2018

TIGP: Advanced Nanotechnology (A)

Part 1: Photonic Crystals and Devices

Lecture #2

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Comparison of Quantum Mechanics and Electridynamics

Table 1 Extended comparison between quantum mechanics in a periodic potential and electromagnetism in a periodic dielectric.

	QUANTUM MECHANICS IN A PERIODIC POTENTIAL (CRYSTAL)	**ELECTROMAGNETISM IN A PERIODIC DIELECTRIC (PHOTONIC CRYSTAL)**
What is the "main function" that contains all of the information?	The scalar wave function $\Psi(\bar{r},t)$.	The magnetic vector field $H(\bar{r},t)$.
How do we separate out the time dependence of the function (into normal modes)?	$\Psi(\bar{r},t)=\sum_E C_E \Psi_E(\bar{r})e^{i\bar{E}t/h}$ Expand in a set of energy eigenstates $\Psi_E(r)$	$\overline{H}(\bar{r},t)=\sum_\omega C_\omega \overline{H}_\omega(\bar{r})e^{i\omega t}$ Expand in a set of harmonic modes $H_\omega(r)$.
What is the "master equation "that determines the normal modes of the system?	$\left(\frac{p^2}{2m}+V(\bar{r})\right)\Psi_E(\bar{r})=E\Psi_E(\bar{r})$ The Schrödinger equation.	$\nabla\times\frac{1}{\varepsilon(\bar{r})}\nabla\times\overline{H}_\omega(\bar{r})=\frac{\omega^2}{c^2}H_\omega(\bar{r})$ The Maxwell equations.
Are there any other conditions on the main function?	Yes, it must be normalizable.	Yes, the field must be both normalizable and transverse: $\nabla\cdot H=0$
Where does the periodicity	The potential:	The dielectric: $\varepsilon(\bar{r})=\varepsilon(\bar{r}+\overline{R})$,

	QUANTUM MECHANICS IN A PERIODIC POTENTIAL (CRYSTAL)	**ELECTROMAGNETISM IN A PERIODIC DIELECTRIC (PHOTONIC CRYSTAL)**
of the system enter?	$V(\bar{r}) = V(\bar{r} + \bar{R})$, for all lattice vectors R.	for all lattice vectors R.
Is there any interaction between normal modes?	Yes, there is an electron-electron repulsive interaction that* makes large-scale computation difficult.	In the linear regime, light modes can pass right through one another undisturbed, and can be calculated independently.
What important properties do the normal modes have in common?	Eigenstates with different energies are orthogonal, they have real eigenvalues, and can be found with a variational principle.	Modes with different frequencies are orthogonal, they have real positive eigenvalues, and can be found with a variational principle.
On what fact about the master equation do the important properties rely?	The Hamiltonian *H* is a linear, Hermitian operator.	The Maxwell operator Θ is a linear, Hermitian operator.
What is the variational theorem we use to determine the normal modes and frequencies?	$E_{\text{var}} = \dfrac{\langle \Psi \mid H \mid \Psi \rangle}{\langle \Psi \mid \Psi \rangle}$ E_{var} is minimized when Ψ is an eigenstate of H*(Hamiltonian)*.	$E_{\text{var}} = \dfrac{\langle \bar{H}, \bar{\Theta}\bar{H} \rangle}{\langle \bar{H}, \bar{H} \rangle}$ E_{var} is minimized when $\bar{H}$*(Field)* is a normal mode of Θ.
What is the heuristic that goes along with the	The wave function concentrates in regions of low potential, while remaining orthogonal to	The fields concentrate their electrical energy in high-ε regions, while remaining orthogonal to lower modes.

	QUANTUM MECHANICS IN A PERIODIC POTENTIAL (CRYSTAL)	**ELECTROMAGNETISM IN A PERIODIC DIELECTRIC (PHOTONIC CRYSTAL)**
variational theorem?	lower states.	
What is the physical energy of the system?	The eigenvalue E of the Hamiltonian.	$E = \left(\frac{1}{8\pi}\right)\int d\bar{r}\left(\frac{1}{\varepsilon}\left\|\overline{D}\right\|^2 + \left\|\overline{H}\right\|^2\right)$ The electromagnetic energy.
Is there a natural length scale to the system?	Usually, because constants such as the Bohr radius set the length scale.	No, solutions are scalable to any length scale.
What is the mathematical statement that says: "A is a symmetry of the system"?	A commutes with the Hamiltonian: $[A,\ H] = 0$.	A commutes with the Maxwell operator: $[A,\ \Theta] = 0$.
How do we classify the normal modes using a system's symmetries?	Distinguish them by how they transform under a symmetry operation A.	Distinguish them by how they transform under a symmetry operation A.
What does the discrete translational symmetry of a crystal allow us to do?	$\Psi_k(\bar{r}) = u_k(\bar{r})e^{i\bar{k}\cdot r}$ Write the wave function in Bloch form.	$\overline{H}_k(\bar{r}) = \bar{u}_k(\bar{r})e^{i\bar{k}\cdot r}$ Write the harmonic modes in Bloch form.
What are the allowable values for the wave v vector k?	They lie in the Brillouin zone in reciprocal space.	They lie in the Brillouin zone in reciprocal space.
What do we mean by the term "band	The functions $E_n(\bar{k})$, which tell us the energies	The functions $\omega_n(\bar{k})$, which tell us the frequencies of the

	QUANTUM MECHANICS IN A PERIODIC POTENTIAL (CRYSTAL)	**ELECTROMAGNETISM IN A PERIODIC DIELECTRIC (PHOTONIC CRYSTAL)**
structure"?	of the allowed eigenstates.	allowed harmonic modes.
What is the physical origin of the band structure?	The electron wave scatters coherently from the different potential regions.	The electromagnetic fields scatter coherently at the interfaces between different dielectric regions.
What happens inside a gap in the band structure?	No propagating electrons in that energy range are allowed to exist, regardless of wave vector.	No extended modes in that frequency range are allowed to exist, regardless of wave vector.
What do we call the bands immediately above and below the gap?	The band above the gap is the *conduction band*; the band below the gap is the *valence band.*	The band above the gap is the *air band*; the band below the gap is the *dielectric band.*
How do we introduce defects into the system?	By adding foreign atoms to the crystal, which breaks the translational symmetry of the atomic potential.	By changing the dielectric constant of certain regions, which breaks the translational symmetry of $\varepsilon(\bar{r})$.
What is the result of introducing a defect?	It might create an allowed state in a band gap, thereby permitting a localized electron state around the defect.	It might create an allowed state in a band gap, thereby permitting a localized mode around the defect.
How do we classify different types of defects?	Donor atoms pull states from the conduction band into the gap; acceptor atoms pull states from the valence	Dielectric defects pull states from the air band into the gap; air defects pull states from the dielectric band into the gap.

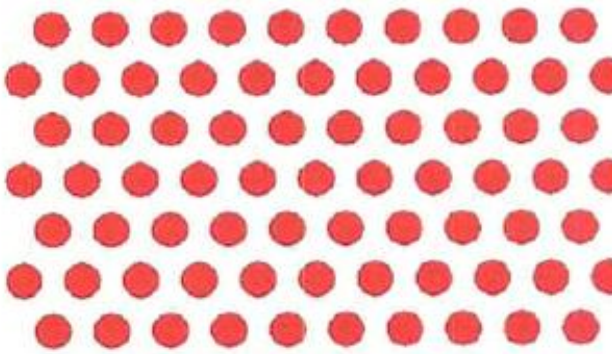
	QUANTUM MECHANICS IN A PERIODIC POTENTIAL (CRYSTAL)	**ELECTROMAGNETISM IN A PERIODIC DIELECTRIC (PHOTONIC CRYSTAL)**
	band into the gap.	
In short, why is the study of the physics of the system important?	We can tailor the electronic properties of materials to our needs.	We can tailor the optical properties of materials to our needs.

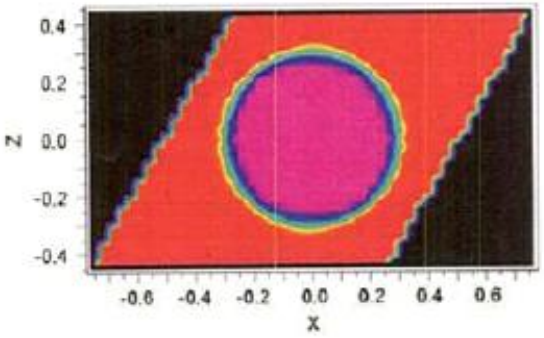
Photonic Crystal Latiice Bandstructure

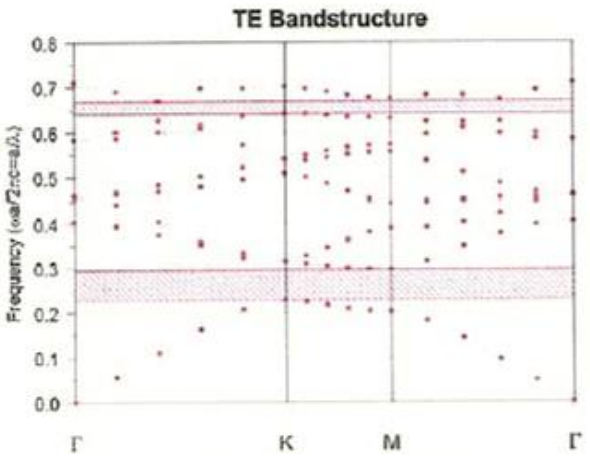
r/a=0.3

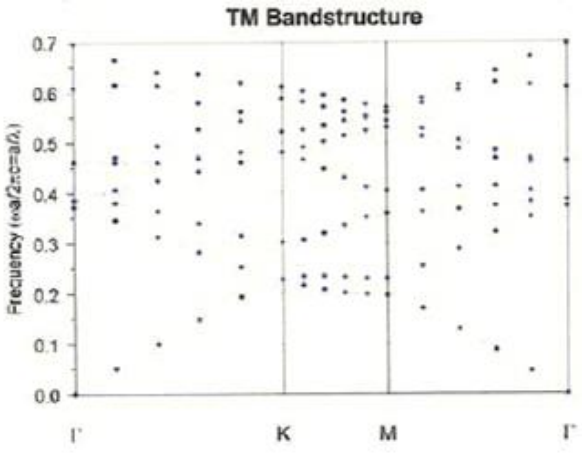
Red region index=1.0

Background index=3.14



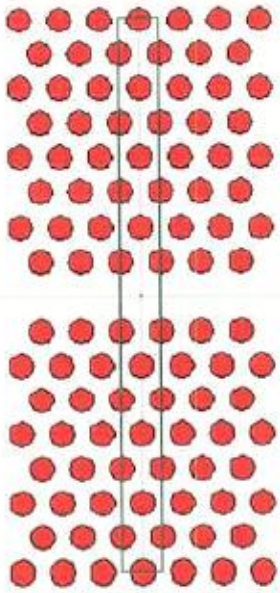




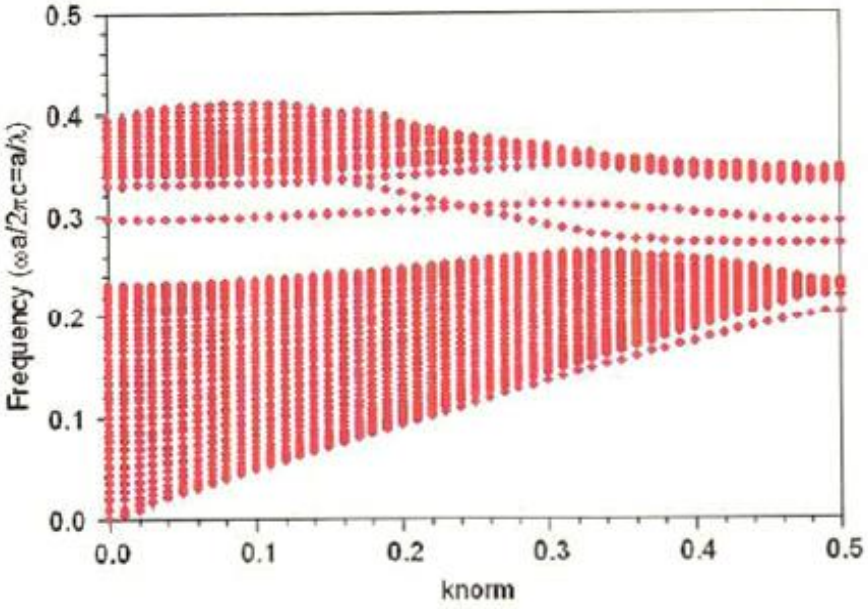


*Calculated by 劉育辰 (NTHU)

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)

We had discussed the band structure for *2-D* photonic crystals. Two popular types of lattices, rectangular & triangular lattices, had been shown in the previous notes.

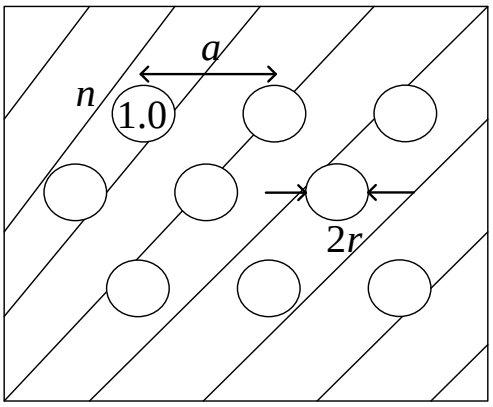
For most of application with photonic crystals, the band gap in the band structure is one of the most important parameters. A lot of applications use the "optical" properties inside or around the photonic band gap, so photonic crystal is one type of photonic band gap materials (PBG) with the control of the band gap characteristics. We can engineer the optical properties of the optical/photonic devices. It's quite similar to the band gap of semiconductor electric material. People can engineer "electronic" properties by controlling the band gap of Si, GaAs or others.

2-D photonic crystals band gap can be decided by the lattice geometry and the parameters $\{n, a, r\}$. Now we are going to discuss how those parameters take some effect for the band gap.

1) "*r/a*" value of photonic crystal holes or rods

Without changing the material or the lattice type, we can

just vary the hole (or rod) radius *r* to modify the band gap frequency (or wave length) and width. Let's consider a *2-D* triangular lattice with air holes embedded in the dielectric material again.



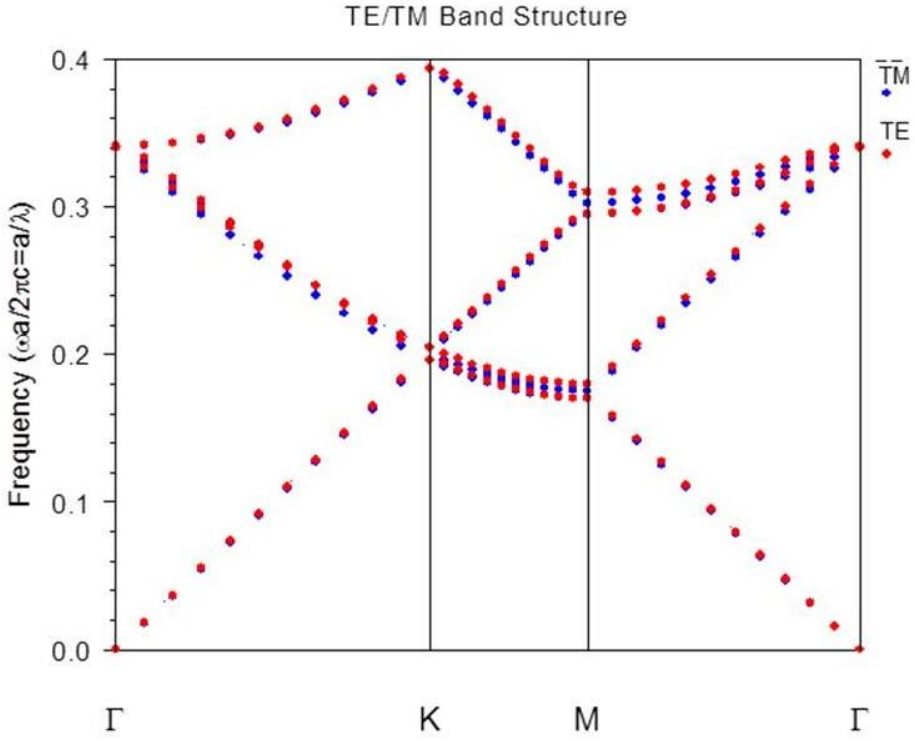
Now we use *n=3.4* and vary *r/a* value of air holes. The band diagram of photonic lattices with the different "*r/a*" values are shown below.

