2018
TIGP: Advanced Nanotechnology (A)

Part 1: Photonic Crystals and Devices

Lecture #1

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Maxwell's equations

In 1846, James Clerk Maxwell wrote down the equations to describe all phenomena in electric & magnetic field from his publication " A dynamic theory of the electromagnetic field" (* philosophical Transaction of the Royal Society of London, 155, pp.459-512, 1865).

The equations were written down for the macroscopic electric & magnetic fields. In semiconductor photonics, we use Maxwell's eqs. to describe light in a mixed dielectric medium, which is a composition of homogeneous dielectric materials. To solve the eqs. in the system, we treat the wave eqs. derived from Maxwell's eqs. as a linear Hermition eigenvalue problem. This treatment is very similar to the Schrödinger's eq. in Q, M.

Maxwell's wgs. In MKS unit are

(1) $\nabla \times \vec{E}(\vec{r},t) = -\frac{\partial \vec{B}(\vec{r},t)}{\partial t}$ (Faraday's induction law)

(2) $\nabla \times \vec{H}(\vec{r},t) = \vec{J}(\vec{r},t) + \frac{\partial \vec{D}(\vec{r},t)}{\partial t}$ (generalized Ampere's law)

(3) $\nabla \cdot \vec{B}(\vec{r},t) = 0$ (Gauss' law for magnetic field)

(4) $\nabla \cdot \vec{D}(\vec{r},t) = \rho(\vec{r},t)$ (Gauss' law for electric field)

Where

$\vec{E}(\vec{r},t)$ = electric field strength $\left({}^{\text{volts}}\!/\!{}_{\text{m}} \right)$

$\vec{B}(\vec{r},t)$ = magnetic flux density $\left({}^{\text{webers}}\!/\!{}_{\text{m}^2} = \text{tesla} \right)$

$\vec{H}(\vec{r},t)$ = magnetic field strength $\left({}^{\text{Amperes}}\!/\!{}_{\text{m}} \right)$

$\vec{D}(\vec{r},t)$ = electric displacement $\left({}^{\text{coul}}\!/\!{}_{\text{m}^2} \right)$

$\vec{J}(\vec{r},t)$ = electric current density $\left({}^{\text{Ampers}}\!/\!{}_{\text{m}^2} \right)$

$\vec{\rho}(\vec{r},t)$ = electric charge density $\left({}^{coul}\!/\!{}_{m^3} \right)$

Taking the divergence of 2nd & introducing 4th eg. , we have In MKS unit are

$$(5)\quad \nabla \cdot \vec{J}(\vec{r},t) + \frac{\partial}{\partial t}\rho(\vec{r},t) = 0$$

This is the conservation law for electric charge and current densities.

We also need to characterized material media by so-called constitutive relations.

In most of problems, we assume that sources of electromagnetic fields are given. Thus $\vec{J}$ and ρ are known and satisfy the conservation eq. So far , in Maxwell's eqs we have 12 scalar unknowns for 4 field vector $\vec{E}$, $\vec{H}$, $\vec{B}$ and $\vec{D}$. We also understand, eqs (3) & (4) are not independent eqs, and can be derived from eg (1), (2) & (5). The independent eqs are (1) & (2), which constitute 6 scalar eqs. Thus we need 6 more scalar eqs. These are the constitutive relations.

For an isotropic medium, the constitutive relations can be written as

$$\vec{D} = \varepsilon\vec{E}$$

$$\vec{B} = \mu\vec{H}$$

where

ε = permittivity & μ = permeability.

In free space, $\mu = \mu_0$ & $\varepsilon = \varepsilon_0$

$$\mu_0 = 4\pi \times 10^{-7} \quad (\text{henry}/\text{m})$$

$$\varepsilon_0 = 8.85 \times 10^{-12} \ (Farad / m)$$

SI (MKSA) **unit and Gaussian unit：**

There are two separate sets of units used for electromagnetic. In page 2, the system of units is *SI* or *MKSA*. All units are defined in term of {kg, m, second, amprer}

$$Wb = \frac{kg \cdot m^2}{Amp\ s^2} \qquad Coul = Amp \cdot s \qquad Volt = \frac{kg \cdot m^2}{Amp \cdot\ s^3}$$

$$Henry = \frac{kg \cdot m^2}{Amp^2 \cdot s^2} \qquad Farad = \frac{Amp^2 \cdot s^4}{kg \cdot m^2}$$

There is another system of units, called Gaussian system. It defines all units in terms of **3** (not 4) quantities：

$$\left\{ \begin{matrix} \text{length} & \text{mass} & \text{time} \\ \text{cm,} & \text{g,} & \text{second} \end{matrix} \right\}.$$

In Gaussian units, Maxwells egs. are

$$\nabla \times \vec{E}(\vec{r},t) = -\frac{1}{c}\frac{\partial \vec{B}(\vec{r},t)}{\partial t}$$

$$\nabla \times \vec{H}(\vec{r},t) = \frac{1}{c}\frac{\partial \vec{D}(\vec{r},t)}{\partial t} + \frac{4\pi}{c}\vec{J}(\vec{r},t)$$

$$\nabla \cdot \vec{B}(\vec{r},t) = 0$$

$$\nabla \cdot \vec{D}(\vec{r},t) = 4\pi\rho$$

In Gaussian units, the unit for charge is *esu* (electrostatic unit) = stat. coulomb = $\dfrac{cm^{3/2}\ g^{1/2}}{s}$

The relation between *SI* & Gaussian systems for charge is

$$q_{(SI)}\frac{1}{\sqrt{4\pi\varepsilon_0}}=q_{(Gaussian)}$$

or $$\frac{1}{\sqrt{4\pi\varepsilon_0}}coul=3\times10^{9}\,stat\ coul$$

or

$$\frac{1\,A\cdot S}{\sqrt{4\pi 18.85\times10^{-12}\,F/m}}=\frac{1\,A\cdot S}{\sqrt{1.112\times10^{-10}\,\frac{A^2S^4}{kg\cdot m^3}}}=\frac{1}{\sqrt{1.112\times10^{-10}\,\frac{S^2}{kg\cdot m^3}}}$$

$$=3\times10^{9}\,\frac{cm^{3/2}g^{1/2}}{s}$$

$$=3\times10^{9}\ \text{stat coul}\ .$$ #

The wave equation

Consider a "source-free" medium $(\rho = 0,\ J = 0)$, We can have wave eq. from eq (1) in page 2,

$$\nabla \times \nabla \times \vec{E}(\vec{r},t) = -\frac{\partial}{\partial t}\nabla \times \vec{B}(\vec{r},t)$$

use the identity

$$\nabla \times \nabla \times \vec{V} = \nabla(\nabla \cdot \vec{V}) - \nabla^2 \vec{V}$$

we have

$$\nabla(\nabla \cdot \vec{E}) - \nabla^2 \vec{E} = -\frac{\partial}{\partial t}\nabla \times \vec{B} \qquad (6)$$

Here we just assume the simple constitutive relation

$$\vec{B} = \mu \vec{H} \quad \& \quad \vec{D} = \varepsilon \vec{E} \qquad (7)$$

where $\mu \,\&\, E$ are scalar constants.

Since source-free $(\rho = 0)$

$$\nabla \cdot \vec{D} = 0 = \nabla \cdot (\varepsilon \vec{E})$$

$$= \vec{E} \cdot (\nabla \varepsilon) + \varepsilon \nabla \cdot \vec{E}$$

$$\downarrow$$

$$0 \quad \because \varepsilon \ is \ scalar$$

$$\Rightarrow \nabla \cdot \vec{E} = 0 \qquad (8)$$

Apply eq. (7) & (8) into eq. (6) , we get

$$-\nabla^2 \vec{E} = -\frac{\partial}{\partial t} \nabla \times (\mu \vec{H})$$

$$= -\mu \frac{\partial}{\partial t} (\frac{\partial \vec{D}}{\partial t})$$

$$= -\mu\varepsilon \frac{\partial^2 \vec{E}}{\partial t^2}$$

use eg. (2) in page 2 & source-free $\vec{J} = 0$

The wave eg. for electric field $\vec{\varepsilon}$ is

$$\nabla^2 \vec{E} - \mu\varepsilon \frac{\partial^2 \vec{E}}{\partial t^2} = 0 \tag{9}$$

in free space.

$$c = \frac{1}{\sqrt{\mu_0 \varepsilon_0}}$$

or $$\nabla^2 \vec{E} - \frac{1}{C^2} \frac{\partial^2 \vec{E}}{\partial t^2} = 0 \tag{10}$$

In an isotropic, source-free medium, a solution of eg (9) is a plane wave

$$\vec{E}(\vec{r}, t) = \vec{E}_0 e^{i(\vec{k} \cdot \vec{r} - wt)} \tag{11}$$

substituting eq (11) into (9), we have

$$(\nabla^2 + \omega^2 \mu\varepsilon)\vec{E}_0 e^{i\vec{k}\cdot\vec{r}} = 0$$

$$\Rightarrow (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} + \omega^2 \mu\varepsilon)\vec{E}_0 e^{i\vec{k}\cdot\vec{r}} = 0$$

$$\vec{k} = k_x \hat{x} + k_y \hat{y} + k_z \hat{z}$$

So we have the dispersion relation $\omega(\vec{k})$

$$(-k_x^{\ 2} - k_y^{\ 2} - k_z^{\ 2} + \omega^2 \mu\varepsilon) = 0$$

or

$$k_x^{\ 2} + k_y^{\ 2} + k_z^{\ 2} = k^2 = \omega^2 \mu\varepsilon$$

$$\Rightarrow \omega^2 = \frac{1}{\mu\varepsilon} k^2$$

for free space

$$\omega^2 = c^2 k^2, \quad c^2 = \frac{1}{\mu_0 \varepsilon_0} \qquad (12)$$

So we can replace $\vec{\nabla}$ by $i\vec{k}$ in Maxwell' eqs.

we have

$$\vec{k} \times \vec{E} = \omega\mu\vec{H} \qquad (13-1)$$

$$\vec{k} \times \vec{H} = -\omega\varepsilon\vec{E} \qquad (13-2)$$

$$\vec{k} \cdot \vec{E} = 0 \qquad (13-3)$$

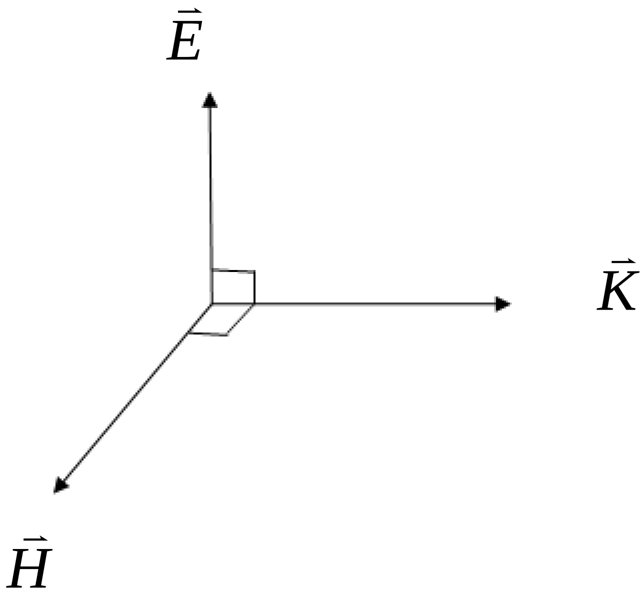
$$\vec{k} \cdot \vec{H} = 0 \qquad (13-4)$$

from eq. (13-1), we can have magnetic field

$$\frac{1}{\mu\omega}\vec{k}\times\vec{E}=\vec{H}$$

also we have $\vec{k}\cdot\vec{E}=0\ \&\ \vec{k}\cdot\vec{H}=0$

i.e. $\vec{E}\ \&\ \vec{H}$ are $\perp$ to $\vec{k}$



x x x

However, for most of cases, $\varepsilon\ \&\ \mu$ are not scalars.

