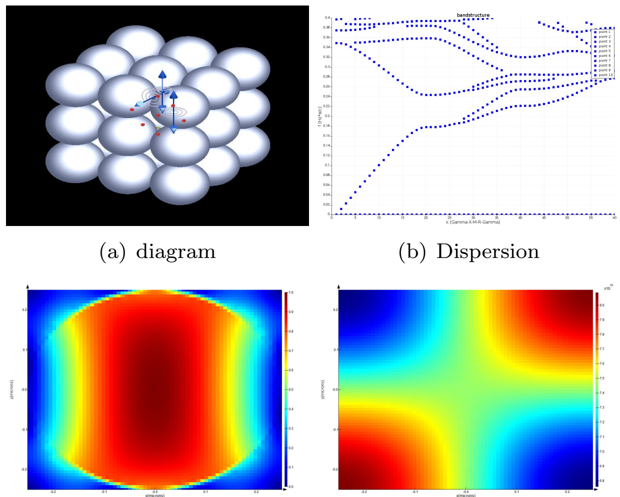


Figure 5: Dispersion of 2-D photonic crystal. Parameters: n_1=1,n_2=2,$f = 0.4$. The horizontal axis is scaled by points in the first Brillouin zone of square lattice: Γ-the center point; X-the center point of an edge; M-the corner.

4 3-D Photonic Crystals



(a) diagram (b) Dispersion

(c) E-field (d) H-field

Figure 6: FDTD simulation for 3-D square lattice photonic crystal.

References

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