We have the band structure of TE and TM modes with the "*r/a*" values. Apparently, the bands shift to higher frequency as the *r/a* value increases. However, the shifts might be different because of the different polarizations. i.e. $TE \neq TM$. The band gap, which is shaded in the band diagrams, is not always existed for all *r/a* values. In this example, the *TE* band gap start to show up when the *r/a* value is large than 0.18. The band gap is around

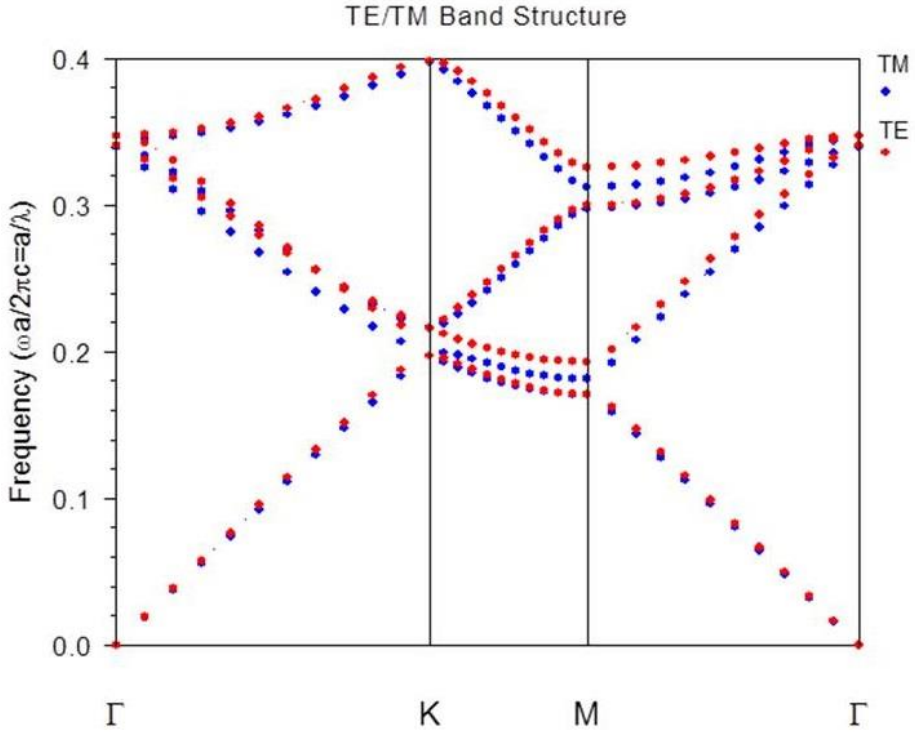
normalized frequency 0.2. We can plot the photonic band gap position versus the *r/a* value which is shown in the page 86. The higher curve is the frequency position of the top boundary of the band gap, while the lower curve is frequency of bottom boundary of the band gap. The region surrounded by the two curves is the band gap region with varied *r/a* values. This band gap region goes to higher frequency area when *r/a* value increase. The width of the photonic band gap, which is the difference between two curves in top-left figure is plotted in the bottom figure. The band gap width increases as *r/a* value increase, and it reaches the maximum 0.18 normalized frequency at *r/a* value 0.42.

After the maximum point, the gap width start to decrease as *r/a* value increases. For this case, we had realized

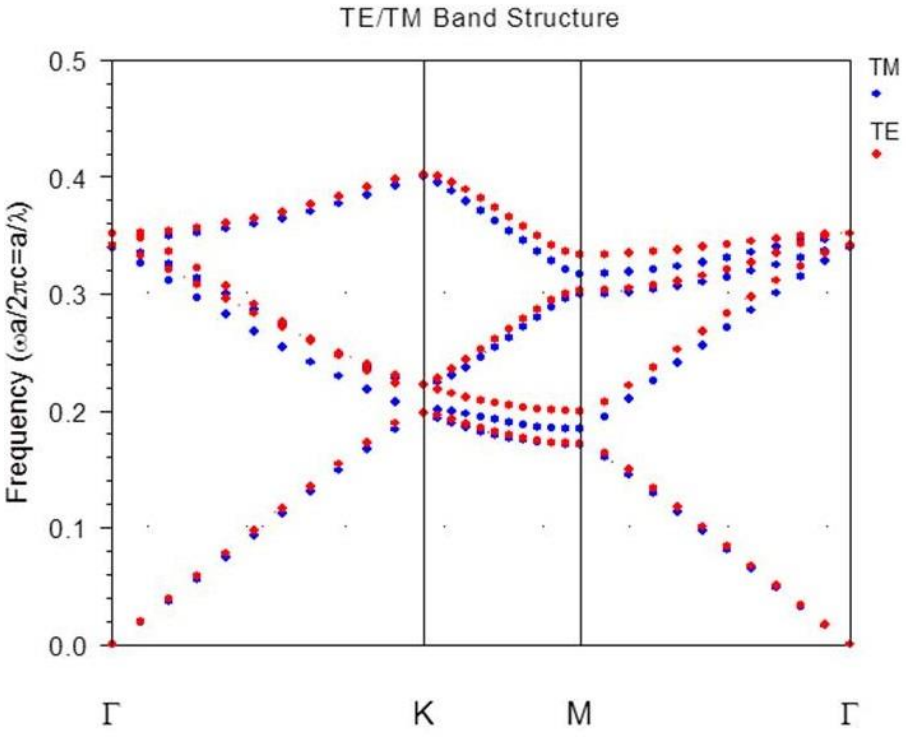
(1) The photonic band gap can be shifted by varying *r/a* value. It means that the device operated wave length can be controlled by the r/a value of photonic lattices.


TE/TM Band Structure
Frequency (ωa/2πc=a/λ)
0.4
0.3
0.2
0.1
0.0
TM
TE
Γ
K
M
Γ

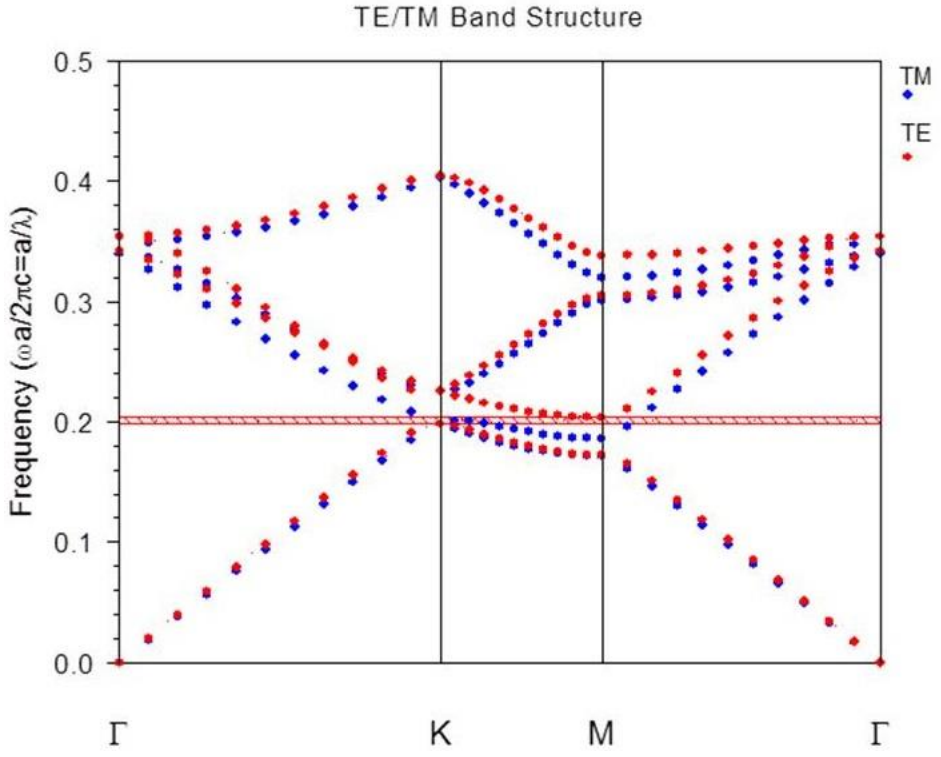
r/a=0.1


TE/TM Band Structure
Frequency (ωa/2πc=a/λ)
0.4
0.3
0.2
0.1
0.0
TM
TE
Γ
K
M
Γ

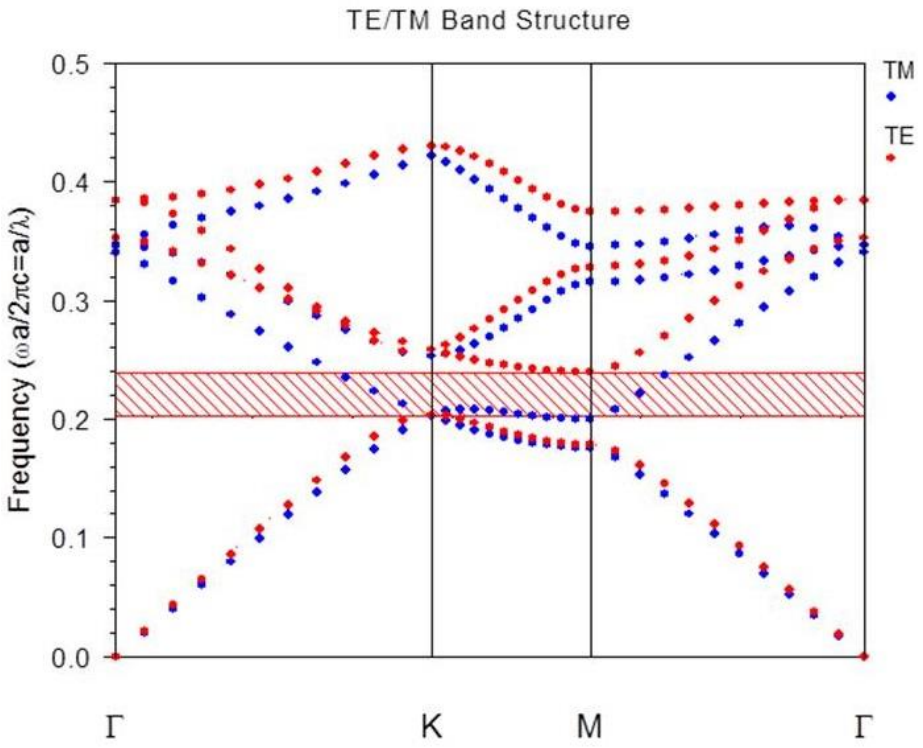
r/a=0.15


TE/TM Band Structure
Frequency (ωa/2πc=a/λ)
0.5
0.4
0.3
0.2
0.1
0.0
TM
TE
Γ
K
M
Γ

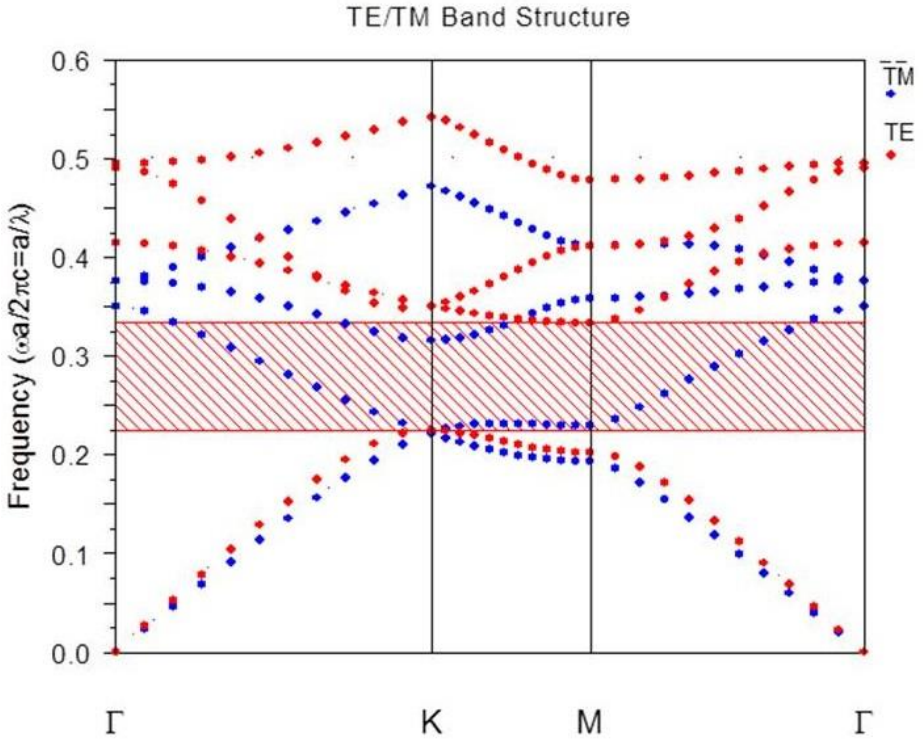
r/a=0.17


TE/TM Band Structure
Frequency (ωa/2πc=a/λ)
0.5
0.4
0.3
0.2
0.1
0.0
TM
TE
Γ
K
M
Γ

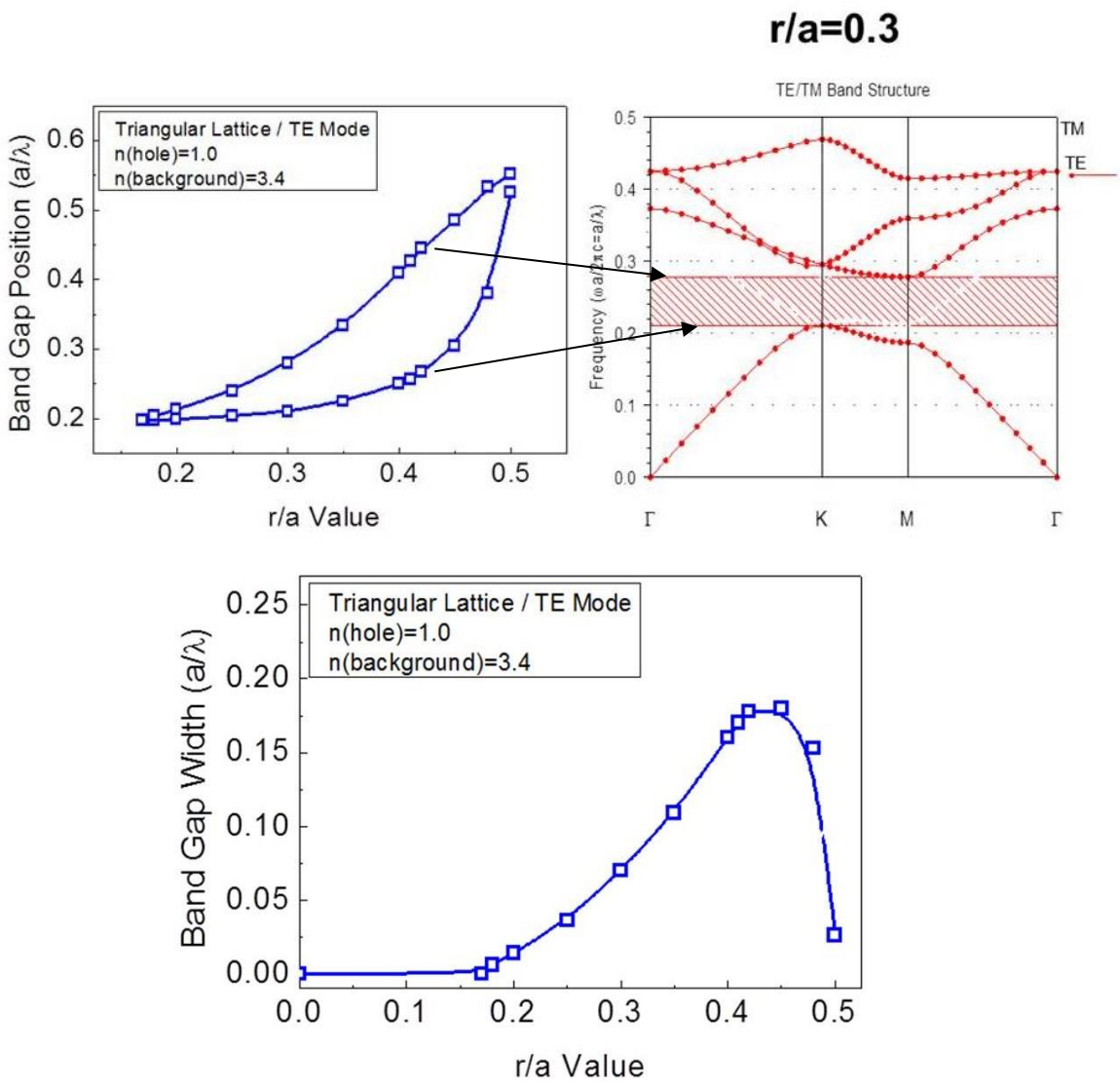
r/a=0.18


TE/TM Band Structure
Frequency (ωa/2πc=a/λ)
0.5
0.4
0.3
0.2
0.1
0.0
TM
TE
Γ
K
M
Γ

r/a=0.25


TE/TM Band Structure
Frequency (ωa/2πc=a/λ)
0.6
0.5
0.4
0.3
0.2
0.1
0.0
TM
TE
Γ
K
M
Γ

r/a=0.35

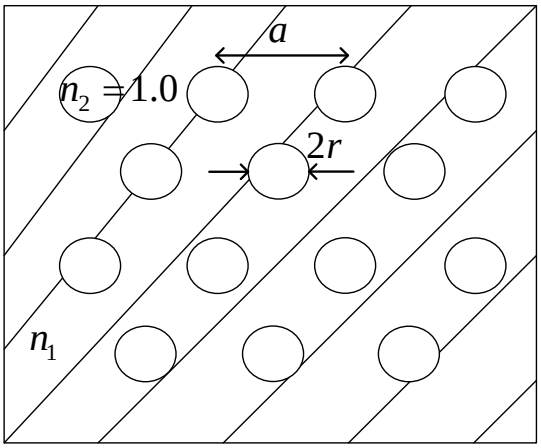


(2) The width of photonic band gap can be modified with the different *r/a* value. Larger band gap gives us more degree of freedom to design the photonic crystal devices and more defect modes or bands from the photonic crystal defect cavities or waveguides.