They are space & frequency dependent.

$$\varepsilon=\varepsilon(\vec{r},\omega)$$
$$\mu=\mu(\vec{r},\omega)$$

Now, we assume

(1) ε is a pure real-valued function, and the freq.

dependence can be ignored i.e. $\varepsilon(\vec{r})$

$$\vec{D}(\vec{r},t) = \varepsilon(\vec{r})\vec{E}(\vec{r},t)$$

(2) Consider nonmagnetic materials only, i.e. $\mu(\vec{r})=1$

$$\Rightarrow \vec{B}(\vec{r},t) = \mu(\vec{r})\vec{H}(\vec{r},t) = \vec{H}(\vec{r},t)$$

then Maxwell's eqs become,

$$\nabla\times\vec{E}(\vec{r},t) = -\frac{\partial}{\partial t}\vec{H}(\vec{r},t) \qquad (14-1)$$

$$\nabla\times\vec{H}(\vec{r},t) = \varepsilon(\vec{r})\frac{\partial}{\partial t}\vec{E}(\vec{r},t) \qquad (14-2)$$

$$\nabla\cdot[\varepsilon(\vec{r})\vec{E}(\vec{r},t)] = 0 \qquad (14-3)$$

$$\nabla\cdot[\vec{H}(\vec{r},t)] = 0 \qquad (14-4)$$

Apply plane wave solutions into eq (14-1) & (14-2)

$$\vec{E}(\vec{r},t) = \vec{E}(\vec{r})e^{i\omega t}$$

$$\vec{H}(\vec{r},t) = \vec{H}(\vec{r})e^{i\omega t}$$

we have

$$\nabla\times\vec{E}(\vec{r}) + i\omega\vec{H}(\vec{r}) = 0$$

$$\nabla\times\vec{H}(\vec{r}) - i\omega\varepsilon(\vec{r})\vec{E}(\vec{r}) = 0$$

we can obtain the wave eg. for $\vec{H}(\vec{r})$

$$\nabla\times[\frac{1}{\varepsilon(\vec{r})}\nabla\times\vec{H}(\vec{r})] = \omega^2\vec{H}(\vec{r}) \qquad (15)$$

& use 2nd eq. to obtain $\vec{E}(\vec{r})$

$$\vec{E}(\vec{r}) = [\frac{-i}{\omega\varepsilon(\vec{r})}]\nabla \times \vec{H}(\vec{r}) \qquad (16)$$

we can write a eigenvalue eg, from eg. (15)

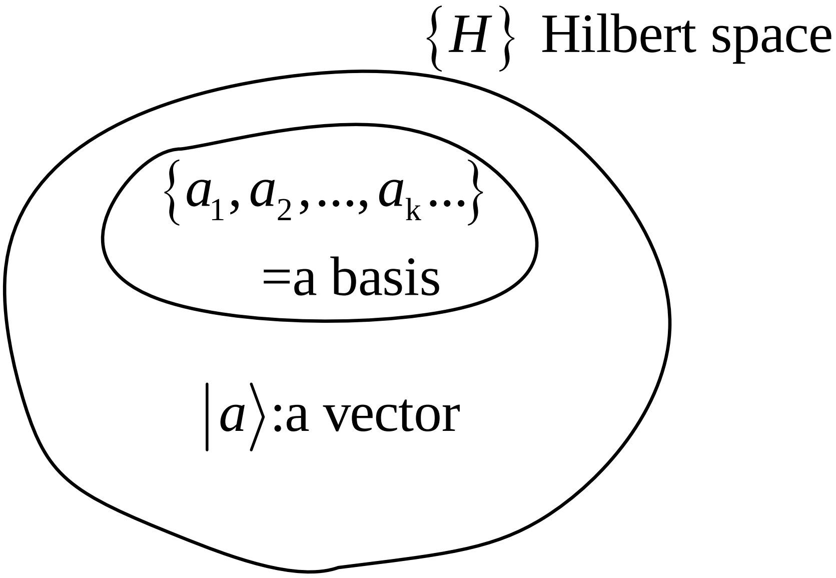
$$\hat{\Theta}\vec{H}(\vec{r}) = \omega^2 \vec{H}(\vec{r})$$

where

$$\hat{\Theta} \equiv \nabla \times (\frac{1}{\varepsilon(\vec{r})}\nabla \times)$$

$\hat{\Theta}$ is a linear differential operator, and $\vec{H}(\vec{r})$ are the eigenvectors associated to eigenvalues ω^2. Since $\hat{\Theta}$ is linear, any linear combination of solutions for $\vec{H}(\vec{r})$ is one of solutions of this eigenvalue eq.

Linear Vector Space and Linear Operators in Hilber Space



Now, let's consider the *EM* wave eqs. as an eigenvalue problem. The Maxwell curl eqs. for time-harmonic field in a source-free region are

$$\nabla \times \vec{E} = -i\omega\mu\vec{H}$$
$$\nabla \times \vec{H} = i\omega\varepsilon\vec{E}$$

Here assume μ is a scalar, but ε is $\varepsilon(r,\omega)$. From 2nd eq. , we can have

$$\nabla \times \frac{1}{\varepsilon(r)} \nabla \times \vec{H} - i\omega\nabla \times \vec{E} = 0$$

then use the first equation, we get

$$\nabla \times \frac{1}{\varepsilon(r)} \nabla \times \vec{H} = \omega^2 \mu \vec{H}$$

or $$\frac{1}{\mu} \nabla \times \frac{1}{\varepsilon(r)} \nabla \times \vec{H} = \omega^2 \vec{H}$$

this become an eigenvalue problem

$$\hat{\Theta} \times \vec{H} = \omega^2 \vec{H}$$

Where ω^2 is the eigenvalue and the differential operator $\hat{\Theta}$ is

$$\hat{\Theta} = \frac{1}{\mu} \nabla \times \frac{1}{\varepsilon(r)} \nabla \times$$

Also, the eigenvector, of course, is the $\vec{H}$ field. We also can write an eigenvalue eq. For $\vec{D}$,

$$\frac{1}{\mu} \nabla \times \nabla \times \frac{1}{\varepsilon(r)} \vec{D} = \omega^2 \vec{D}$$

or $$\hat{O}_D = \omega^2 \vec{D}$$

where the differential operator $\hat{O}_D = \frac{1}{\mu} \nabla \times \nabla \times \frac{1}{\varepsilon(r)}$

Note

These 2 operators are linear operators. Linear operators have the property that if *A* and *B* are eigenvectors of operator $\hat{O}$ with the same eigenvalue O^2

$$\hat{O}A = O^2 A \qquad \&$$

$$\hat{O}\; B = \;\overset{2}{O}$$

then $\alpha A + \alpha B$ is also an eigenvector of $\hat{O}$.

Before we examine $\hat{\Theta}$ & $\hat{O}_D$ for Hermitian operator, we should know something about Hermitian operators.

Hermitian operators are important in *Q.M.*, as well as in *EM* wave. Let’s consider the inner product

$$\langle g | f \rangle = \int_a^b \vec{g}^*(x)\vec{f}(x)dx$$

$$\& \ \langle g | f \rangle^* = \int_a^b \vec{g}\ (x) \cdot \vec{f}^*(x)dx = \langle f | g \rangle$$

For the system, we have an operator $\hat{O}$ & its adjoint operator $\hat{O}^+$, i.e.

$$\langle \hat{O}^+ g | f \rangle = \langle g | \hat{O} f \rangle$$

The operator $\hat{O}$ is Hermitian if

$$\hat{O} = \hat{O}^+$$

or $\left\langle \hat{O}\, g \middle| f \right\rangle = \left\langle g \middle| \hat{O} f \right\rangle$

An Hermitian (or self-adjoint) operator with appropriate boundary conditions have three nice properties.

(1) The eigenvalues of an Hermitian operator are real.

(2) The eigenfunctions of an Hermitian operator are orthogonal.

(3) The eigenfunctions of an Hermitian operator form a complete set.

We'll demonstrate first two properties.

(1) Consider a eigenvalue eq.

$$\hat{O}\left| f \right\rangle = \omega^2 \left| f \right\rangle$$

form the inner product with $\left\langle f \right|$

$$\left\langle f \middle| \hat{O} \middle| f \right\rangle = \omega^2 \left| f \right\rangle$$

If $\hat{O}$ is a Hermitian operator,

i.e. $\left\langle \hat{O}\, g \middle| f \right\rangle = \left\langle g \middle| \hat{O} \middle| f \right\rangle$

then we have

$$\left\langle f \middle| \hat{O} \middle| f \right\rangle^* = \left\langle \hat{O} f \middle| f \right\rangle = \left\langle f \middle| \hat{O} \middle| f \right\rangle$$

so $\left\langle f \middle| \hat{O} \middle| f \right\rangle$ is real. And $\left\langle f \middle| f \right\rangle$ is also real.

Since $\langle f|\hat{O}|f\rangle$ and $\langle f|f\rangle$ are both real, we have a real eigenvalue ω^2. It means eigenvalues of an Hermitian operator are real.