2) Refractive index *n* of photonic crystal lattices

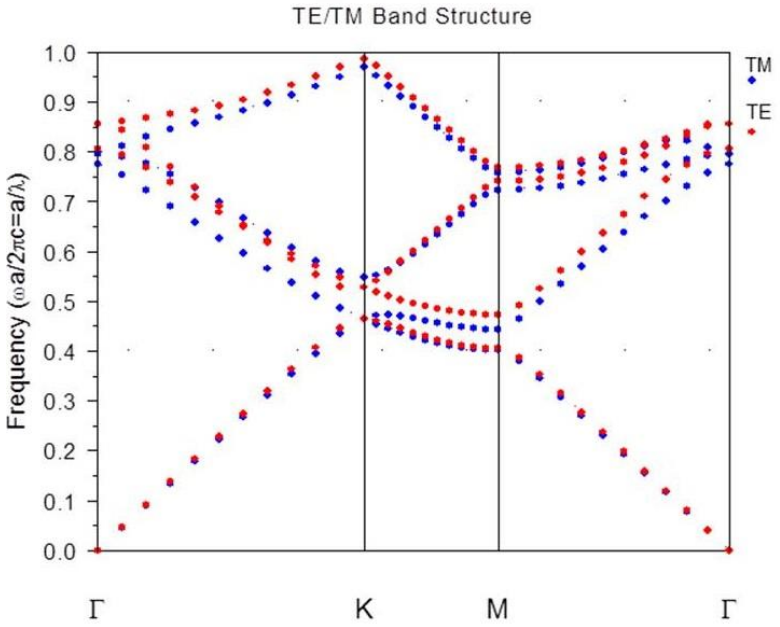
In next example, we are going to examine the effect due to the variation of the refractive index of the photonic crystal lattices. We still take the triangular lattices with air holes as an example.

Now we fix the r/a=0.3 and index of air holes, 1.0. The background index, *n*, is varied from 1.5 to 3.5.

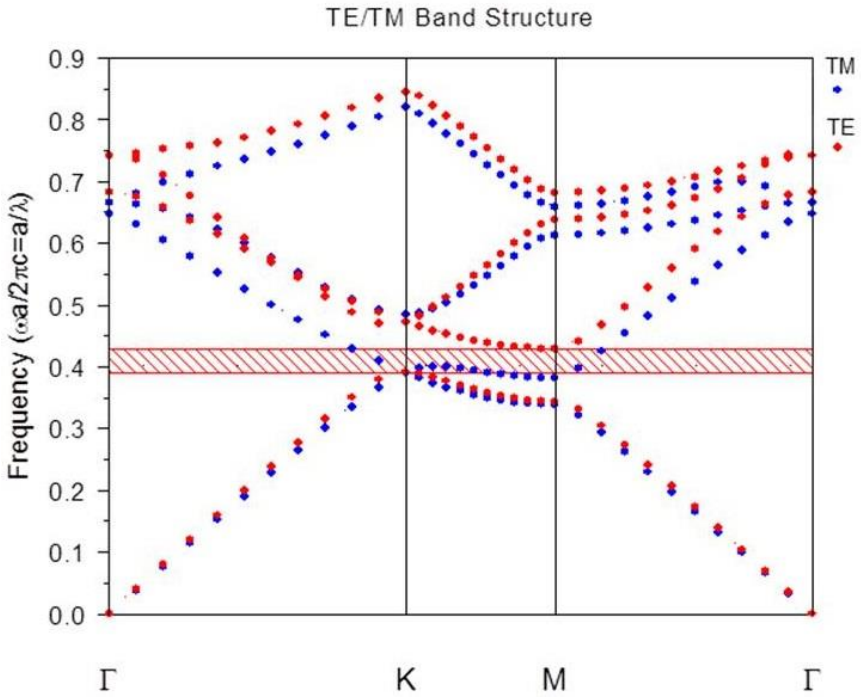


$r/a = 0.3$

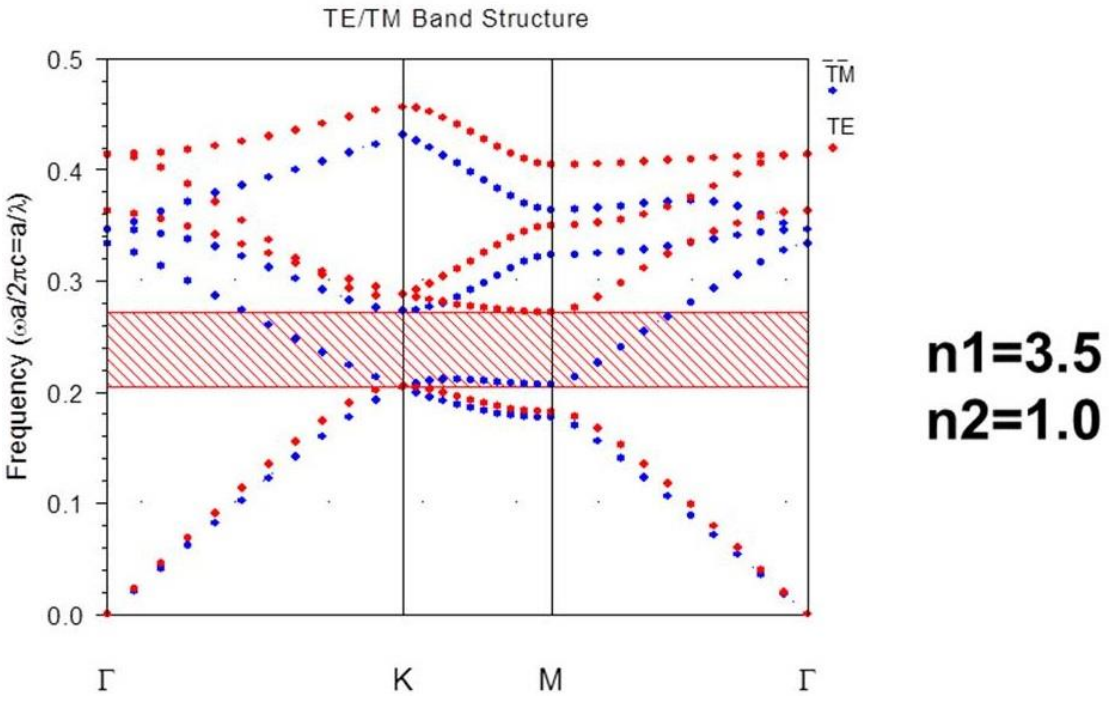
$n(\text{hole}) = 1.0$



n1=1.5
n2=1.0

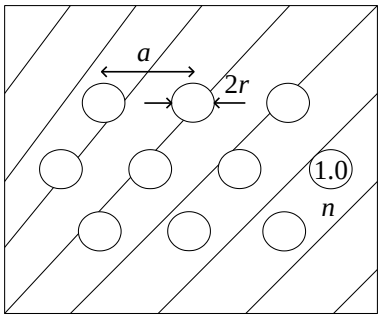


n1=1.8
n2=1.0



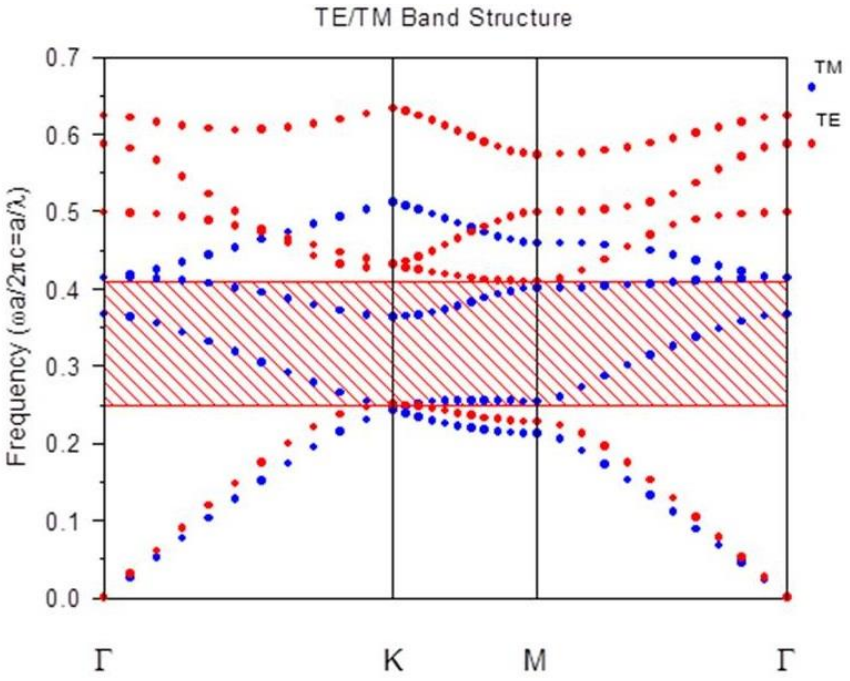
3) <u>Complete band gap for both polarizations</u>

In the previous examples, some have the photonic band gap for *TE* modes, some have band gap only for *TM* mode, and some even have no band gap for the both polarizations. Is it possible to have the photonic band gap for both *TE* and *TM* polarizations simultaneously?

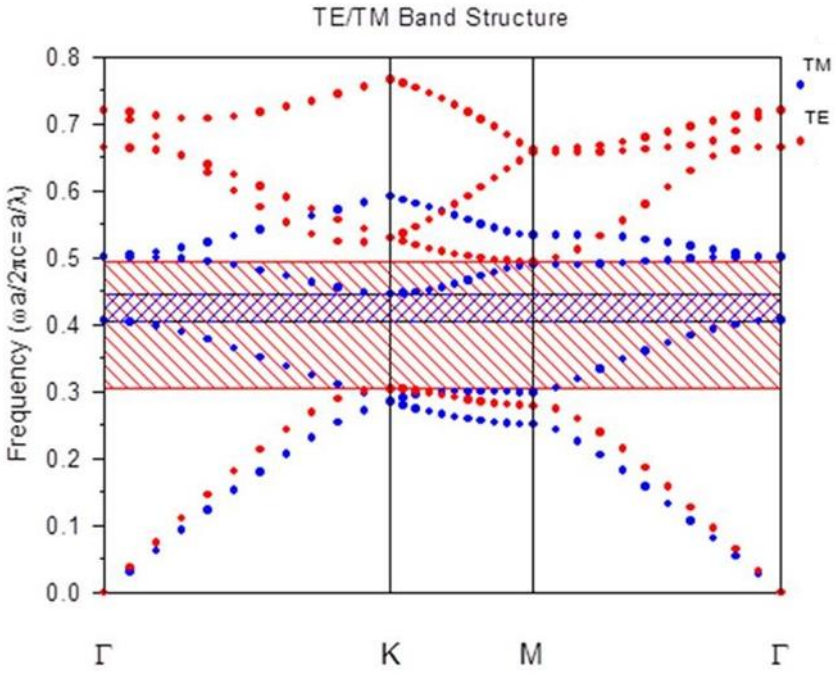


The answer is Yes! Now let's take a look to an example first, then we'll analyze the reason for *TE* and *TM* band gaps. Consider a *2-D* triangular photonic crystal lattices with the air holes again. This time we'll let *n=3.4*

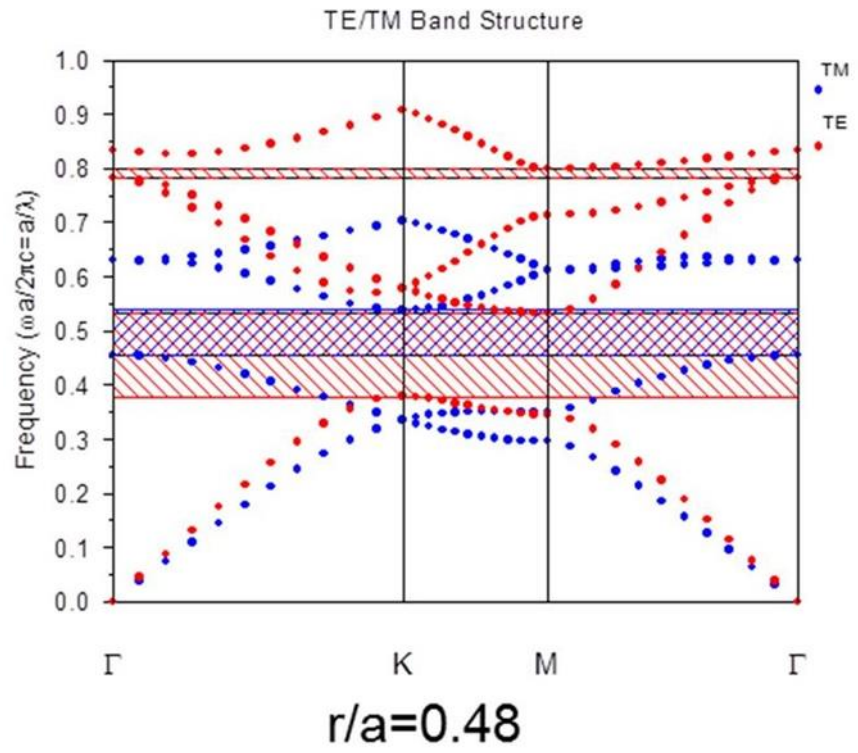
and *r/a* value varied from 0.35 to 0.50. The band structures of *TE* and *TM* modes with these r/a values are shown below.



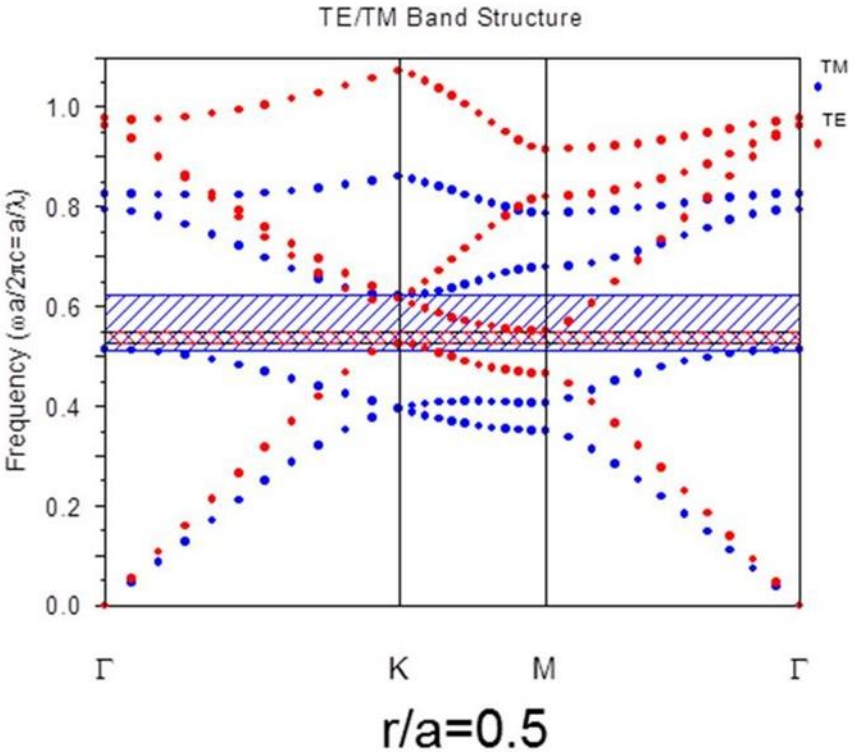
r/a=0.4



r/a=0.45



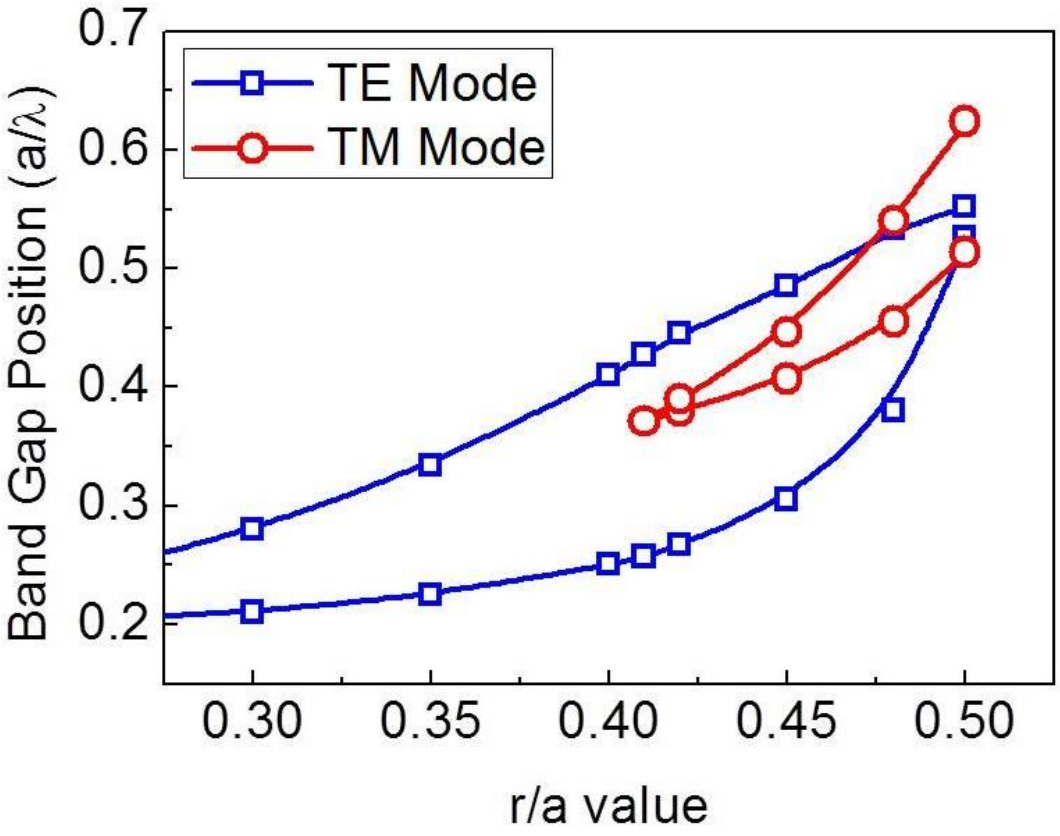
r/a=0.48

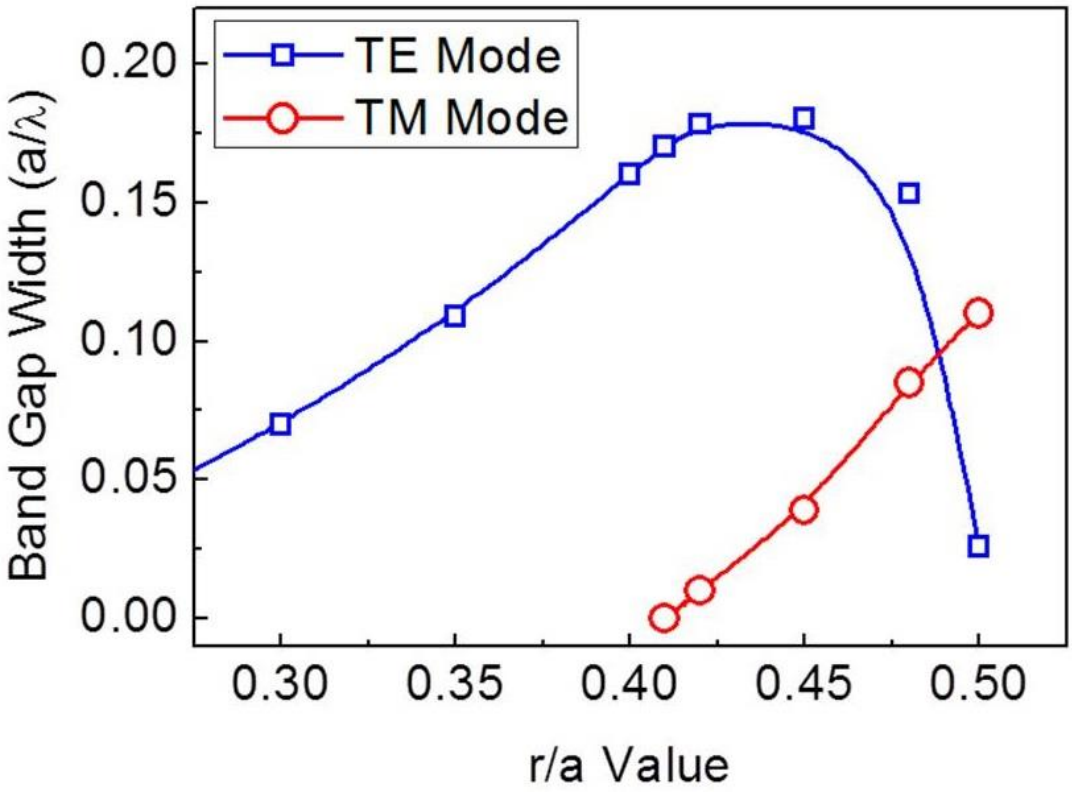


r/a=0.5

According to the band diagrams in the previous pages, we can plot the band gap position in normalized frequency versus *r/a* value like we did in the page 92. In the top figure of page 92,

the square-curves are the top & bottom boundaries for *TE* band gap while the circle-curves are the band gap boundaries versus r/a value for *TM* mode. We also plot the width of band gaps for *TE* & *TM* modes versus r/a value of lattices in the bottom figure.




TE Mode
TM Mode
Band Gap Width (a/λ)
0.20
0.15
0.10
0.05
0.00
0.30
0.35
0.40
0.45
0.50
r/a Value

What's important for the photonic crystal band gap?

We have done several examples for the different photonic crystals, and plotted their band diagrams and the photonic band gaps. To apply photonic crystals in the real devices and engineer their optical properties around the band gap region, we should discuss several key issues for the photonic band gap.

1) Scaling properties of photonic crystals

In EM , there is no fundamental length scale other than the assumption that the system is macroscopic. Therefore, in photonic crystals, there is no fundamental constant with the dimensions of length. The relationship between EM problems is the difference only by a contraction or expansion of all distances.

Consider the eigenvalue equation for $\vec{H}(\vec{r})$

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

Now we make a compression or expansion for the structure $\varepsilon'(\vec{r})$, then

$$\varepsilon'(\vec{r}) = \varepsilon(\frac{\vec{r}}{s})$$

where s is a scale factor.

We can also make changes of the variables

$$\vec{r}' = s\vec{r}$$

$$\nabla' = \frac{\nabla}{s}$$

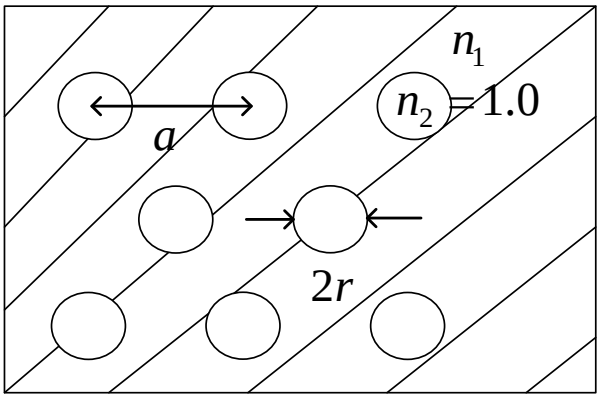
then the above equation becomes

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

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

This is just the same eigenvalue equation with the mode $\vec{H}'(\vec{r}') = \vec{H}(\frac{\vec{r}'}{s})$ and frequency $\omega' = \frac{\omega}{s}$. This means that we can obtain the new mode and new frequency just scale a factor, s, from the original solutions of the Maxwell's equations.

To understand the scaling properties of photonic crystals, let's consider the followed example.



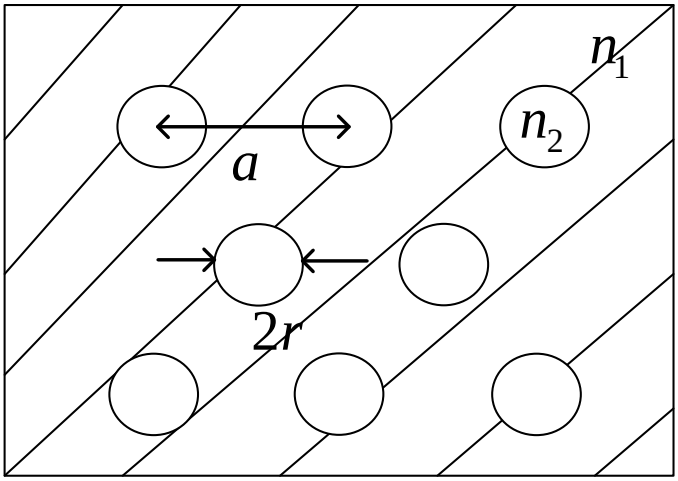
Now we fixed n_1 & n_2, and $\frac{r}{a} = 0.3$, but we vary the lattice constant, a to study the changes in the band structure & band gaps. In page 97, we plot the band diagrams for a =1000 nm and a =2000 nm. We realized that 2 band structures looks same in the normalize frequency unit ($\frac{a}{\lambda}$). It means the frequency vary linearly with the scale of the lattice const.

i.e. $\frac{1}{\lambda} \propto a$

2) The ratio of different dielectric constants.

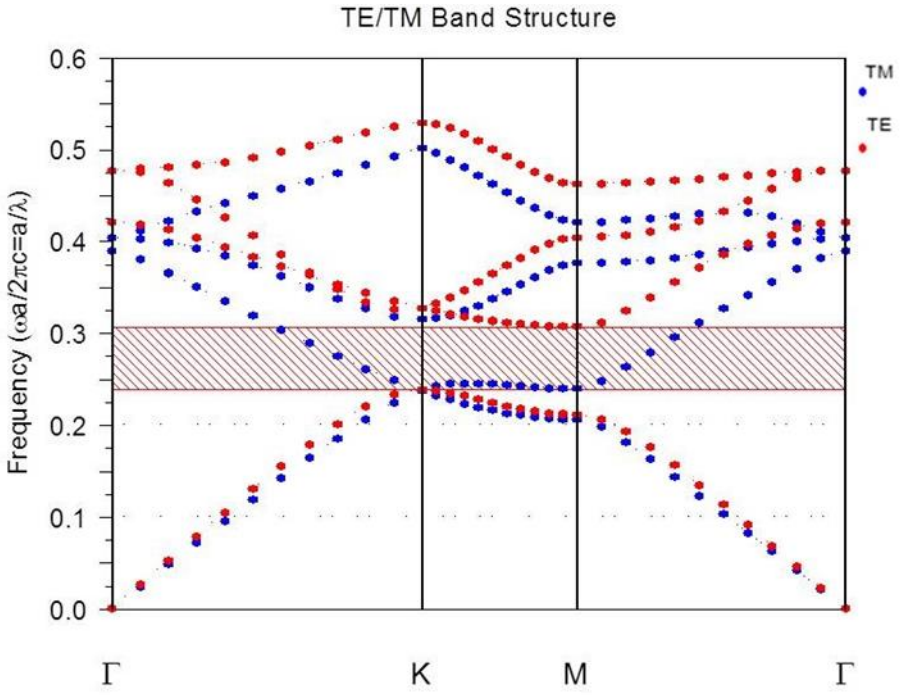
In the previous discussion for *2-D* photonic crystal band structures, we had examined the bands and band gaps vary with the different dielectric constants. However, is the absolutely value of a dielectric constant the key parameter for the band gap?

Actually what is really important is the ratio of the 2 different constants, not the actual values. Let's consider this example.

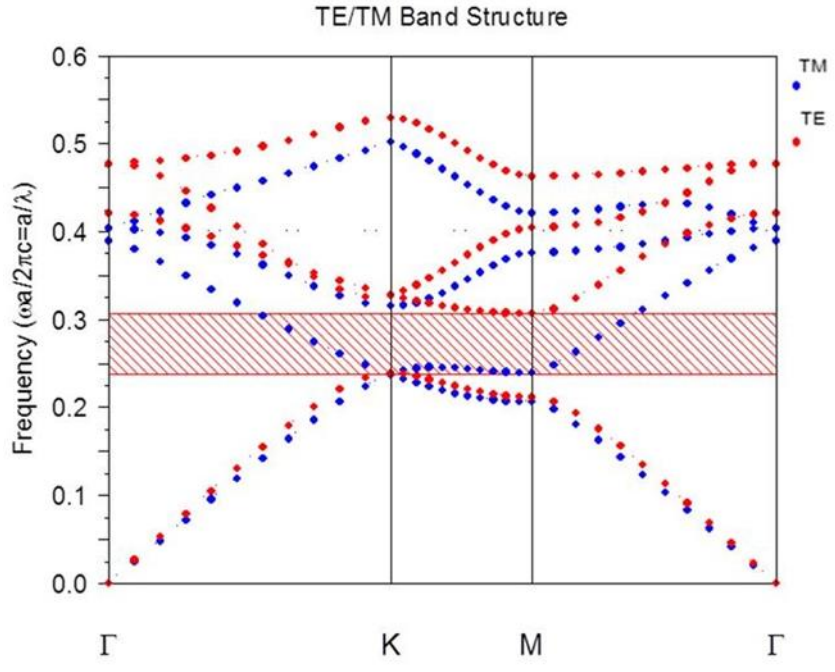


Now we fixed *a* & *r* in the lattices. We also fixed the ration of two refractive indices, $\frac{n_1}{n_2}$, but varied the actual values from $\frac{n_1}{n_2}=\frac{3}{1}$ to $\frac{n_1}{n_2}=\frac{6}{2}$.

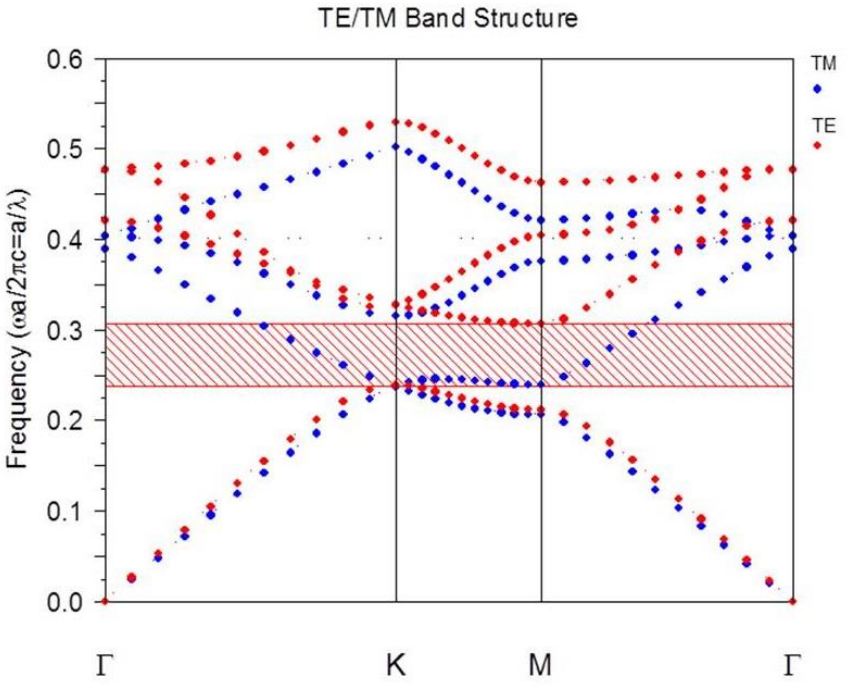
The band diagrams are plotted in the page 98.