(2) Consider two eigenvectors of $\hat{O}$ with different eigenvalues:

$$\hat{O}|f_1\rangle = \omega_1^{\ 2}|f_1\rangle$$
$$\hat{O}|f_2\rangle = \omega_2^{\ 2}|f_2\rangle$$

where $\omega_1 \neq \omega_2$

we have

$$\omega_1^{\ 2}\langle f_2|f_1\rangle = \langle f_2|\hat{O}|f_1\rangle$$
$$= \left\langle \hat{O}f_2 \middle| f_1 \right\rangle \qquad \because \hat{O} \textit{ is Hermitian}$$
$$= \omega_2^{\ 2}\langle f_2|f_1\rangle$$

or $(\omega_1^{\ 2} - \omega_2^{\ 2})\langle f_2|f_1\rangle = 0$

$$\because \omega_1^{\ 2} \neq \omega_2^{\ 2} \Rightarrow \langle f_2|f_1\rangle = 0$$

i.e. $|f_1\rangle$ and $|f_2\rangle$ are orthogonal.

Now, we'll start to prove

$$\hat{\Theta} = \frac{1}{\mu}\nabla\times\frac{1}{\varepsilon(r)}\nabla\times$$

is a Hermitian operator for *EM* fields.

consider the field vectors $\vec{A}(r)$ and $\vec{B}(r)$, and we assume $\varepsilon(r)$ is real, i.e. lossless media.

$$\langle A|\hat{O}|B\rangle = \int d^3r\vec{A}^*(r)\cdot\frac{1}{\mu}\nabla\times\frac{1}{\varepsilon(r)}\nabla\times\vec{B}(r)$$

$$= \frac{1}{\mu}\int d^3r\vec{A}^*(r)\cdot\nabla\times\frac{1}{\varepsilon(r)}\nabla\times\vec{B}(r) \qquad \mu \text{ is a scalar}$$

Then we need the first Green's identity for this prove.

$$\int_V (\nabla\times\vec{P}\cdot\nabla\times\vec{Q} - \vec{P}\cdot\nabla\times\nabla\times\vec{Q})dV = \int_S (\vec{P}\times\nabla\times\vec{Q})\cdot\hat{n}da$$

or

$$\int_v \vec{P}\cdot\nabla\times\nabla\times\vec{Q}dV = \int_V \nabla\times\vec{P}\cdot\nabla\times\vec{Q}d\vec{V} - \int_S (\vec{P}\times\nabla\times\vec{Q})\cdot\hat{n}da$$

Since the fields are zero on a surface at infinity, we can ignore the surface integral. $\Rightarrow \int_S (\vec{P}\times\vec{V}\times\vec{Q})\cdot\hat{n}da = 0$

With the above identity, we can have

$$\langle A|\hat{O}|B\rangle = \frac{1}{\mu}\int d^3r\nabla\times\vec{A}^*(r)\cdot\frac{1}{\varepsilon(r)}\nabla\times\vec{B}(r) \quad \because \text{no differential op. on } \varepsilon(r)$$

$$= \frac{1}{\mu}\int d^3r\underbrace{\frac{1}{\varepsilon(r)}\nabla\times\vec{A}^*(r)}_{\vec{P}}\cdot\nabla\times\vec{B}(r)$$

Next, use the Green’s first identity again by letting.

$$\vec{P} = \frac{1}{\varepsilon(r)} \nabla \times \vec{A}^*, \quad \nabla \times \vec{Q} = \vec{B}$$

then we get

$$\left\langle A \middle| \hat{O} \middle| B \right\rangle = \frac{1}{\mu} \int d^3 r \, \nabla \times \frac{1}{\varepsilon(r)^*} \nabla \times \vec{A}^*(r) \cdot \vec{B}(r)$$

$$= \left\langle \hat{O} A \middle| B \right\rangle$$

$[\varepsilon(r) \textit{ is real}, \varepsilon(r) = \varepsilon^*(r)]$

so

$$\hat{O} = \frac{1}{\mu} \nabla \times \frac{1}{\varepsilon(r)} \nabla \times$$ is a hermitian operator.

Also, we can prove

$$\hat{O}_D = \frac{1}{\mu} \nabla \times \nabla \times \frac{1}{\varepsilon(r)}$$

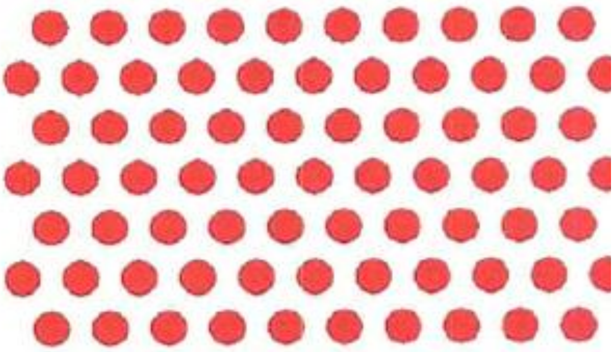
is not hermitian.

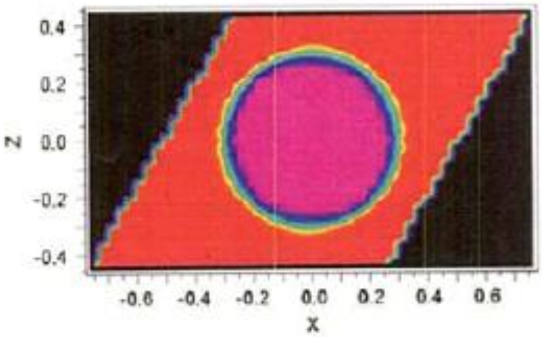
Photonic Crystal Latiice Bandstructure

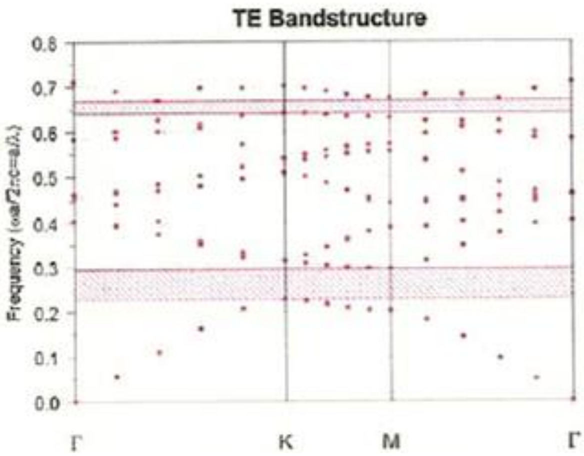
r/a=0.3

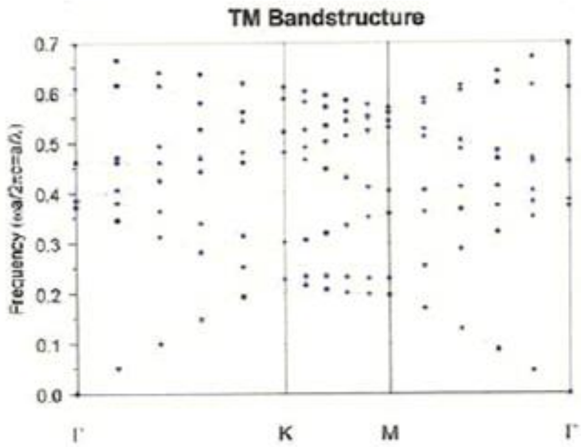
Red region index=1.0

Background index=3.14



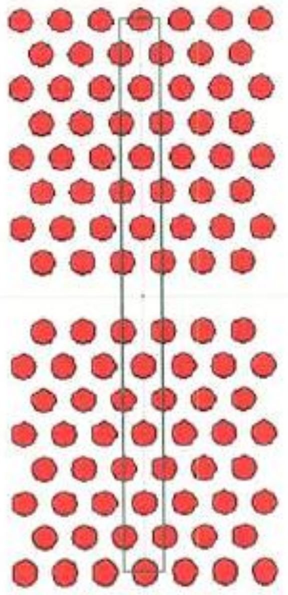




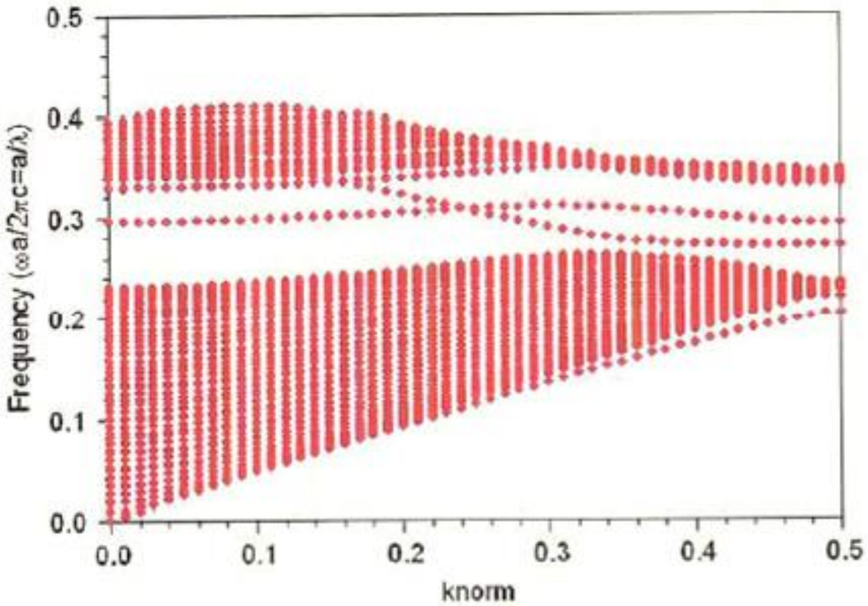


*Calculated by 劉育辰 (NTHU)

Photonic Crystal Waveguide Bandstructure



r/a=0.3
紅色區index = 1
白色區index = 2.5~3.4



*Calculated by 張子倉 (NTHU)

Plane-Wave Expansion Method for Photonic Crystal Band Structure

For photonic band structure, we need to solve the eigenvalue problem

$$\hat{\Theta}\vec{H}_{\vec{k}}(\vec{r}) = \omega^2 \vec{H}_{\vec{k}}(\vec{r}), \quad \hat{\Theta} = \frac{1}{\mu}\nabla\times\frac{1}{\varepsilon(\vec{r})}\nabla\times \quad \text{or}$$

(1) $$\frac{1}{\mu}\nabla\times\frac{1}{\varepsilon(\vec{r})}\nabla\times\vec{H}_{\vec{k}}(\vec{r}) = \omega^2\vec{H}_{\vec{k}}(\vec{r})$$

where $\vec{H}_{\vec{k}}(\vec{r})$ is a Bloch state

(2) $$\vec{\mathrm{H}}_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{-i\vec{k}\cdot\vec{r}} \vec{u}_{\vec{k}}(\vec{r})$$

Ω is the volume of the crystal included here for normalization. The orthogonality relations for Bloch states are

(3) $$\int \vec{H}^*_{n',\vec{k}'}(\vec{r})\mu(\vec{r})\cdot\vec{H}_{n,\vec{k}}(\vec{r})d^3r = \delta_{n,n'}\delta_{\vec{k},\vec{k}'} \quad \&$$

(4) $$\int \vec{E}^*_{n',\vec{k}'}(\vec{r})\varepsilon(\vec{r})\cdot\vec{E}_{n,\vec{k}}(\vec{r})d^3r = \delta_{n,n'}\delta_{\vec{k},\vec{k}'}$$

where *n* is band label.