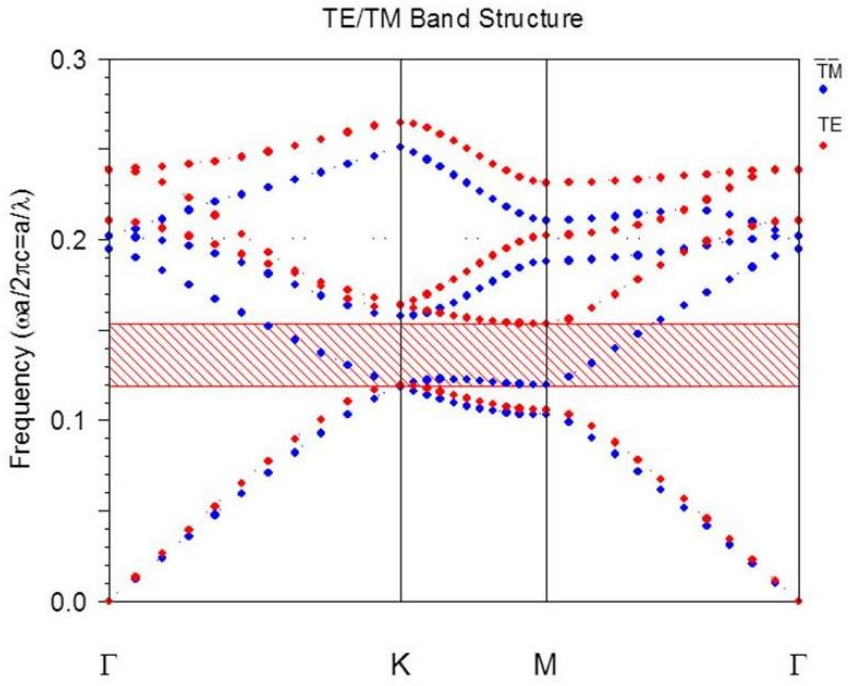
a=1000 nm



a=2000 nm



n_1/n_2= 3/1

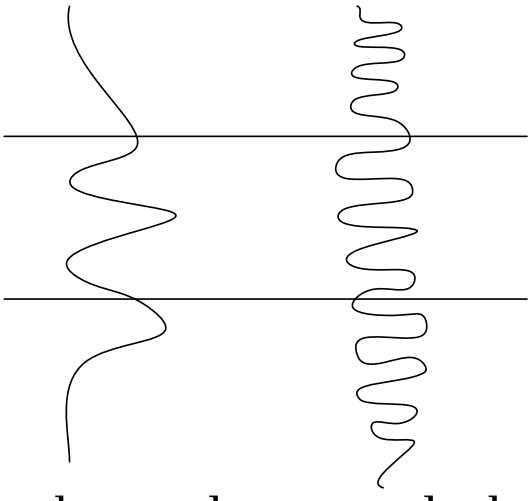


n_1/n_2= 6/2

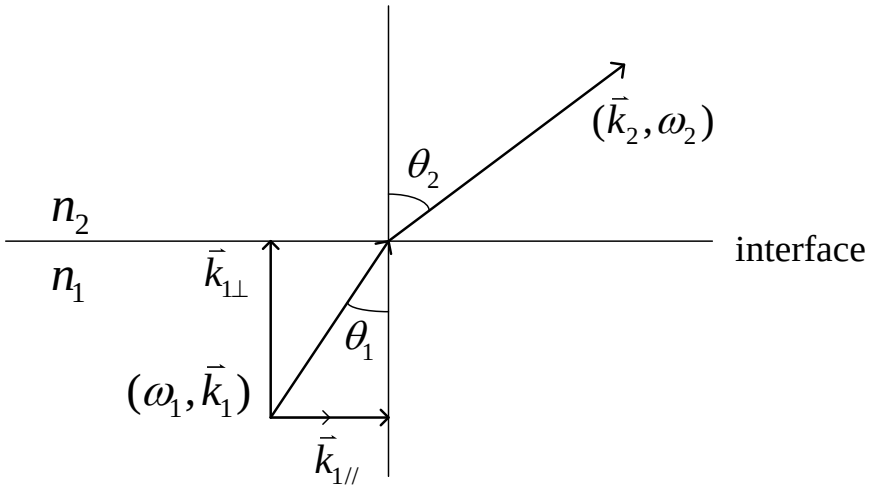
So as long as the ration fixed, we can just scale the dielectric constants to whatever we want, and the optical properties will be same.

Concept of the Light Cone/Line

In *2-D* photonic crystal, we assumed the periodic structure in x-y plane, and infinite thickness in z-axis. However, for most of the cases, we have the finite thickness in the photonic crystal slab structure. It is important to consider whether light coming from an outside homogeneous medium can couple to the inside modes through the entrance boundary plane. This kind of coupling mode called the leaky mode because it is not an eigenmode it is not an eigenmode of the structure and it's energy leak to the outside space through the coupling.



Non-leaky mode leaky mode



Now consider 2 mediums with index n_1 & n_2. In medium 1, the signal has wave vector $\vec{k}_1$ and frequency ω_1 . In medium 2, the signal has $(\vec{k}_2, \omega_2)$. In coupling process, the energy conservation and momentum conservation energy to interface must be valid so

$$\omega_1 = \omega_2$$

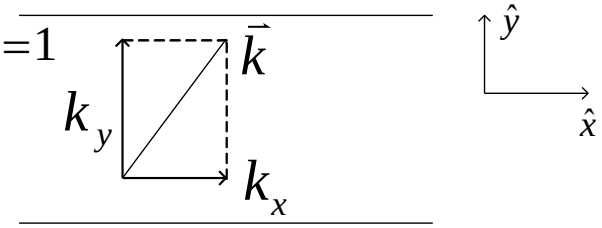
and

$$\vec{k}_{1//} = \vec{k}_{2//}$$

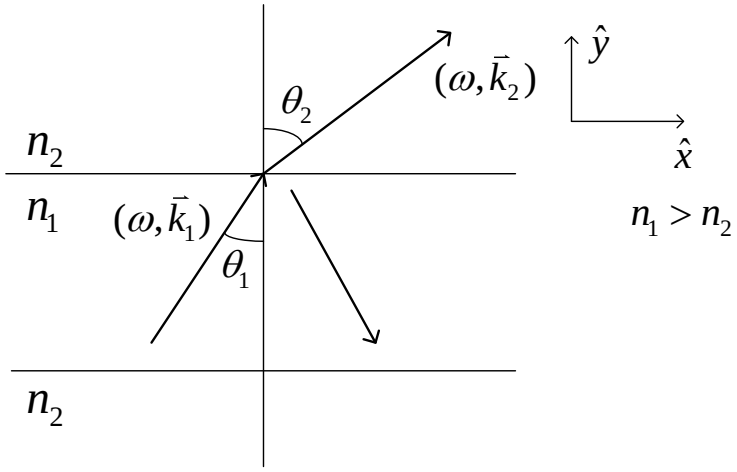
In a homogeneous medium with index *n*, the light cone can be described by the relation

$$\omega = \frac{c}{n}\left|\vec{k}_{//}\right| = c \cdot \beta$$

When n=1 (i.e. in air), then the light line $\omega = ck_x$



Now let's use the 2 layer structure to describe the concept of light line (cone).



Consider the above structure, medium 1 is embedded by medium 2, and the refractive index of medium1, n_1 is larger than the refractive index of medium2, n_2. Assume a mode in medium 1 with the wave vector $\vec{k}_1$ and a propagation angle θ_1. After pass through the interface into the medium 2, the mode has the wave vector $\vec{k}_2$ and the propagation angle θ_2. Note, we have the Snell's law

$$\left|\vec{k}_1\right| \sin\theta_1 = \left|\vec{k}_2\right| \sin\theta_2$$

or

$$\left|\vec{k}_{1//}\right| = \left|\vec{k}_{2//}\right|$$

or

$$n_1 \sin\theta_1 = n_2 \sin\theta_2$$

For a mode confined in the medium 1, it means that we need have a mode total reflective from the interface.

i.e. $\theta_1 > \theta_c$

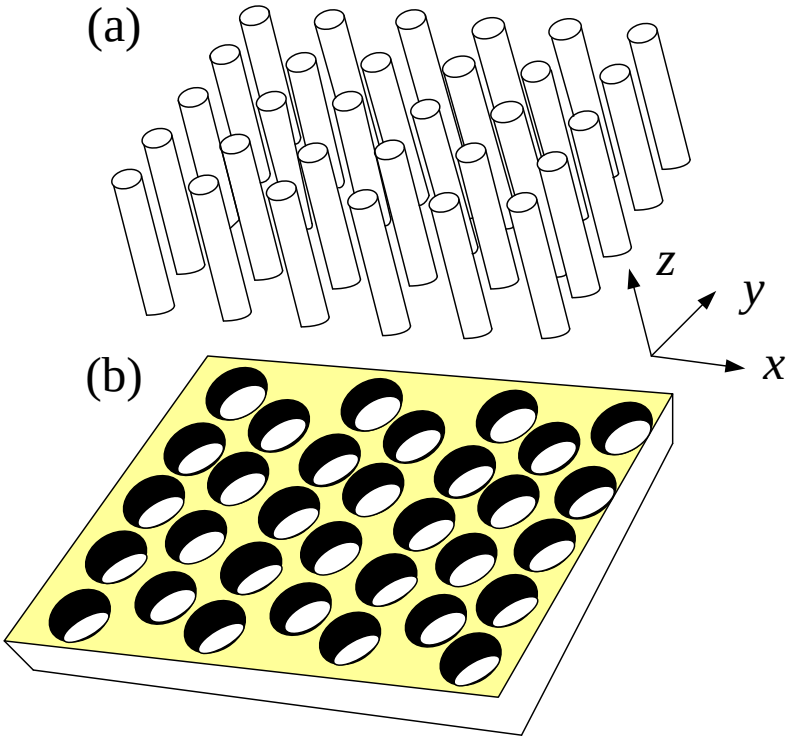
where $\sin\theta_c = \frac{n_2}{n_1}$

or $n_1 \sin\theta_c = n_2 \sin(\frac{\pi}{2})$

so once $\theta > \theta_c$, there is no wave propagate into the medium 2 from the interface. However this doesn't indicate the light field vanishes completely in the medium 2. See the leaky and non-leaky modes in the figure of page 99.

Photonic Crystal Slab Structure

So far we had discussed the photonic crystals which the lattice is periodic in *2-D* and infinitely extended in the $\hat{z}$ axis. Now we are going to consider the photonic crystals with a finite thickness.



Adding the finite thickness for the *2-D* photonic crystal lattices means we have to deal with the propagation vector in the $\hat{z}$ -axis. Even for propagation in-plane (x-y plane), the dielectric slab will have guided modes which there k_z is not zero.

There are some effects from this finite thickness of the slab

structure.

1) There is no longer a complete photonic band gap. It's still possible to have the band gaps for the guided modes of the slab.
2) Modes cannot be classified as "pure" *TE* or *TM* modes.

So let's discuss the two issues one by one.

1) First thing is the **disappearance of a complete band gap**. This is due to the non-zero k_z. Even in two-dimensional photonic crystals that are infinite in the third dimensional (Here is the $\hat{z}$-axis), the photonic band gap disappears when we allow out-of-plane ($k_z \neq 0$) propagation.

Here we show the band diagrams from *2-D* photonic crystals. They are periodic in x-y plane and infinitely in the $\hat{z}$-axis.

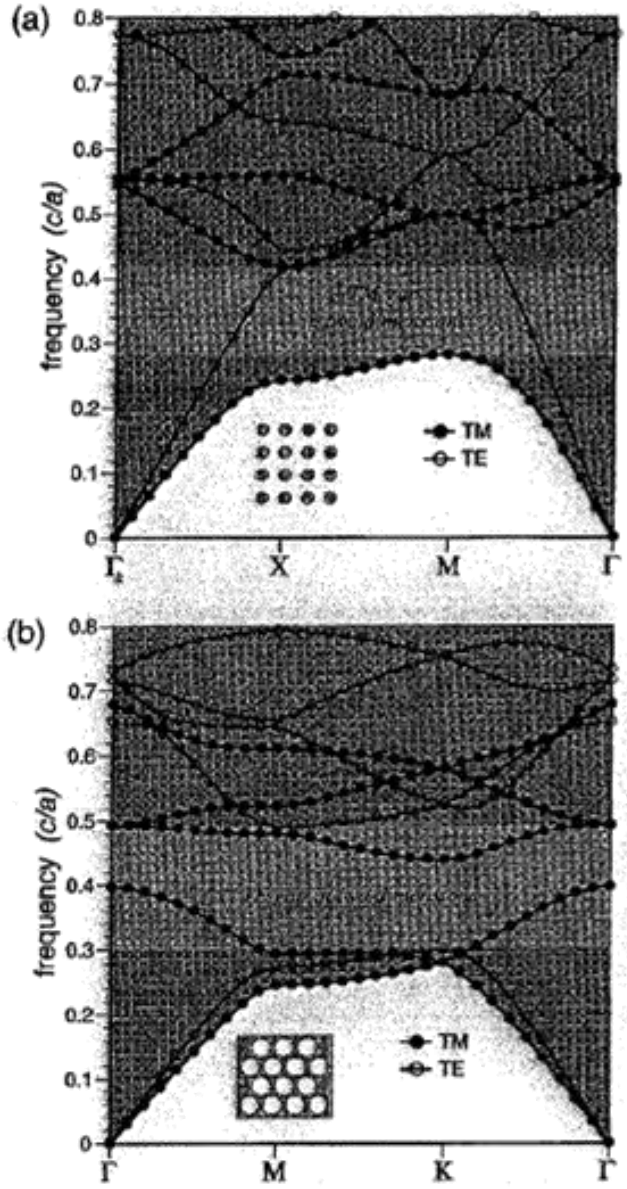
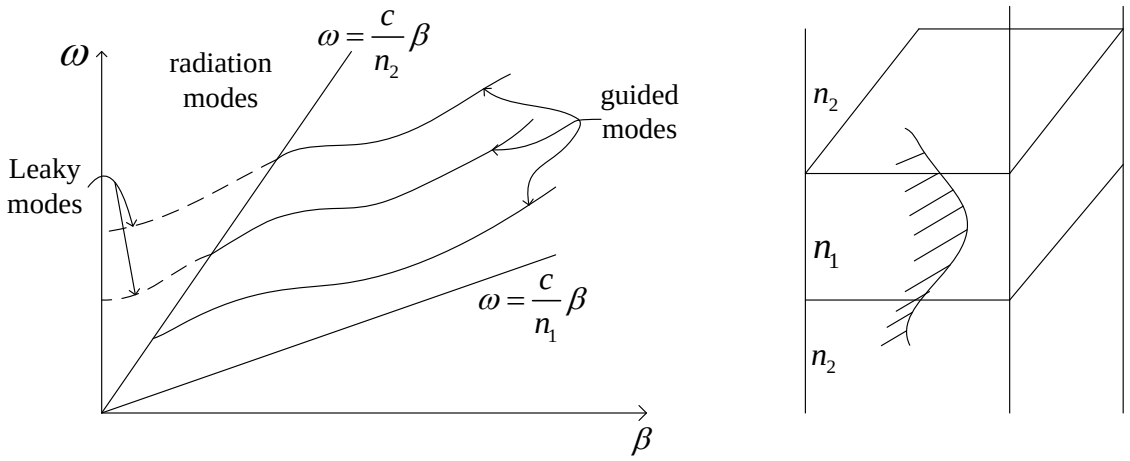


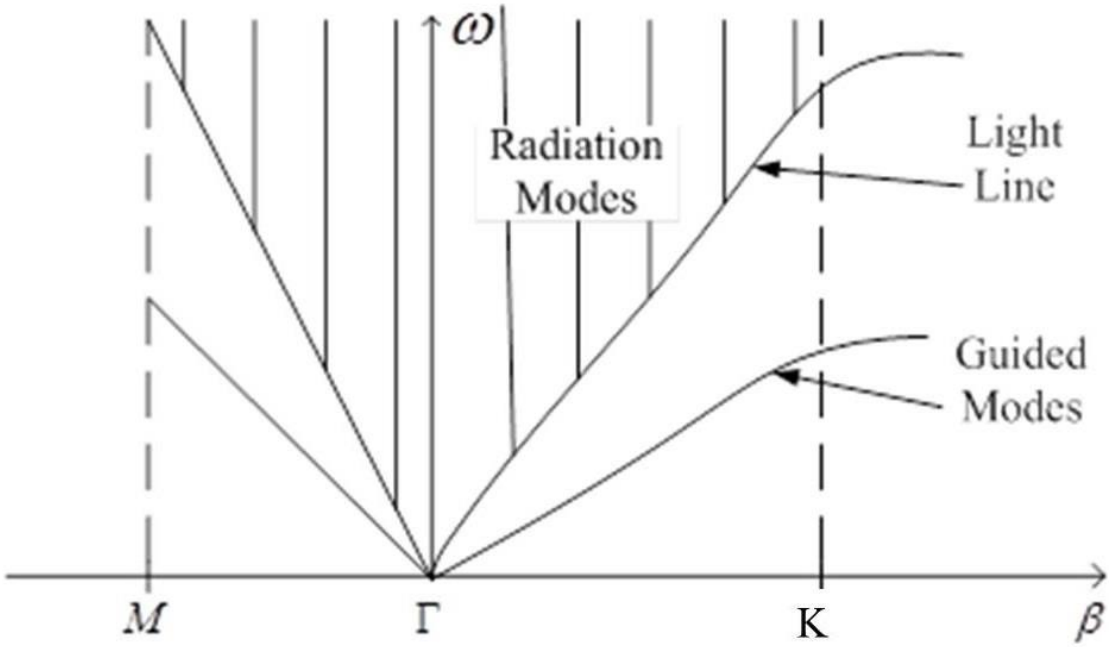
Fig2. Band diagrams for the photonic crystals from (a) Fig.1 (a) and (b) Fig.1 (b). The shaded region indicates the frequencies of states introduced when vertical propagation (i.e. perpendicular to the plane of periodicity) is permitted.