Let plug equation (2) into equation (1), we have

$$(5)\quad \frac{1}{\mu}\nabla\times\frac{1}{\varepsilon(\vec{r})}\nabla\times e^{-i\vec{k}\cdot\vec{r}}u_{\vec{k}}(\vec{r}) = \omega^2 e^{-i\vec{k}\cdot\vec{r}}\vec{u}_{\vec{k}}(\vec{r})$$

In equation (5) ,

$$\nabla\times e^{-i\vec{k}\cdot\vec{r}}u_{\vec{k}}(\vec{r}) = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ e^{-\vec{k}\cdot\vec{r}}u_x & e^{-\vec{k}\cdot\vec{r}}u_y & e^{-\vec{k}\cdot\vec{r}}u_z \end{vmatrix}$$

$$= \hat{x}(\frac{\partial}{\partial y}e^{-i\vec{k}\cdot\vec{r}}u_z - \frac{\partial}{\partial z}e^{-i\vec{k}\cdot\vec{r}}u_y) - \hat{y}(\frac{\partial}{\partial x}e^{-i\vec{k}\cdot\vec{r}}u_z - \frac{\partial}{\partial z}e^{-i\vec{k}\cdot\vec{r}}u_x)$$

$$+ \hat{z}(\frac{\partial}{\partial x}e^{-i\vec{k}\cdot\vec{r}}u_y - \frac{\partial}{\partial y}e^{-i\vec{k}\cdot\vec{r}}u_x)$$

$$= \hat{x}\left\{-ik_y e^{-i\vec{k}\cdot\vec{r}}u_z + e^{-i\vec{k}\cdot\vec{r}}\frac{\partial u_z}{\partial y} - (-ik_z)e^{-i\vec{k}\cdot\vec{r}}u_y - e^{-i\vec{k}\cdot\vec{r}}\frac{\partial u_y}{\partial z}\right\}$$

$$- \hat{y}\left\{-ik_x e^{-i\vec{k}\cdot\vec{r}}u_z + e^{-i\vec{k}\cdot\vec{r}}\frac{\partial u_z}{\partial x} - (-ik_y)e^{-i\vec{k}\cdot\vec{r}}u_x - e^{-i\vec{k}\cdot\vec{r}}\frac{\partial u_x}{\partial z}\right\}$$

$$+ \hat{z}\left\{-ik_x e^{-i\vec{k}\cdot\vec{r}}u_y + e^{-i\vec{k}\cdot\vec{r}}\frac{\partial u_y}{\partial x} - (-ik_z)e^{-i\vec{k}\cdot\vec{r}}u_x - e^{-i\vec{k}\cdot\vec{r}}\frac{\partial u_x}{\partial y}\right\}$$

$$= e^{-i\vec{k}\cdot\vec{r}}(-i\vec{k} + \nabla)\times\vec{u}_{\vec{k}}(\vec{r})$$

Similarly, we can replace the next ∇ by $-i\vec{k} + \nabla$. So we have the eigenvalue equation

$$(6)\quad e^{-i\vec{k}\cdot\vec{r}}\,\frac{1}{\mu}(-i\vec{k}+\nabla)\times\frac{1}{\varepsilon(r)}(-i\vec{k}+\nabla)\times\vec{u}_{\vec{k}}(\vec{r})=\omega^2 e^{-i\vec{k}\cdot\vec{r}}\,\vec{u}_{\vec{k}}(\vec{r})$$

or

$$(7)\quad \underbrace{\frac{1}{\mu}(-i\vec{k}+\nabla)\times\frac{1}{\varepsilon(r)}(-i\vec{k}+\nabla)\times}_{\hat{O}\,\vec{u}_{\vec{k}}(\vec{r})}\vec{u}_{\vec{k}}(\vec{r})=\omega^2\vec{u}_{\vec{k}}(\vec{r})\,.$$

here $\vec{k}$ can be consider as a parameters, and $\vec{u}_{\vec{k}}(r)$ follow the condition

$$\vec{u}_{\vec{k}}(r)=\vec{u}_{\vec{k}}(\vec{r}+\vec{R})$$

The Hermitian operator $\hat{O}$ with the periodic boundary condition has a complete set of eigenvectors, $u_{\vec{k}}(\vec{r})$. The spectrum contains an infinite set of discrete eigenvalues for each $\vec{k}$. We label this infinite set of modes by the band index, *n*. The Bloch modes form a complete set for each $\vec{k}$.

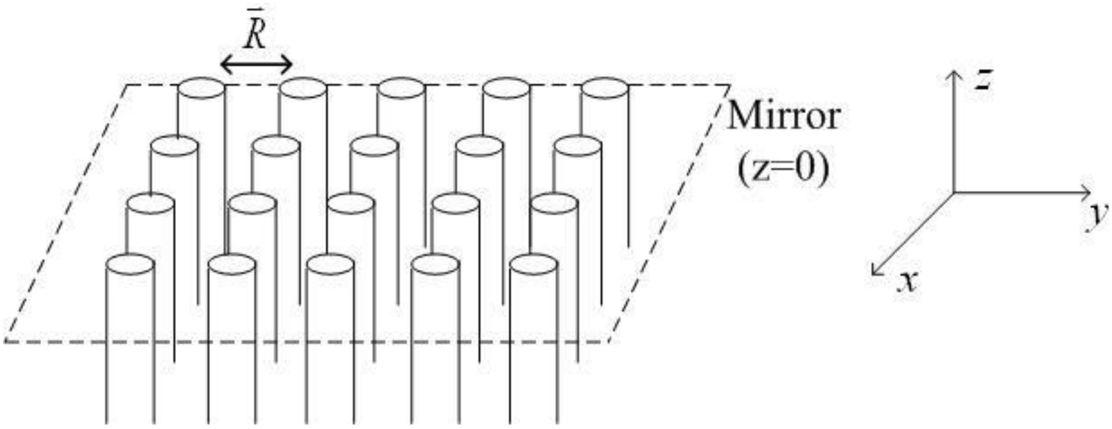
There are couple things we should note before we start to solve this eigenvalue problem. Solving the problem for photonic crystal band structure is quite similar to finding electronic band structure for solid. However, there are couple differences.

(1)EM wave in Maxwells' equations are vectors while electron waves in Schrödinger's equations are scalar.

(2)Pauli exclusion principle doesn't apply to photonic band structure since photons are spin-one particles. (Note: electrons are spin-half particles)

(3)Solving Maxwells' equations for a single EM wave can lead to exact results since photon-photon interaction are negligible. But solving single-electron Schrödinger equations can't be exact solution since electron-electron interactions are significant.

Now let's consider a two-dimensional photonic crystal lattice, for example, an array of dielectric rods with the infinite height in $\hat{z}$ -axis.



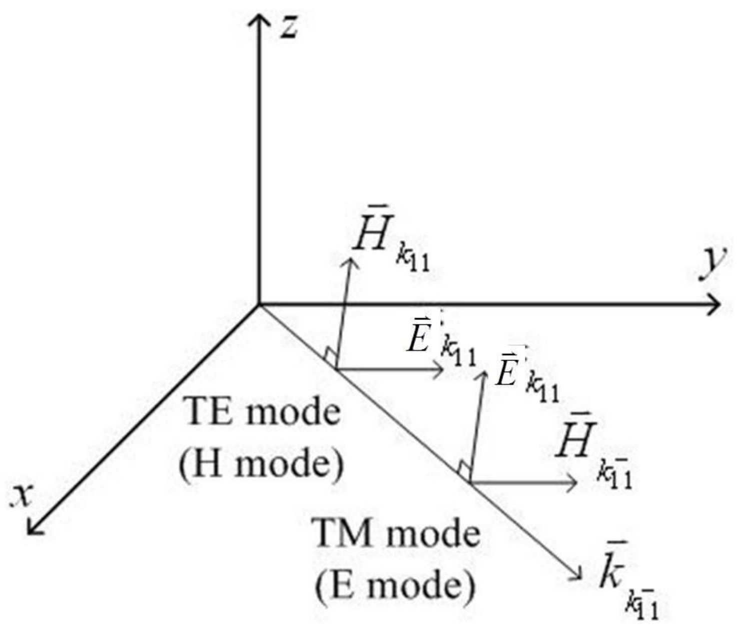
For this system, we have EM fields components $\{E_x, E_y, E_z, H_x, H_y, H_z\}$. We can group them into 2 parities. An "even" parity mode is a mode which has an $\vec{E}$ field invariant under mirror reflection in x-y plane, namely $\vec{E}$ and the vector plane-wave involved are polarized within x-y plane. Its parity is even, because a vector in the x-y plane is invariant by the mirror in the x-y plane. The $\vec{H}$ field is directed in the $\hat{z}$ direction, perpendicularly to the $\vec{E}$ field. This is called transverse electric (TE) mode.

The "odd"-parity mode has $\vec{E}$ field in the $\hat{z}$ -direction. In this case the mirror reflection turns a $\hat{z}$ -directed polarization vector to a $\hat{z}$ -directed vector. This is the transverse magnetic (TM) mode. Very often the TE and TM modes are called $\vec{H}$ mode and $\vec{E}$ mode, respectively.

In summary,

TE has $\{E_x, E_y, H_z\}$; TM has $\{H_x, H_y, E_z\}$.

For three-dimensional lattice, this separation is not possible, and modes cannot be classified as either TE or TM.



So we can solve the scalar field H_z for TE polarization and the scalar E_z field for TM polarization.

Let's start with TE modes. The solution of the form

(8) $$\vec{H}(x,y,z,t) = H_z(x,y)e^{i\varpi t}\hat{z}$$

(9) $$\vec{E}(x,y,z,t) = e^{i\omega t}\left\{E_x(x,y)\hat{x} + E_y(x,y)\hat{y}\right\}$$

The Maxwell's curl equations

(10) $$\nabla \times \vec{E} = -i\omega\mu\vec{H}$$

(11) $$\nabla \times \vec{H} = i\omega\varepsilon\vec{E}$$

Plug-in equation (8) & (9) into equation (10) & (11), we have

(12) $$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = -i\omega\mu\vec{H}_Z$$

(13) $$\frac{\partial H_z}{\partial y} = -i\omega\varepsilon E_x$$

(14) $$-\frac{\partial H_z}{\partial x} = i\omega\varepsilon E_y$$

Now use equation (13) & (14) to eliminate E_x and E_y from equation (12), i.e.

$$E_x = \frac{1}{i\omega\varepsilon}\frac{\partial H_z}{\partial y}$$

&

(15) $$\frac{\partial E_x}{\partial y} = \frac{1}{i\omega}\frac{\partial}{\partial y}\left(\frac{1}{\varepsilon}\frac{\partial H_z}{\partial y}\right)$$

Similarly

$$E_y = \frac{-1}{iw\varepsilon}\frac{\partial H_z}{\partial x}$$

&

(16) $$\frac{\partial E_y}{\partial x} = -\frac{1}{iw}\frac{\partial}{\partial x}(\frac{1}{\varepsilon}\frac{\partial H_z}{\partial x})$$

equation (15) & (16) $\rightarrow$ equation (12), we get

$$-\frac{1}{i\omega}\frac{\partial}{\partial x}(\frac{1}{\varepsilon}\frac{\partial H_z}{\partial x}) - \frac{1}{i\omega}\frac{\partial}{\partial y}(\frac{1}{\varepsilon}\frac{\partial H_z}{\partial y}) = -i\omega\mu H_z$$

or (17) $$\frac{\partial}{\partial x}(\frac{1}{\varepsilon}\frac{\partial H_z}{\partial x}) + \frac{\partial}{\partial y}(\frac{1}{\varepsilon}\frac{\partial H_z}{\partial y}) + \omega^2 \mu H_z = 0$$

Now we expand $\frac{1}{\varepsilon}$ and H_z

(18) $$\frac{1}{\varepsilon(x,y)} = \sum_{\vec{G}'} \kappa(\vec{G}')e^{-i\vec{G}\cdot\vec{\rho}}$$

(19) $$H_z = \frac{1}{\sqrt{\Omega}}\sum_{\vec{G}} C_k(\vec{G})e^{-i(\vec{k}+\vec{G})\cdot\vec{\rho}}$$

where Ω : sample volume for normalization

$\vec{\rho}$: in-plane position vector

$\vec{G},\vec{G}'$: reciprocal lattice vectors

Now plug equation (18) & (19) into equation (17), we have

$$\frac{1}{\sqrt{\Omega}}\sum_{\vec{G}}\sum_{\vec{G}'}\frac{\partial}{\partial x}\left[\kappa(\vec{G}')e^{-i\vec{G}'\cdot\vec{\rho}}C(\vec{G})(-i)(k_x+G_x)e^{-i(\vec{k}+\vec{G})\cdot\vec{\rho}}\right]$$
$$+\frac{1}{\sqrt{\Omega}}\sum_{\vec{G}}\sum_{\vec{G}'}\frac{\partial}{\partial y}\left[\kappa(\vec{G}')e^{-i\vec{G}'\cdot\vec{\rho}}C(\vec{G})(-i)(k_y+G_y)e^{-i(\vec{k}+\vec{G})\cdot\vec{\rho}}\right]$$
$$+\frac{1}{\sqrt{\Omega}}\sum_{\vec{G}}C(\vec{G})\omega^2\mu e^{-i(\vec{k}+\vec{G})\cdot\vec{\rho}}=0$$

$$\Rightarrow\frac{1}{\sqrt{\Omega}}\sum_{\vec{G}}\sum_{\vec{G}'}\kappa(\vec{G}')C(\vec{G})(-i)(G_x+G_x'+k_x)(-i)(k_x+G_x)e^{-i(\vec{G}+\vec{G}'+\vec{k})\cdot\vec{\rho}}$$
$$+\frac{1}{\sqrt{\Omega}}\sum_{\vec{G}}\sum_{\vec{G}'}\kappa(\vec{G}')C(\vec{G})(-i)(G_y+G_y'+k_y)(-i)(k_y+G_y)e^{-i(\vec{G}+\vec{G}'+\vec{k})\cdot\vec{\rho}}$$
$$+\frac{1}{\sqrt{\Omega}}\sum_{\vec{G}}C(\vec{G})\omega^2\mu e^{-i(\vec{k}+\vec{G})\cdot\vec{\rho}}=0$$

The first two line can be added, we have

$$-\frac{1}{\sqrt{\Omega}}\sum_{\vec{G}}\sum_{\vec{G}'}\kappa(\vec{G}')C(\vec{G})(\vec{k}+\vec{G})(\vec{G}+\vec{G}'+\vec{k})e^{-i(\vec{G}+\vec{G}'+\vec{k})\cdot\vec{\rho}}$$
$$+\frac{1}{\sqrt{\Omega}}\sum_{\vec{G}}C(\vec{G})\omega^2\mu e^{-i(\vec{k}+\vec{G})\cdot\vec{\rho}}=0$$

We multiply $\frac{1}{\sqrt{\Omega}}e^{i(\vec{G}''+\vec{k})\cdot\vec{\rho}}$ and integrate over the crystal volume Ω,

(20)

$$-\frac{1}{\Omega}\sum_{\vec{G}}\sum_{\vec{G}'}\kappa(\vec{G}')C(\vec{G})(\vec{k}+\vec{G})(\vec{G}+\vec{G}'+\vec{k})\int_{\Omega}d\rho e^{-i(\vec{G}+\vec{G}'+\vec{k}-\vec{G}''-\vec{k})\cdot\vec{\rho}}$$
$$+\frac{1}{\sqrt{\Omega}}\sum_{\vec{G}}\omega^{2}\mu C(\vec{G})\int_{\Omega}d\rho e^{-i(\vec{G}+\vec{k}-\vec{G}''-\vec{k})\cdot\vec{\rho}}$$

and we have the relation

(21) $$\frac{1}{\Omega}\int_{\Omega}d\rho e^{i\vec{k}\cdot\rho}=\delta_{\vec{k},0}$$

Plug equation (21) into equation (20), we have

$$-\sum_{\vec{G}}\sum_{\vec{G}'}\kappa(\vec{G}')C(G)(\vec{G}+\vec{K})\cdot(\vec{G}+\vec{G}'+\vec{K})\delta_{\vec{G},\vec{G}''-\vec{G}'}$$
$$+\sum_{G}w^{2}\mu C(\vec{G})\delta_{\vec{G},\vec{G}''}=0$$
$$\Rightarrow-\sum_{\vec{G}''-\vec{G}}\kappa(\vec{G}')C(\vec{G}''-\vec{G})(\vec{G}''-\vec{G}'+\vec{k})\cdot(\vec{G}''+\vec{k})+w^{2}\mu C(\vec{G}'')=0$$

Let $\vec{G}_1=\vec{G}''-\vec{G}' \Leftrightarrow \vec{G}'=\vec{G}''-\vec{G}_1$

Then we have an equations for the coefficients $C(\vec{G}'')$.

(22) $$\sum_{\vec{G}_1}\kappa(\vec{G}''-\vec{G}_1)C(\vec{G}_1)(\vec{G}_1+\vec{k})\cdot(\vec{G}''+\vec{k})=\omega^{2}\mu C(\vec{G}'')$$

This is the matrix form of the eigenvalue problem for TE modes.

Note the matrix is symmetric $(a_{ij}=a_{ji})$.

The TM modes work similarly. The fields for TM are

(23) $\vec{E}(x,y,z,t) = E_z(x,y)e^{i\omega t}\hat{z}$

$$\vec{H}(x,y,z,t) = e^{i\varpi t}(H_x(x,y)\hat{x} + H_y(x,y)\hat{y})$$

Plug equation (23) into curl equation of Maxwell's equations,

we can have

(24) $\frac{1}{\varepsilon(x,y)}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2})E_z + \omega^2 \mu E_z = 0$

and expanding E_z

(25) $E_z = \frac{1}{\sqrt{\Omega}} \sum_{\vec{G}} B(\vec{G}) e^{i(\vec{k}+\vec{G})\cdot\vec{\rho}}$.

Then we'll have a matrix form of eigenvalue problem for TM

modes.

(26) $\sum_{\vec{G}'} \kappa(\vec{G} - \vec{G}')(\vec{k} + \vec{G}')^2 B(\vec{G}') = \omega^2 \mu B(\vec{G})$

However, the matrix in equation (26) is not symmetric.

Now let $C(\vec{G}) = \left|\vec{k} + \vec{G}\right| \vec{B}(\vec{G})$.

We get

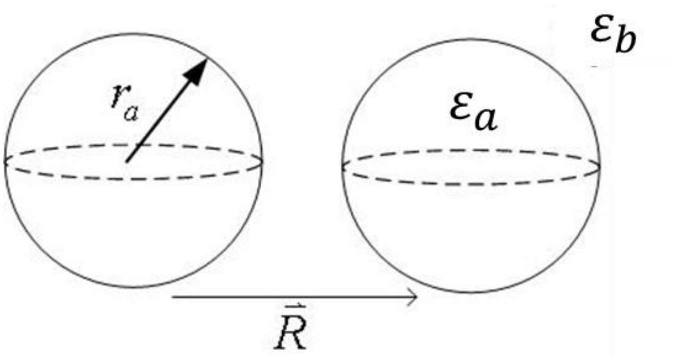
$$\sum_{\vec{G}'} \kappa(\vec{G} - \vec{G}')\left|\vec{k} + \vec{G}'\right|^2 \frac{C(\vec{G}')}{\left|\vec{k} + \vec{G}'\right|} = \omega^2 \mu \frac{C(\vec{G})}{\left|\vec{k} + \vec{G}\right|} \quad \Rightarrow$$

(27) $$\sum_{\vec{G}'} \kappa(\vec{G}-\vec{G}')\left|\vec{k}+\vec{G}'\right|\left|\vec{k}+\vec{G}\right| C(\vec{G}') = \omega^2 \mu C(\vec{G})$$

This is an eigenvalue problem for a symmetric matrix. There are several things we should note. ①This numerical method, plane-wave expansion (PWE) method, which is based on the Fourier expansion of the EM waves and the dielectric functions. ②In the real numerical calculation of photonic bands, the $\sum$ in equation (22) & (26) is calculated up to a sufficiently large number *N* of $\vec{G}_1(\text{or } \vec{G}_1')$, and an eigenvalue problem for each *k* is solved, which is equivalent to the diagonalization of the matrix defined by the left-hand side of equation (22) & (26). ③The dimension of the matrix that should be 3*N*. However it could be 2*N* since $\vec{\mathrm{H}}(x,y,z,t)$ is perpendicular to $\vec{k}+\vec{G}$ with polarization, and its degree of freedom is two. Hence, the matrix in the equation has the dimension of $3N \times 3N$, generally. In fact, the converge of the plane-wave expansion method is not good when the variation of dielectric constant is large, and numerical error exceeds 5% in certain cases even *N* >3000.