If we restrict the photonic lattice to a finite thickness then we expect that there will be modes guided by the dielectric slab and radiation modes (or leaky modes).

The dispersion relation for a slab waveguide is followed



The band structure for a slab photonic crystal lattice has the similar situation.



Bands below the light line are guided by the dielectric slab. Bands above the light line are the leaky waves. Their energy is

not confined inside the dielectric slab. There is also a continuum of radiation modes above the light line. The light line is given as in the case of the slab waveguide by the free propagation (plane wave) dispersion relation of the cladding.

The pressure of the radiation modes eliminates the complete band gap. It is still possible, however, to obtain gaps in the guided spectrum. Light in the frequency range corresponding to the gap in the guided modes can’t propagate in the plane of the slab.

According to the above arguments, once we have a finite thickness for the *2-D* photonic crystals, the band diagrams of *2-D* lattices in the page 110 will become the band diagrams shown in the next page.

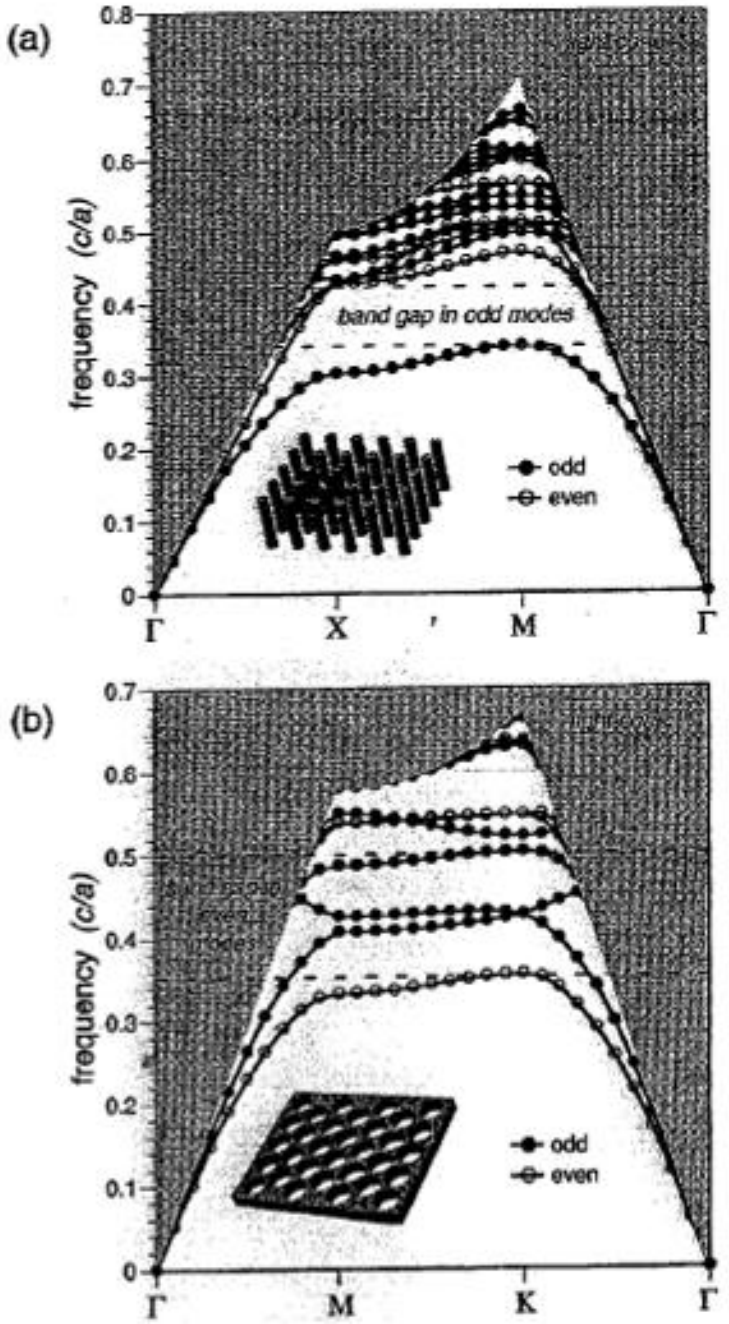
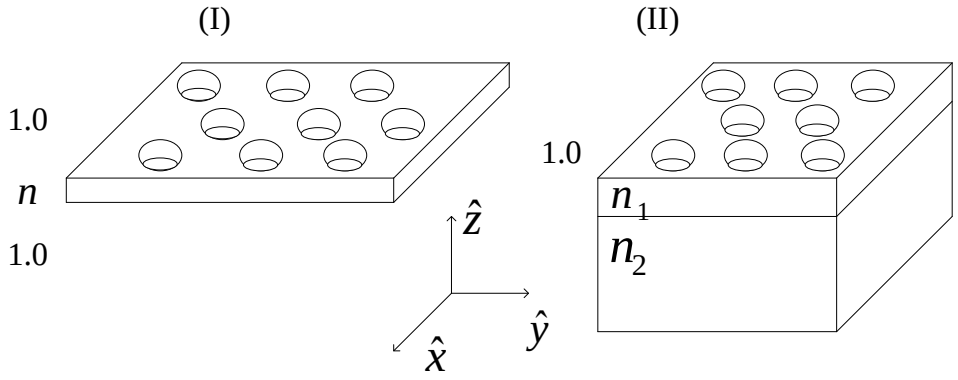


Fig.4. Projected band diagrams corresponding to the two slabs in Fig.3. Whether states are even or odd with respect to the horizontal mirror plane of the slab is indicated by open or filled circles, respectively.

The shaded regions above the light cone are radiation modes or leaky modes for the 2-D photonic crystal slabs. Only the bands below the light cones are considered as the guided (or

confined) modes in the slab. We are most likely to use those modes for the real devices.

2) Now let's talk about the **polarization of slab photonic crystals.** Since the symmetry under reflection through x-y plane is no longer valid for all *z*, the slab modes can not be classified as even or odd modes for all *z*. However, it is possible to separate the slab modes into even to odd at some points. Consider the two examples



Example (I) is a suspended membrane photonic crystal structure which has air cladding above and bottom of the slab. In this case, we'll have reflection symmetry at x-y plane of $z = 0$ (i.e. at center of the slab). We therefore have separated even and odd modes at $z = 0$. In the x-y plane of the center of the slab, the even modes are *TE*, and the odd modes are *TM*. However, at all other *z*, the even modes are only *TE*-like and the odd modes are

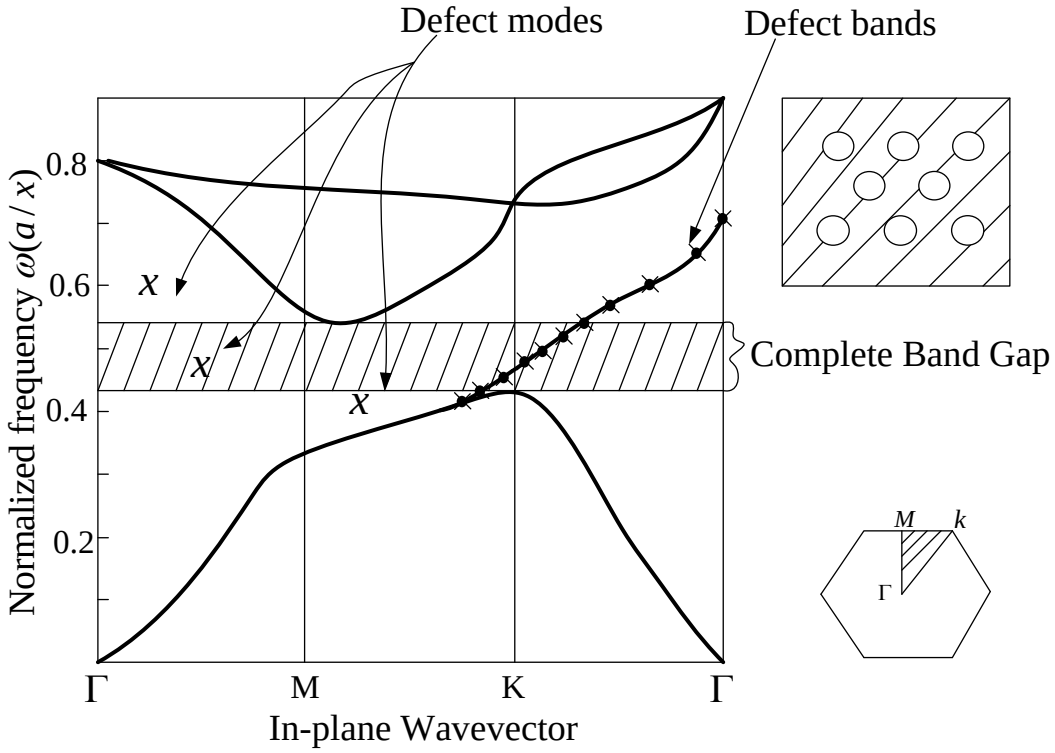
only *TM*-like. They are not rigorously *TE* or *TM*.

In example (II), we cannot have any *z* which has the reflection symmetry for the photonic crystal system. For this case, we only have *TE*-like (or even-like) modes and *TM*-like (or odd-like) modes.

Defects and defect modes from the photonic crystals

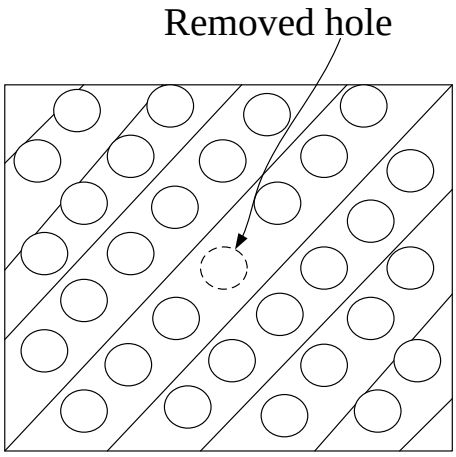
After the discussion of non-defect photonic crystal lattices, we are going to study the photonic crystals with the defects or the defect lines.

For a triangular photonic crystal with the defect, we have the band diagram for TE mode.

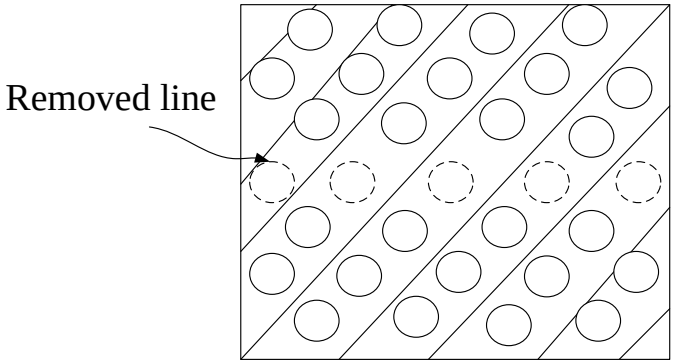


Now if we create a defect point by removing an air hole from the lattices to form a defect cavity.

(* Confine photon intensity inside the defect)



Then we'll simultaneously have some defect modes in the photonic band gap regions. The modes describe the photon / wave behavior associated with the defect we created.



If we remove a line from the lattice to form a waveguide, we'll have the defect bands in the gap region to describe the character of the wave propagation inside or around the defect line area.

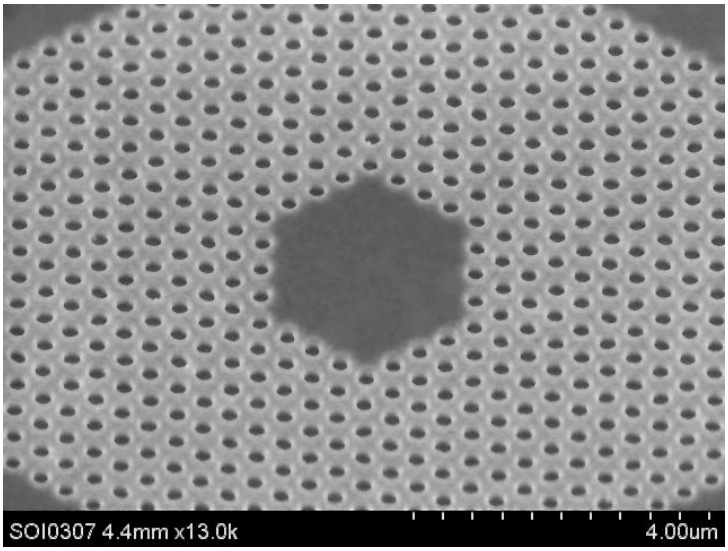
There are several notes we should mention for the defect modes / bands of the photonic crystals,

(1) The defect modes, which are formed by removing some

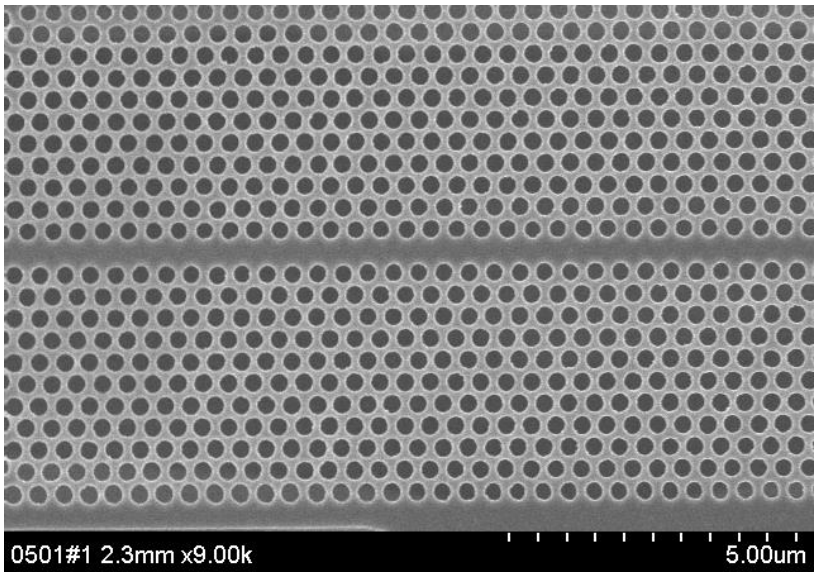
lattice points, are only the “isolated” modes in the band gaps. It means that there is no allowed modes / states between those defect modes for the photonic crystal cavity.

(2) The defect bands, which are created by removing a line of lattices, are composed by “many” defect modes in the gaps. Since the defects in the lattices open one-dimensional degree of freedom, any point (or state) on the defect bands is the allowed state for the photonic crystal waveguide.

(3) The defect modes and bands are not only located inside the “completely” band gap regions, but also in the gap region outside the complete band gap.



(Cavity) The D_4 photonic crystal defect cavity on a SOI substrate.



(Waveguide) The with photonic crystal waveguide in a GaAs suspended membrane.

Quality factor (Q) and photon lifetime

Quality factor (Q) is an important parameter for a cavity. It mainly describes the photo life time inside the cavity, or the energy stored in the cavity. There are several definitions (or descriptions) for the quality factor of a cavity.