Now, we start to calculate the Fourier coefficients, $\kappa(\vec{G})$, of $\dfrac{1}{\varepsilon(x,y)}$

Case 1 Dielectric Sphere



Consider a dielectric sphere array with lattice vector $\vec{R}$. The radius of sphere is r_a, and the dielectric constants inside and outside the sphere are ε_a & ε_b, respectively.

We can write down the dielectric function

(28) $$\frac{1}{\varepsilon(\vec{r})} = \frac{1}{\varepsilon_b} + (\frac{1}{\varepsilon_a} - \frac{1}{\varepsilon_b})S(\vec{r})$$

where $S(\vec{r})$ is defined such that

(29) $$S(\vec{r}) = \begin{cases} 1\ , & |\vec{r}| \le r_a \\ 0\ , & |\vec{r}| > r_a \end{cases}$$

Then the Fourier coefficients are

(30) $\kappa(\vec{G}) = \dfrac{1}{V_c}\int_V d\vec{\rho} e^{i\vec{G}\cdot\vec{\rho}} \dfrac{1}{\varepsilon(\vec{\rho})}$ V_c : volume of unit cell

Equation (28) & (29) $\rightarrow$ equation (30), we have

(31) $\kappa(\vec{G}) = \dfrac{1}{\varepsilon_b}\delta_{\vec{G},0} + \dfrac{1}{V_C}(\dfrac{1}{\varepsilon_a} - \dfrac{1}{\varepsilon_b})\int_V d\vec{\rho}\, S(\vec{\rho})\, e^{-i\vec{G}\cdot\vec{\rho}}$

In order to calculate equation (31), we use spherical coordinates (r,θ,ϕ), and assume the direction of $\vec{G}$ is $\theta = 0$.

For $\vec{G} \neq 0$, the integral in equation (31) is

$$\int_V d\vec{\rho} S(\vec{\rho}) e^{-i\vec{G}\cdot\vec{\rho}}$$

$$= 2\pi \int_0^{r_a} dr \int_0^{\pi} d\theta\, r^2 \sin\theta e^{-iGr\cos\theta}$$

$$= \frac{4\pi}{G^3}\left[\sin(Gr_a) - Gr_a\cos(Gr_a)\right] \quad , G = \left|\vec{G}\right|$$

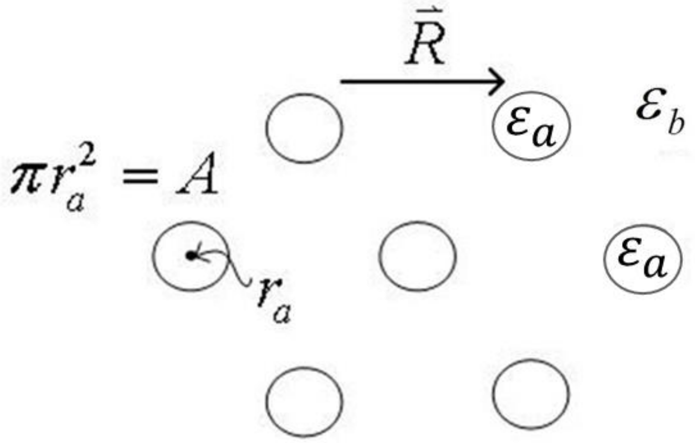
For $\vec{G}$=0 , the integral became $\int_V d\vec{\rho} S(\vec{\rho}) e^{-i\vec{G}\cdot\vec{\rho}}$

$$= \int_V dr\ S(r) = \frac{4\pi}{3} r_a^{\ 3} = V_a$$

So we have the Fourier coefficients for the dielectric spheres.

$$
(32)\quad \kappa(\vec{G}) = \begin{cases} \dfrac{1}{\varepsilon_b} + \left(\dfrac{1}{\varepsilon_a} - \dfrac{1}{\varepsilon_b}\right)\dfrac{V_a}{V_c} & ,for\ \vec{G} = 0 \\ 3\left(\dfrac{1}{\varepsilon_a} - \dfrac{1}{\varepsilon_b}\right)\dfrac{V_a}{V_c}\left[\dfrac{\sin(Gr_a)}{(Gr_a)^3} - \dfrac{\cos(Gr_a)}{(Gr_a)^2}\right] & ,for\ \vec{G} \neq 0 \end{cases}
$$

Case 2 Dielectric Rods (or Holes)



Consider a 2-D dielectric rods (or holes) array in x-y plane, and they are infinite along z axis. The dielectric function can be described as

$$\frac{1}{\varepsilon(x,y)} = \frac{1}{\varepsilon_b} + \left(\frac{1}{\varepsilon_a} - \frac{1}{\varepsilon_b}\right)\sum_{\vec{R}} S(\vec{\rho} - \vec{R}) \qquad (33)$$

Where $S(\vec{\rho}) = \begin{Bmatrix} 1 & ,\rho \in A \\ 0 & ,\rho \notin A \end{Bmatrix}$

The Fourier coefficients are

$$\kappa(\vec{G}) = \frac{1}{a_c}\int_a d\vec{\rho} e^{i\vec{G}\cdot\vec{\rho}} \frac{1}{\varepsilon(\vec{\rho})}$$
$$= \frac{1}{\varepsilon_b}\delta_{\vec{G},0} + \left(\frac{1}{\varepsilon_a} - \frac{1}{\varepsilon_b}\right)\frac{1}{a_c}\int_a d\vec{\rho} e^{i\vec{G}\cdot\vec{\rho}} s(\vec{\rho})$$

For $\vec{G}=0$

(34) $$\kappa(\vec{G})=\frac{1}{\varepsilon_b}+(\frac{1}{\varepsilon_a}-\frac{1}{\varepsilon_b})\frac{1}{a_c}\int_a d\vec{\rho}S(\vec{\rho})$$

$$=\frac{1}{\varepsilon_b}+(\frac{1}{\varepsilon_a}-\frac{1}{\varepsilon_b})\frac{A}{a_c}$$

$d\vec{\rho}S(\rho)=A$

A: *the cross section of the rods or holes*

For $\vec{G}\neq 0$, we need to evaluate the integral

(35) $$\frac{1}{a_c}\int_A d\vec{\rho}e^{i\vec{G}\vec{\rho}}=\frac{1}{a_c}\int_0^R rdr\int_0^{2\pi} d\varphi e^{iGr\cos\varphi}$$

,where φ is the angle between G and r.

Using the integral representation for $J_o(x)$

(36) $$J_o(x)=\frac{1}{2\pi}\int_0^{2\pi} e^{ix\cos\theta}d\theta$$

Compare equation (35) and (36), we get the integral

(37) $$\frac{2\pi}{a_c}\int_0^{r_a} rdrJ_0(Gr)$$

Then we can use the relation of Bessel functions

(38) $$\frac{d}{dx}\left[x^n J_n(x)\right]=x^n J_{n-1}(x)$$

we have

(39) $$\int dx x^n J_{n-1}(x)=x^n J_n(x)$$

Let $x = Gr$, $dx = Gdr$ or $dr = \frac{dx}{G}$.

Equation (37) became

$$\frac{2\pi}{a_c}\int_0^{Gr_a}\frac{xdx}{G^2}J_o(x) = \frac{2\pi}{a_c G^2}\times J_1(x)\Big|_0^{Gr_a}$$

$$= \frac{2\pi}{a_c G^{2}} G r_a J_1(Gr_a)$$

$$= \frac{2A}{a_c}\frac{J_1(Gr_a)}{Gr_a}$$

,where $A = \pi r_a^2$

So we obtain the Fourier coefficients

$$\kappa(\vec{G}) = \begin{cases} \frac{1}{\varepsilon_b} + (\frac{1}{\varepsilon_a} - \frac{1}{\varepsilon_b})\frac{A}{a_c} & ,for\ \vec{G} = 0 \\ (\frac{1}{\varepsilon_a} - \frac{1}{\varepsilon_b})\frac{A}{a_c}\frac{2J_1(Gr_a)}{Gr_a} & ,for\ \vec{G} \neq 0 \end{cases}$$

, where r_a is the radius of the rods or holes,

and J_1 is a Bessel function.

Now given a particular lattice, the $\vec{G}$ vector can be determined and the eigenvalues can be calculated.

The Irreducible Brillouin Zone

Photonic crystals usually have translation invariance and symmetries in the structures simultaneously. It means a photonic crystal might be invariant under periodic translation, mirror reflection or rotation with specific angles.

Now we consider a rotation symmetry for the photonic crystals. Let $\hat{R}(\hat{n},\alpha)$ be an operator which rotates the vector by an angle α about the $\hat{n}$ axis. The vector field operator $\hat{O}_R$ is defined as

$$\hat{O}_R \vec{H}(\vec{r}) = \hat{R}(\hat{n},\alpha)\vec{H}(\tilde{R}^{-1}(\hat{n},\alpha)\vec{r})$$

($\because$ To rotate a vector field, we rotate the vector by $\tilde{R}$ and the argument by $\tilde{R}^{-1}$)

If a rotation by $\tilde{R}$ leaves the crystal invariant, then

$$[\hat{\Theta},\hat{O}_R] = 0$$

where

$$\hat{\Theta} = \frac{1}{\mu}\nabla\times\frac{1}{\varepsilon(\vec{r})}\nabla\times$$

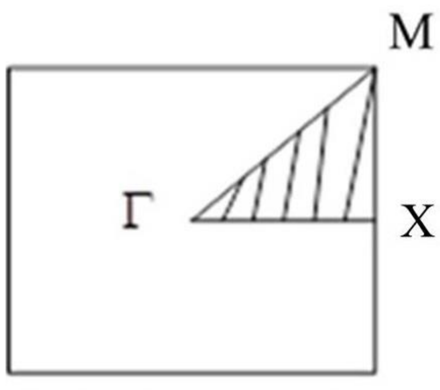
so

$$\hat{\Theta}(\hat{O}_R\vec{H}_{n\vec{k}}) = \hat{O}_R(\hat{\Theta}\vec{H}_{n\vec{k}})$$
$$= \omega^2 \hat{O}_R \vec{H}_{n\vec{k}}$$

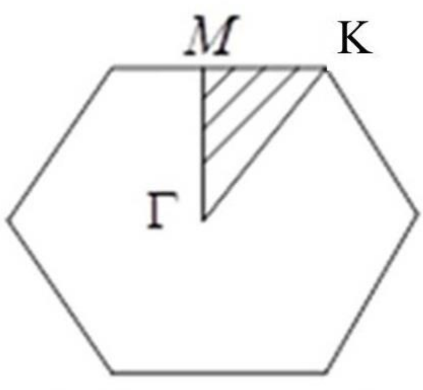
It means $\hat{O}_R\vec{H}_{n\vec{k}}$ is an eigenstate of $\hat{\Theta}$ with the same eigenvalue as $\vec{H}_{n\vec{k}}$. It can also be shown that $\hat{O}_R\vec{H}_{n\vec{k}}$ is just the Bloch state with wave vector $\tilde{R}\vec{k}$. Then we have

$$\omega_n(\tilde{R}\vec{k}) = \omega_n(\vec{k})$$

The dispersion relation $\omega_n(\vec{k})$ has the full symmetry of the crystal. Therefore, we don't need to consider the entire Brillouin zone, because different portions are related with others through symmetry. The smallest region of the Brillouin zone for $\omega_n(\vec{k})$ is called irreducible *BZ*. This *BZ* is not related by symmetry.



Brillouin zone for a square lattice with the irreducible zone shaded.



Brillouin zone for a triangular lattice with the irreducible zone shaded.

Two-Dimensional Photonic Crystals

After discussing the properties of *1-D* photonic crystals, we'll start to talk about *2-D* photonic crystals. In this part, we are going to study the "*2-D*" crystals which are periodic in 2 directions ("usually" x-y plane) and homogeneous in the third direction ("usually" $\hat{z}$ direction).

In *1-D* system, we consider the modes with the Bloch form, say $\vec{H}$ field

(1) $H_{n\vec{k}}(\vec{r}) \sim e^{-i\vec{k}\cdot\vec{r}} u_{n\vec{k}}(z) \sim e^{-i\vec{k}_{//}\cdot\vec{\rho}} e^{-ik_z z} u_{n\vec{k}}(z)$

if the layer structure is along $\hat{z}$ axis. Now, for *2-D* system, the Bloch state will be

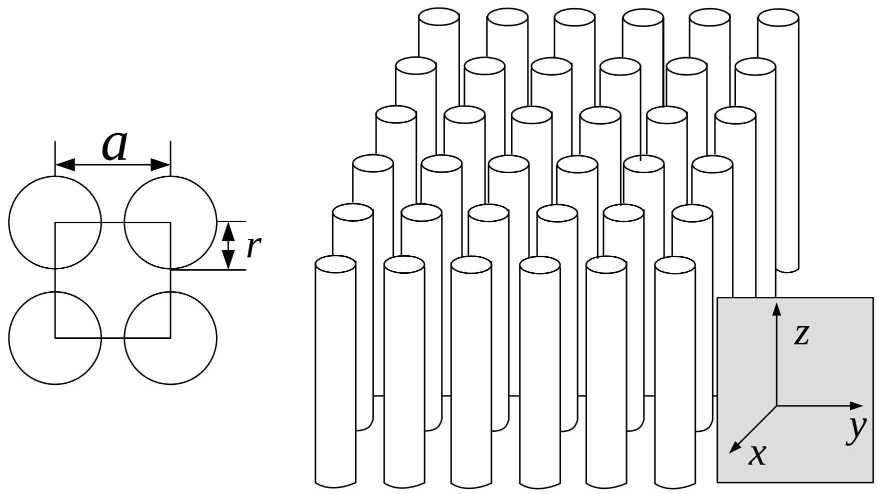
(2) $H_{n\vec{k}}(\vec{r}) \sim e^{-i\vec{k}\cdot\vec{r}} u_{n\vec{k}}(x,y) \sim e^{-ik_z z} e^{-i\vec{k}_{//}\cdot\vec{\rho}} u_{n\vec{k}}(\rho)$

if the *2-D* photonic crystals are in x-y plane. Like *1-D* case, here $u_{n\vec{k}}$ is a periodic function,

$u_{n\vec{k}}(\vec{\rho}) = u_{n\vec{k}}(\vec{\rho}+\vec{R})$ for all lattice vector $\vec{R}$.

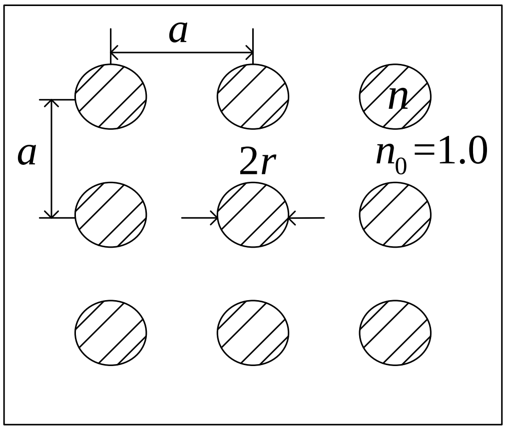
The main difference between equation (1) & equation (2) is that in *2-D* case, $\vec{k}_{//}$ is restricted to the *BZ* in x-y plane and k_z is un-restricted. However, in *1-D* case, k_z is restricted to *BZ* along $\hat{z}$ axis, and $\vec{k}_{//}$ is not.

Here is a example of *2-D* photonic crystals. It contains a square lattice of dielectric rods with a radians of *r* and a dielectric constant of ε . The background is air ($\varepsilon_0 = 1$). The dielectric rods are periodic in x-y plane with lattice constant *a*, and infinite along $\hat{z}$ direction.

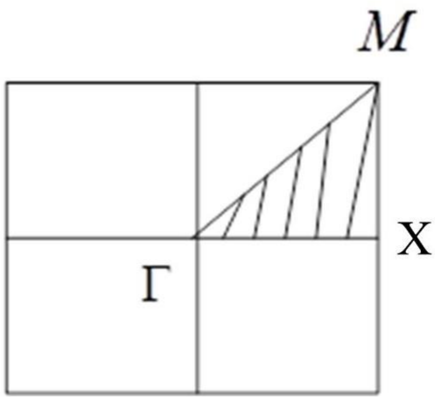


Conventionally, we choose x-y plane as the symmetry plane. Then the system is invariant under reflections through this symmetry plane. Like we discuss in page 40-44, we can classify 6 components of $\vec{E}$ and $\vec{H}$ fields and group them into 2 polarizations. The transverse-electric (TE) modes have $\{H_z, E_x, E_y\}$. The transverse-magnetic TM modes have $\{E_z, H_x, H_y\}$. The band structure for TE and TM modes can be completely different. And the band gap night not appear in both polarizations. It means that there are band gaps for TE mode, but no band gap for TM mode in some cases.

Let's consider in *2-D* photonic crystals with the rectangular dielectric rod array. The lattices have a lattice constant of *a* and the rod radius of *r*. The refractive indices of the rods and background are *n* and 1, respectively. Here is the illustration of the *2-D* photonic crystal lattices.

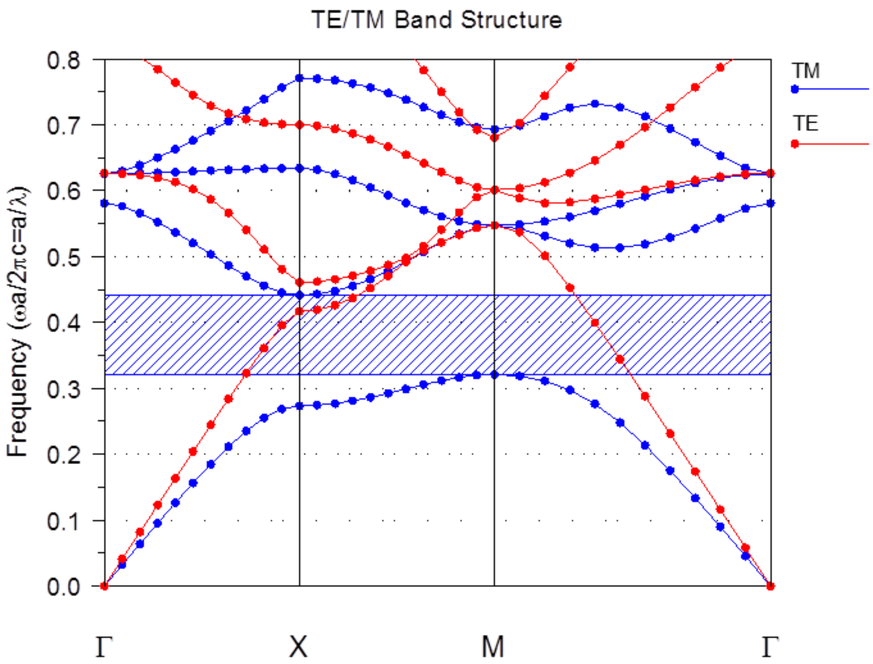


The 3 important parameters, $\{n, a, r\}$, are going to decide the properties of this structure. The irreducible Brillouin zone of the rectangular lattice is shown below



The irreducible *BZ* is the shaded region. The whole square is the first *BZ*, and the rest of first *BZ* can be related to the irreducible *BZ* by rotational symmetry. The three symmetry points Γ , X , and M correspond to $\beta(k_{//}) = 0$, $\beta = \frac{\pi}{a}\hat{x}$ and $\beta = \frac{\pi}{a}\hat{x} + \frac{\pi}{a}\hat{y}$, respectively.

With plane-wave expansion, we can calculate the band structure $\omega(\beta)$ for the *2-D* photonic crystals. The band structure shown here is for n=3.0 and r/a=0.2 . The red bands are *TE* while the blue are *TM* modes.