(1) $$Q = \frac{2\pi \text{ (energy stored in the system at resonance)}}{\text{(energy lost in a cycle of oscillation)}}$$

$$= \frac{2\pi}{T} \cdot \frac{W}{-dw/dt} \qquad W: \text{ Stored energy}$$

$$= \omega_0 \frac{W}{-dw/dt} \qquad \omega_0: \text{ Resonance freq.}$$

or

$$W(t) = W(0)e^{-\frac{\omega_0 t}{Q}}$$

(2) We can also have Q related to the photon lifetime τ_p

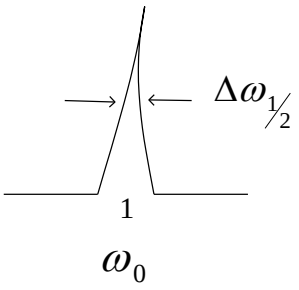
$$\tau_p = \frac{Q}{\omega_0}$$

or

$$Q = \omega_0 \tau_P$$

(3) In experiences, we can obtain the Q value from the spectrum

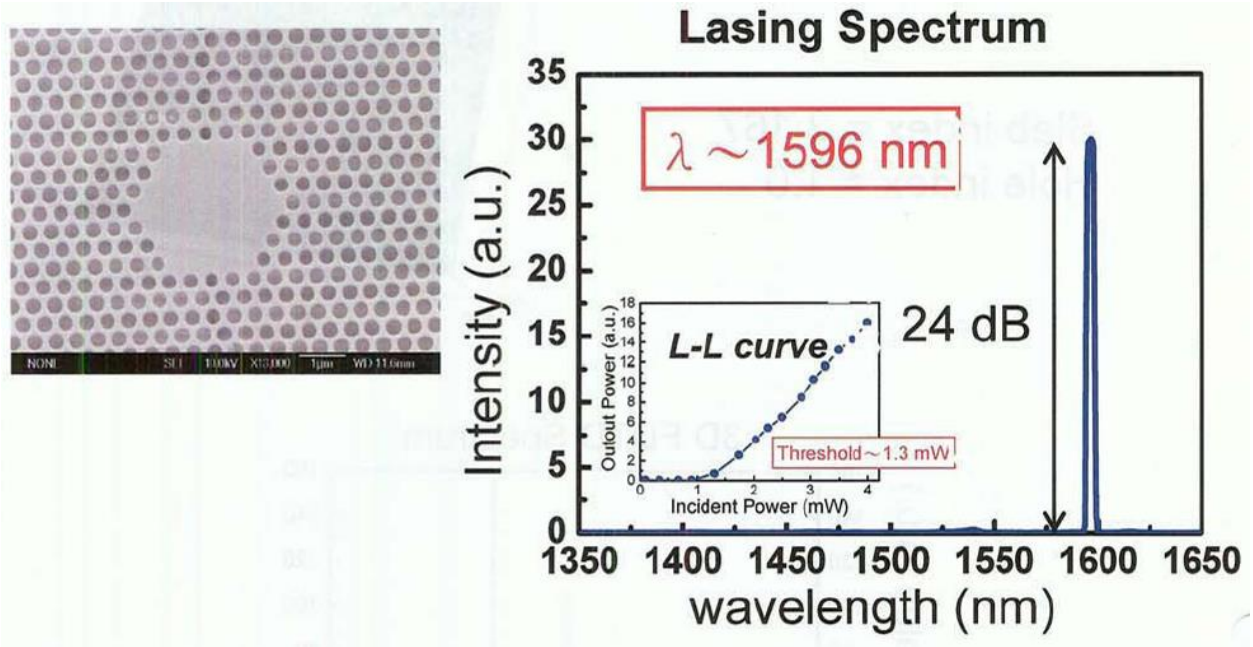
$$Q = \frac{\omega_0}{\Delta\omega_{\frac{1}{2}}}$$

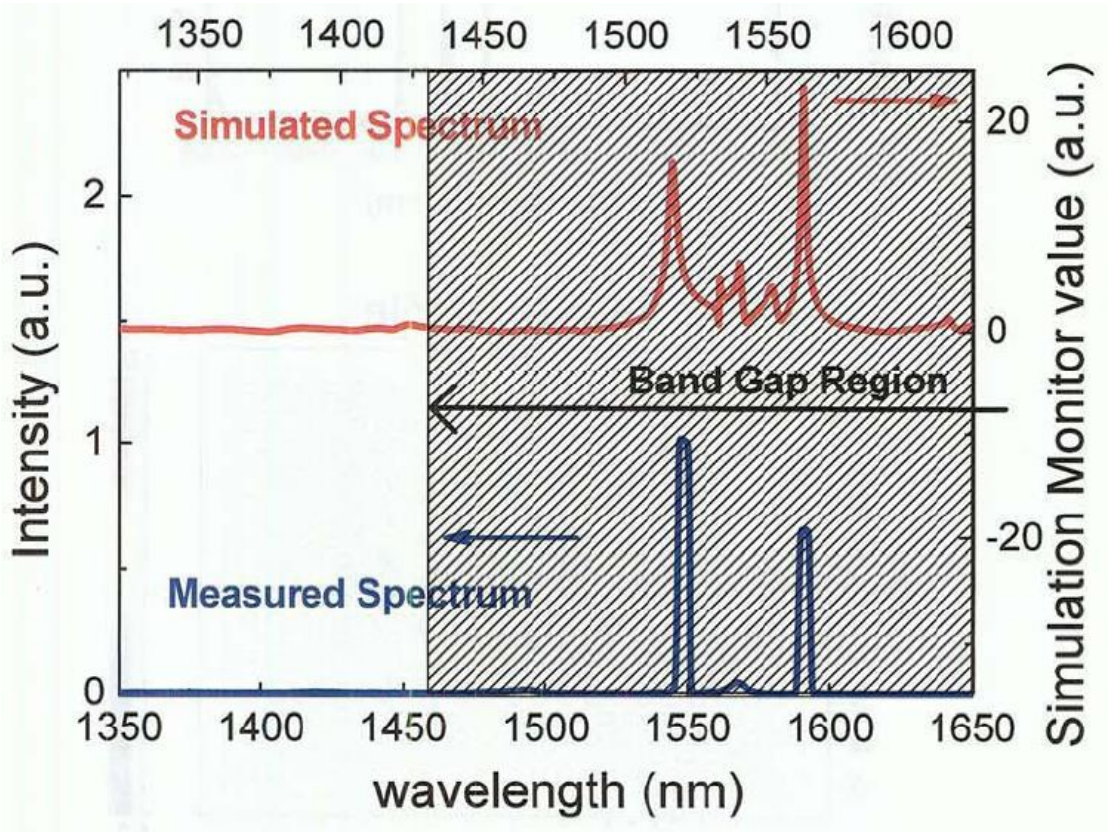


In photonic crystals, we use the photonic crystal defect structure serve as the resonant cavity for the designed defect modes. The quality factor Q will represent a measure of how many oscillations take place inside the cavity before the excited photon energy dissipate out of the cavity. It means that the photon energy for narrow frequency bands be trapped in the cavity for longer period of time if we have a high-Q cavity.

Now the important question becomes how the defect cavity should be designed for introducing the high-Q modes into the structure. There are several examples of the high-Q photonic crystal cavities in the following pages.

Photonic Crystal D4 Lasers in InGaAsP Membrane





Finite-difference time-domain (FDTD) simulation method

The finite-difference time-domain (FDTD) method is widely used to directly solve time-dependent Maxwells' equations now. FDTD was originally proposed for EM waves with long wavelengths, such as microwaves, because the spatial discrimination requirement is small ($\sim\frac{1}{10}-\frac{1}{20}\lambda$). In 1966, Yee described the basis of FDTD numerical technique for EM wave in the time domain on a space grid. (K.S. Yee, IEEE Transaction of Antennas and Propagation 14, 302-307 (1966)). Recently, FDTD method is popular in simulating photonic band gap structure and other photonic devices.

For 3-D simulation of the Maxwell's equations, it become more complicated.

The time-dependent Maxwell's equations are

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

(21) $$\varepsilon\frac{\partial\vec{E}}{\partial t}=\nabla\times\vec{H}$$

Their {x, y, z} component representations are

(22) $$-\mu\frac{\partial H_x}{\partial t}=\frac{\partial E_z}{\partial y}-\frac{\partial E_y}{\partial z}$$

(23) $$-\mu\frac{\partial H_y}{\partial t}=\frac{\partial E_x}{\partial z}-\frac{\partial E_z}{\partial x}$$

(24) $$-\mu\frac{\partial H_z}{\partial t}=\frac{\partial E_y}{\partial x}-\frac{\partial E_x}{\partial y}$$

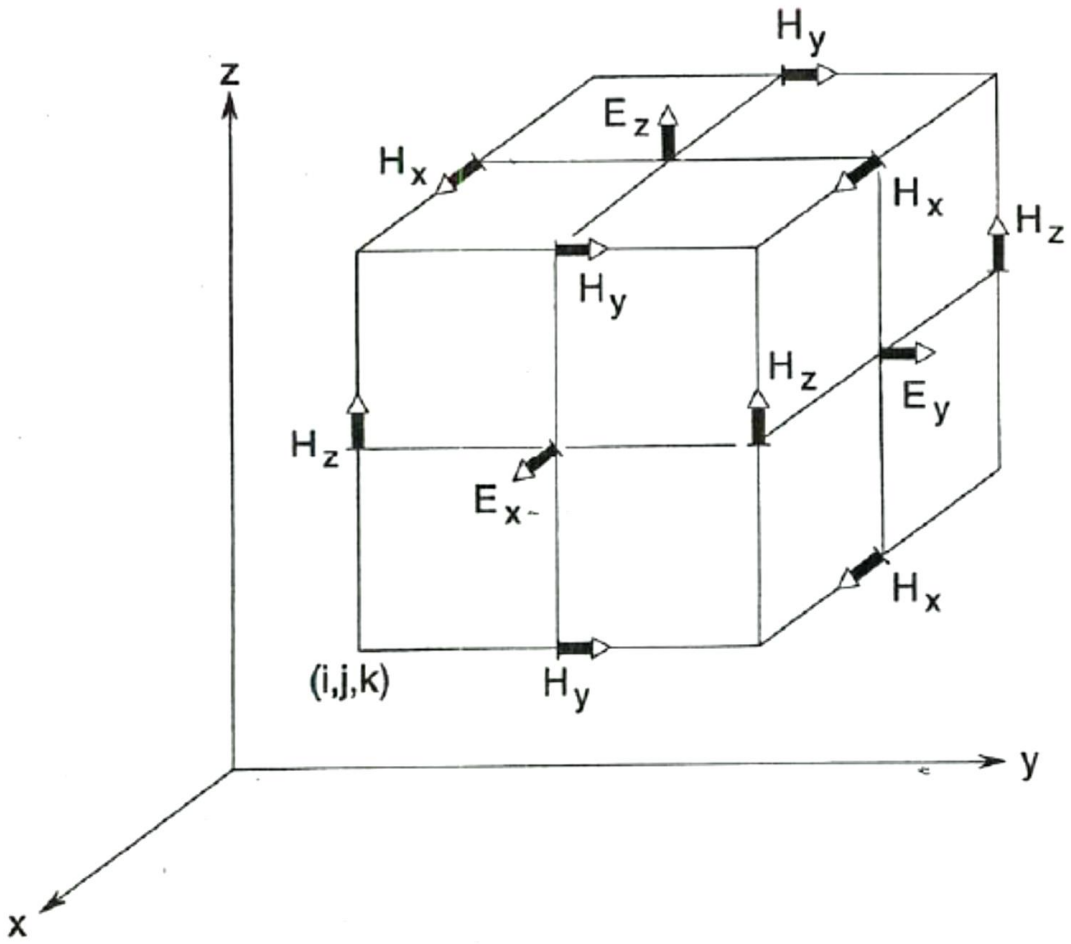
(25) $$\varepsilon\frac{\partial E_x}{\partial t}=\frac{\partial H_z}{\partial y}-\frac{\partial H_y}{\partial z}$$

(26) $$\varepsilon\frac{\partial E_y}{\partial t}=\frac{\partial H_x}{\partial z}-\frac{\partial H_z}{\partial x}$$

(27) $$\varepsilon\frac{\partial E_z}{\partial t}=\frac{\partial H_y}{\partial x}-\frac{\partial H_x}{\partial y}$$

We assume that $\Delta x, \Delta y, \Delta z$ are spatial discretization and that Δt is a time step, the function F(x, y, z, t) is discretized as

(28) $$F(x,y,z,t)=F(i\Delta x,\ j\Delta y, k\Delta z, n\Delta t)=F^n(i,\ j, k)$$



In the paper of 1966, Yee originated a set of finite-difference equations for the time-dependent Maxwell's curl equations for the lossless materials case ($\sigma^* = 0, \sigma = 0$).

The above figure shows Yee space lattice which illustrates the Yee algorithm. This algorithm centers its $\vec{E}$ and $\vec{H}$ components in 3-D space so that every $\vec{E}$ component is surrounded by four circulating $\vec{H}$ components, and each $\vec{H}$ component is surrounded four circulating $\vec{E}$ component.

The Yee algorithm also centers its $\vec{E}$ and $\vec{H}$ components in time. All of the $\vec{E}$ computation in the modeled space are completed and stored in memory for particular time point using previously stored $\vec{H}$ data. Then all of the $\vec{H}$ computations in the space are completed and stored in memory using the $\vec{E}$ data just computed. The cycle begins again with the recomputation of the $\vec{E}$ components based on the new obtained $\vec{H}$. This process continues until time-step finished.

Yee used centered finite-difference (or central-difference) expressions for the space and time derivatives. This way can obtain simpler programing and second-order accuracy. For example, the first spatial derivative of the function $F(x, y, z, t) = F(i\Delta x, j\Delta y, k\Delta z, n\Delta t) = F^n(i, j, k)$ will be

$$\frac{\partial F^n(i, j, k)}{\partial x} = \frac{F^n(i + \frac{1}{2}, j, k) - F^n(i - \frac{1}{2}, j, k)}{\Delta x} + O[(\Delta x)^2]$$

And the first time derivative of $F^n(i, j, k)$ is

$$\frac{\partial F^n(i, j, k)}{\partial t} = \frac{F^{n+\frac{1}{2}}(i, j, k) - F^{n-\frac{1}{2}}(i, j, k)}{\Delta t} + O[(\Delta t)^2]$$

There are two notes we should understand that Yee chose the central-difference in space and time.

1. With the central-difference in space (time), Yee's goal is the second-order accurate central differencing $O[(\Delta x)^2]$ $\{O[(\Delta t)^2]\}$, but the difference is only $\frac{\Delta x}{2}$ instead of Δx.
2. Yee chose he central-difference in space(time) because we can interleave $\vec{E}$ and $\vec{H}$ components in the space lattice at intervals of $\frac{\Delta x}{2}$ ($\frac{\Delta t}{2}$).

With Yee algorithm, we can re-write 3-D Maxwell's equations.

Equation 22 become

$$H_x^{n+1}(i, j+\frac{1}{2}, k+\frac{1}{2}) = H_x^{n-\frac{1}{2}}(i, j+\frac{1}{2}, k+\frac{1}{2}) - \frac{\Delta t}{\mu}\left\{\begin{array}{l}\frac{1}{\Delta y}\left[E_z^n(i, j+1, k+\frac{1}{2}) - E_z^n(i, j, k+\frac{1}{2})\right] \\ -\frac{1}{\Delta z}\left[E_y^n(i, j+\frac{1}{2}, k+1) - E_y^n(i, j+\frac{1}{2}, k)\right]\end{array}\right\}$$

equation 23 become,

$$H_y^{n+1}(i+\frac{1}{2}, j, k+\frac{1}{2}) = H_y^{n-\frac{1}{2}}(i+\frac{1}{2}, j, k+\frac{1}{2}) - \frac{\Delta t}{\mu}\left\{\begin{array}{l}\frac{1}{\Delta z}\left[E_x^n(i+\frac{1}{2}, j, k+\frac{1}{2}) - E_x^n(i+\frac{1}{2}, j, k)\right] \\ -\frac{1}{\Delta x}\left[E_z^n(i+1, j, k+\frac{1}{2}) - E_z^n(i, j, k+\frac{1}{2})\right]\end{array}\right\}$$

equation 24 become,

$$H_z^{n+1}(i+\frac{1}{2}, j+\frac{1}{2}, k) = H_z^{n-\frac{1}{2}}(i+\frac{1}{2}, j+\frac{1}{2}, k) - \frac{\Delta t}{\mu}\left\{\begin{array}{l}\frac{1}{\Delta x}\left[E_y^n(i+\frac{1}{2}, j+\frac{1}{2}, k) - E_y^n(i, j+\frac{1}{2}, k)\right] \\ -\frac{1}{\Delta y}\left[E_x^n(i+\frac{1}{2}, j+1, k) - E_x^n(i+\frac{1}{2}, j, k)\right]\end{array}\right\}$$

Equation 25 become

$$E_x^{n+1}(i+\frac{1}{2},j,k)=E_x^{n}(i+\frac{1}{2},j,k)+\frac{\Delta t}{\varepsilon}\left\{\begin{array}{l}\frac{1}{\Delta y}\left[H_z^{n+\frac{1}{2}}(i+\frac{1}{2},j+\frac{1}{2},k)-H_z^{n+\frac{1}{2}}(i+\frac{1}{2},j-\frac{1}{2},k)\right]\\ -\frac{1}{\Delta z}\left[H_y^{n+\frac{1}{2}}(i+\frac{1}{2},j,k+\frac{1}{2})-H_y^{n+\frac{1}{2}}(i+\frac{1}{2},j,k-\frac{1}{2})\right]\end{array}\right\}$$

equation 26 become

$$E_y^{n+1}(i,j+\frac{1}{2},k)=E_y^{n}(i,j+\frac{1}{2},k)+\frac{\Delta t}{\varepsilon}\left\{\begin{array}{l}\frac{1}{\Delta z}\left[H_x^{n+\frac{1}{2}}(i,j+\frac{1}{2},k+\frac{1}{2})-H_x^{n+\frac{1}{2}}(i,j+\frac{1}{2},k-\frac{1}{2})\right]\\ -\frac{1}{\Delta x}\left[H_z^{n+\frac{1}{2}}(i+\frac{1}{2},j+\frac{1}{2},k)-H_z^{n+\frac{1}{2}}(i-\frac{1}{2},j+\frac{1}{2},k)\right]\end{array}\right\}$$