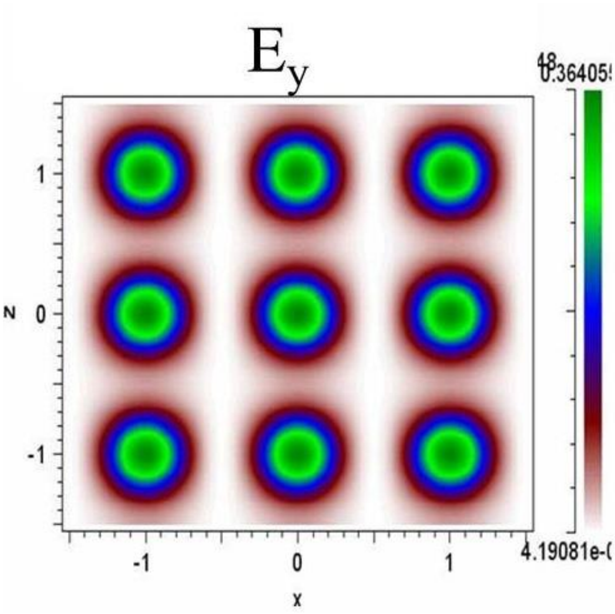


In the band diagram, the horizontal axis is the in-plane wave vector β and Γ, M and X points are the symmetry points in the irreducible *BZ*. The band structure is plotted (or calculated) along. The edge of the irreducible zone, then it returns to Γ point to form a close loop. The vertical axis is the normalized frequency which is the modal frequency normalized to $\frac{a}{\lambda}$ (or $\frac{\omega a}{2\pi c}$). Here *a* &*c* are the lattice constant of lattices and the speed of light.

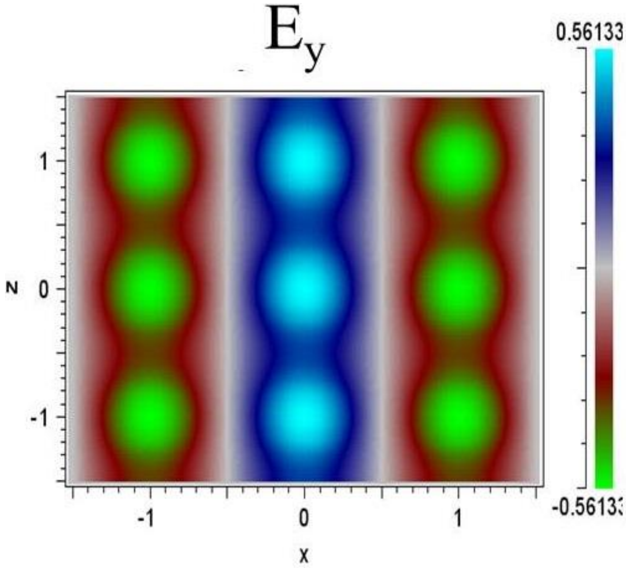
According to this band diagram, there is a band gap from normalized frequency 0.32 to 0.44 for *TM* mode, while there is no band gap for *TE* mode.

Now we are going to take a look for EM field profiles at several symmetry points.

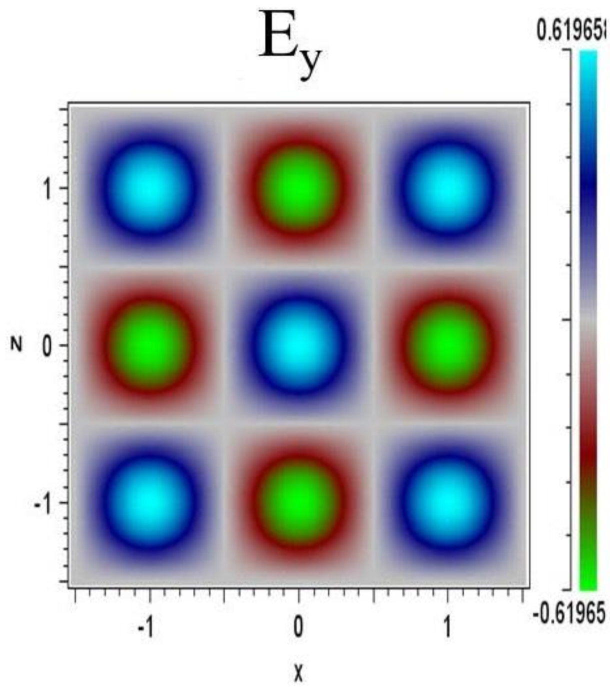
The first figure in the next page is the E field profile at Γ point of the irreducible *BZ* of this rectangular photonic lattices. Since $\beta(\Gamma)=0$, the fields have no in-plane wave vector to propagate in-plane. It means the wave vector of this mode is along $\hat{z}$ axis of the structure, and the fields are the same in each unit cell. The second figure is the E field profile at *x* point of the zone edge. The mode has an in-plane wave vector along $\hat{x}$ direction, i.e. $\beta(x)=\frac{\pi}{a}\hat{x}$. The third profile is the E field profile at *M* point. This mode has a in-plane wave vector along $\hat{x}+\hat{y}$ direction, i.e. $\beta(M)=\frac{\pi}{a}\hat{x}+\frac{\pi}{a}\hat{y}$.



Γ point

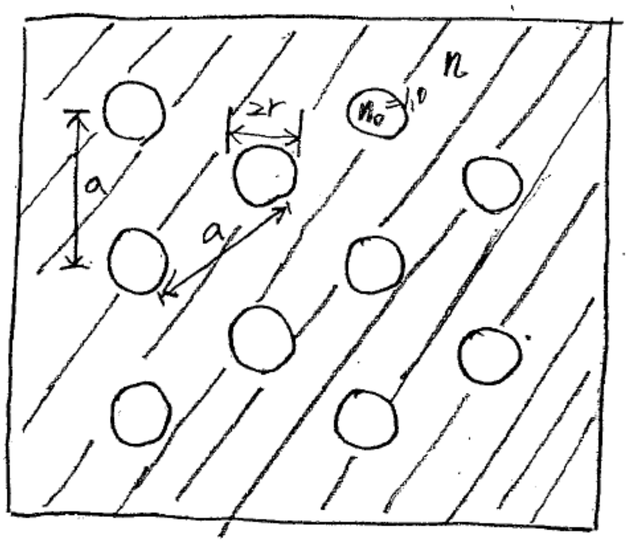


X point

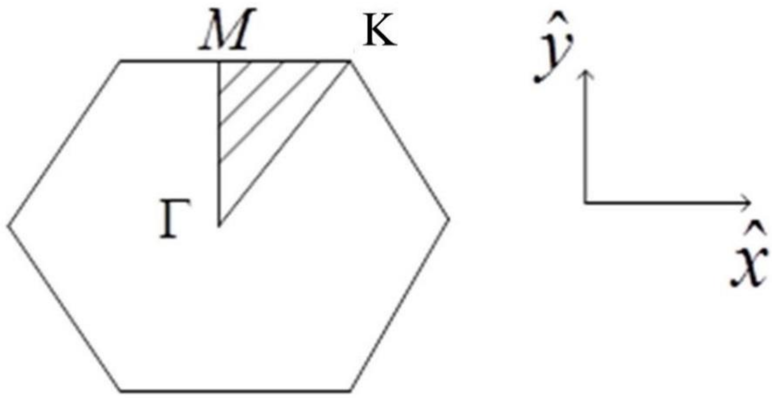


M point

Now, let’s consider a triangular lattices with the embedded air holes surround by the dielectric materials.

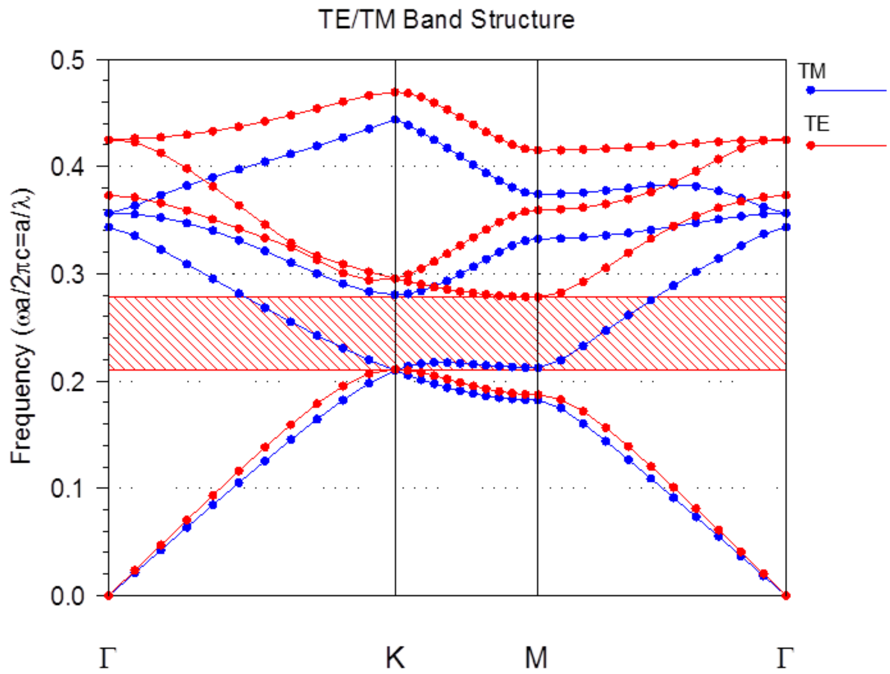


The lattice constant and hole radius are *a* and *r*. And the refractive index of the material is n. The irreducible *BZ* embedded in the first *BZ* is shown below.



The shaded region is the irreducible *BZ*, and three symmetry points Γ, *M* and K are $\beta = 0$, $\beta = \frac{\pi}{a}\hat{y}$ and $\beta = \frac{\pi}{\sqrt{3}a}\hat{x} + \frac{\pi}{a}\hat{y}$.

The band diagram of the triangular lattices with the background index *n*=3.4 and the r/a value 0.3 is shown below.



The red lines are the bands for *TE* mode, and the blue lines are for *TM* mode. In this band diagram, the *TE* mode has a band gap from normalized frequency 0.21 to 0.28 . However, there is no band gap for *TM* mode. If we consider a photonic crystal with a lattice constant of 500 nm, the TE band gap region will allocate at wavelength $\lambda = 1785\ \text{nm} \sim 2380\ \text{nm}$.