Equation 27 become

$$E_z^{n+1}(i,\, j, k+\frac{1}{2}) = E_z^{n}(i,\, j, k+\frac{1}{2})$$
$$+\frac{\Delta t}{\varepsilon}\left\{\begin{array}{l}\frac{1}{\Delta x}\left[H_y^{n+\frac{1}{2}}(i+\frac{1}{2},\, j, k+\frac{1}{2}) - H_y^{n+\frac{1}{2}}(i-\frac{1}{2},\, j, k+\frac{1}{2})\right] \\ -\frac{1}{\Delta y}\left[H_x^{n+\frac{1}{2}}(i,\, j+\frac{1}{2}, k+\frac{1}{2}) - H_x^{n+\frac{1}{2}}(i,\, j-\frac{1}{2}, k+\frac{1}{2})\right]\end{array}\right\}$$

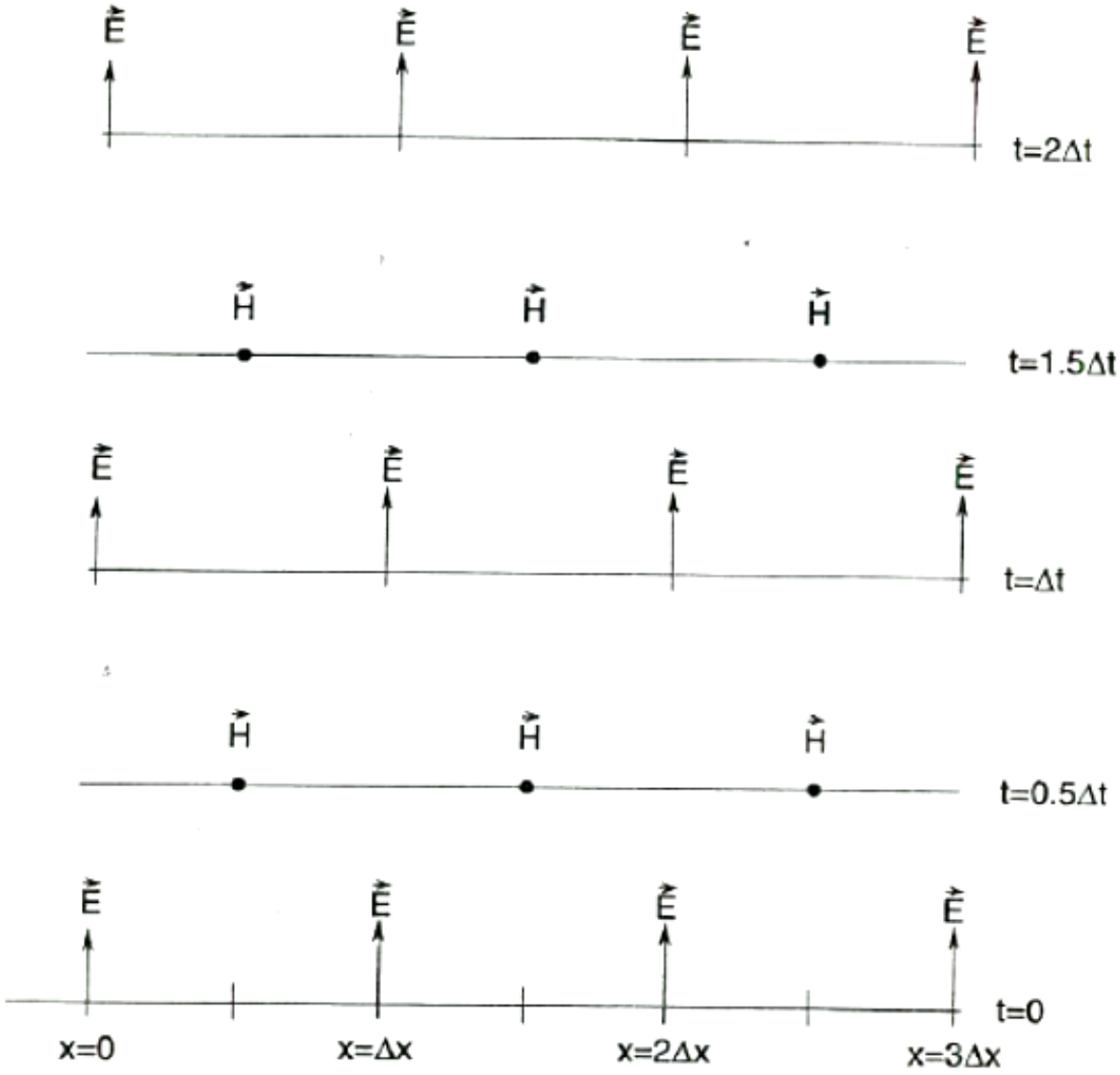


Fig. 3.2 Space-time chart of the Yee algorithm for a one-dimensional wave propagation example showing the use of central differences for the space derivatives and leapfrog for the time derivatives. Initial conditions for both electric and magnetic fields are zero everywhere in the grid.

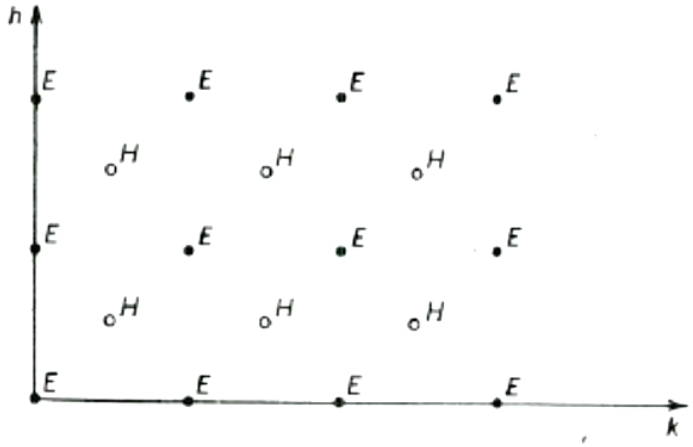


FIGURE 4-1. Mesh for Maxwell's equations in one spatial dimension.

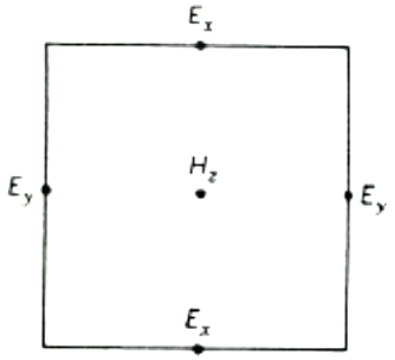


FIGURE 4-2. Typical cell for TE wave

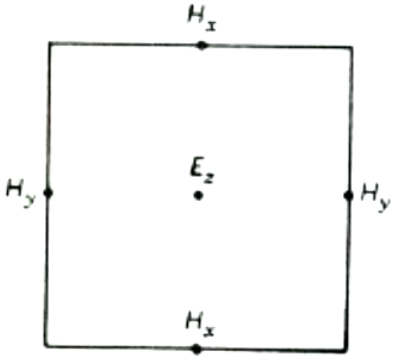
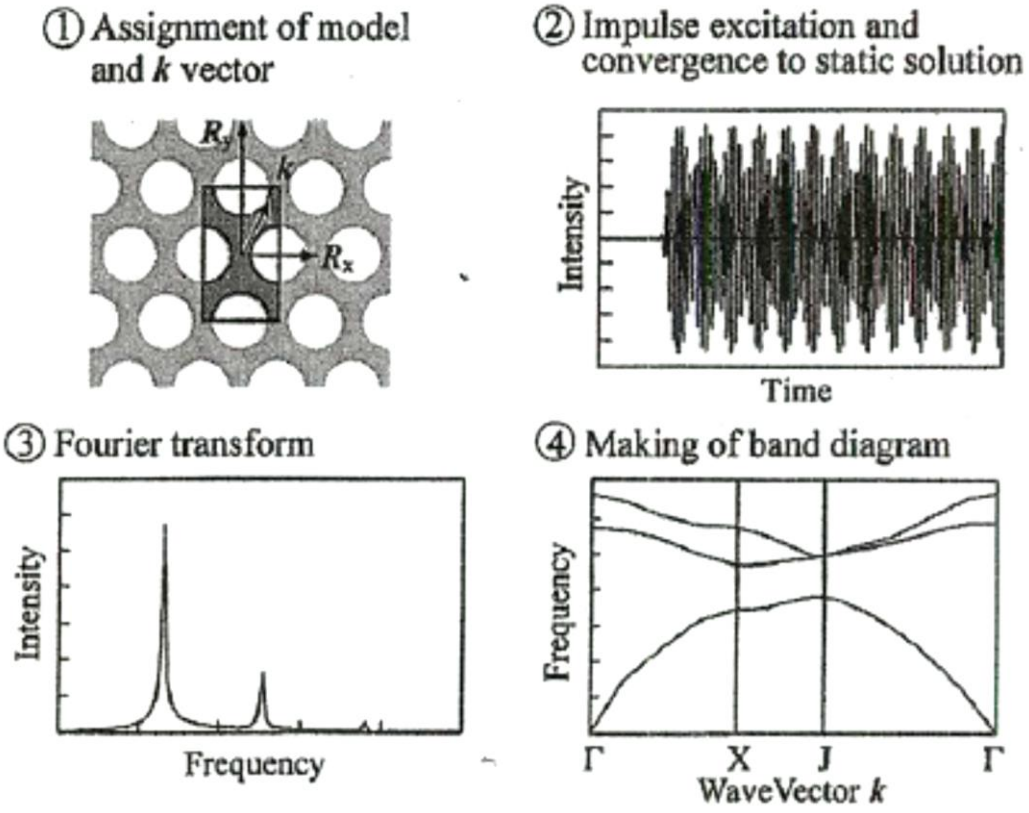


FIGURE 4-3. One version of the typical cell for TM wave.

The following illustration shows how we apply FDTD to real structure.



1. First we construct the structure we want to simulate. The material properties are assigned to corresponded locations. For example, refractive index $n(\vec{r})$ [i.e. dielectric function [$\varepsilon_r(\vec{r})$]. After setting-up the detectors in the designed structure to collect the signal, we can launch the initial sources, and let them

propagating following the FDTD algorithm.

2. The detectors will collect the signal varied with time during the FDTD calculation process. Figure 2 shows an example of the collected intensity versus time from a detector. The impulse initial excitation is usually applied in the simulation. And the collected signal goes stable (or say converge) after amount of simulation time(or simulation steps).

3. After the simulation finishing, the signal is collected, say I(t), by the detectors. The fourier transform will be applied to transfer time-domain spectrum into frequency-domain spectrum. Since “time, t” and “frequency, ω” are the conjugates in the Fourier transformation. Figure 3 is a frequency-domain spectrum which shows the dominant frequencies during the FDTD propagation in the simulated structure.

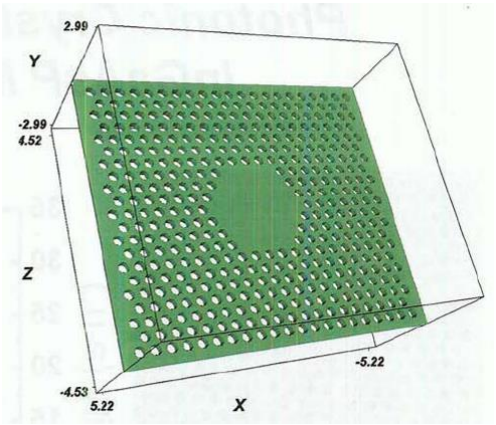
4. Not only frequency-domain information will be obtained from the FDTD simulation, we also can have more details about this structure, like mode profiles

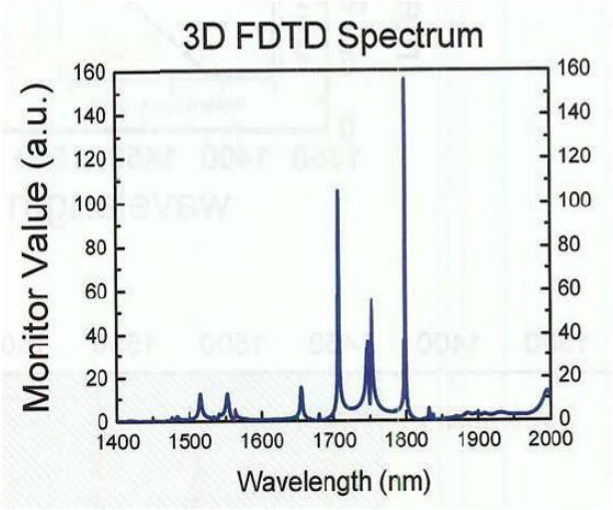
(see attachments), spectrum in wavelength and etc. for example, figure 4 is a band diagram $\omega(\beta)$ (or band structure) of the simulated structure from the frequency-domain spectrum and the initial propagation $\vec{k}$ of the sources.

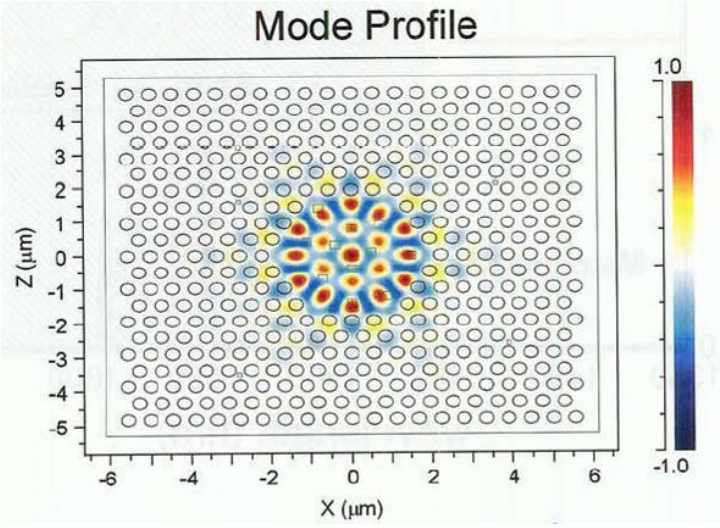
FDTD for D4 cavity

Slab index =3.167

Hole index=1.0







***From Y.C. Yang.**

Quality factor (Q) and photon lifetime

Quality factor (Q) is an important parameter for a cavity. It mainly describes the photo life time inside the cavity, or the energy stored in the cavity. There are several definitions (or descriptions) for the quality factor of a cavity.

(1) $$Q = \frac{2\pi \text{ (energy stored in the system at resonance)}}{\text{(energy lost in a cycle of oscillation)}}$$

$$= \frac{2\pi}{T} \cdot \frac{W}{-dw/dt} \qquad W: \text{ Stored energy}$$

$$= \omega_0 \frac{W}{-dw/dt} \qquad \omega_0: \text{ Resonance freq.}$$

or

$$W(t) = W(0)e^{-\frac{\omega_0 t}{Q}}$$

(2) We can also have Q related to the photon lifetime τ_p

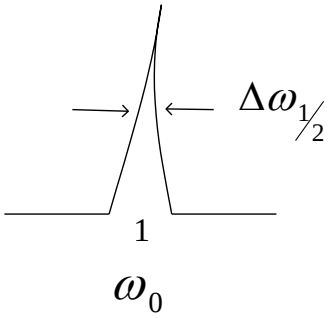
$$\tau_p = \frac{Q}{\omega_0}$$

or

$$Q = \omega_0 \tau_P$$

(3) In experiences, we can obtain the Q value from the spectrum

$$Q = \frac{\omega_0}{\Delta\omega_{\frac{1}{2}}}$$



In photonic crystals, we use the photonic crystal defect structure serve as the resonant cavity for the designed defect modes. The quality factor Q will represent a measure of how many oscillations take place inside the cavity before the excited photon energy dissipate out of the cavity. It means that the photon energy for narrow frequency bands be trapped in the cavity for longer period of time if we have a high-Q cavity.

Now the important question becomes how the defect cavity should be designed for introducing the high-Q modes into the structure. There are several examples of the high-Q photonic crystal cavities in the following pages.