ES 275 Nanophotonics

Lecture 11

Photonic Crystals:

One-Dimensional Photonic Crystals: Off-Axis Modes
Bloch Theorem
Reciprocal Lattice

One-Dimensional Photonic Crystals

From Last Time:

- Wave Equation in 1D:

$$\frac{\partial^2}{\partial z^2}E(z,t) - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\varepsilon(z)E(z,t) = 0 \qquad (10.6)$$

- Periodic Dielectric Permittivity:

$$\varepsilon(z) = \sum_{p=-\infty}^{\infty}\varepsilon_p e^{j\frac{2\pi p}{a}z} \qquad (10.8)$$

- Electric field is of Bloch form:

$$E(z,t) = \sum_{p=-\infty}^{\infty}c_p e^{j(k+p\frac{2\pi}{a})z} e^{-j\omega t} \qquad (11.1)$$

One-Dimensional Photonic Crystals

To find solutions, solve:

$$\det\begin{vmatrix} \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & (k-\frac{2\pi}{a})^2-(\frac{\omega}{c})^2\varepsilon_0 & -(\frac{\omega}{c})^2\varepsilon_{-1} & -(\frac{\omega}{c})^2\varepsilon_{-2} & \cdots \\ \cdots & -(\frac{\omega}{c})^2\varepsilon_1 & (k)^2-(\frac{\omega}{c})^2\varepsilon_0 & -(\frac{\omega}{c})^2\varepsilon_{-1} & \cdots \\ \cdots & -(\frac{\omega}{c})^2\varepsilon_2 & -(\frac{\omega}{c})^2\varepsilon_1 & (k+\frac{2\pi}{a})^2-(\frac{\omega}{c})^2\varepsilon_0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{vmatrix}=0$$

(10.16)

One-Dimensional Photonic Crystal: Off-Axis Modes

- Consider those modes with ***k*** perpendicular to the layers or the film

- Therefore, the guided mode is specified by k_x and k_z

- This time, the wave equation is given by:

$$\frac{\partial^2}{\partial x^2}E(x,z,t)+\frac{\partial^2}{\partial z^2}E(x,z,t)-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\varepsilon(z)E(x,z,t)=0 \qquad (11.2)$$

- The electric field is given by:

$$E(x,z,t)=\sum_{p=-\infty}^{\infty}c_p\, e^{j(k_z+p\frac{2\pi}{a})z}\, e^{jk_x x}e^{-j\omega t} \qquad (11.3)$$

One-Dimensional Photonic Crystal: Off-Axis Modes

- This time, we have:

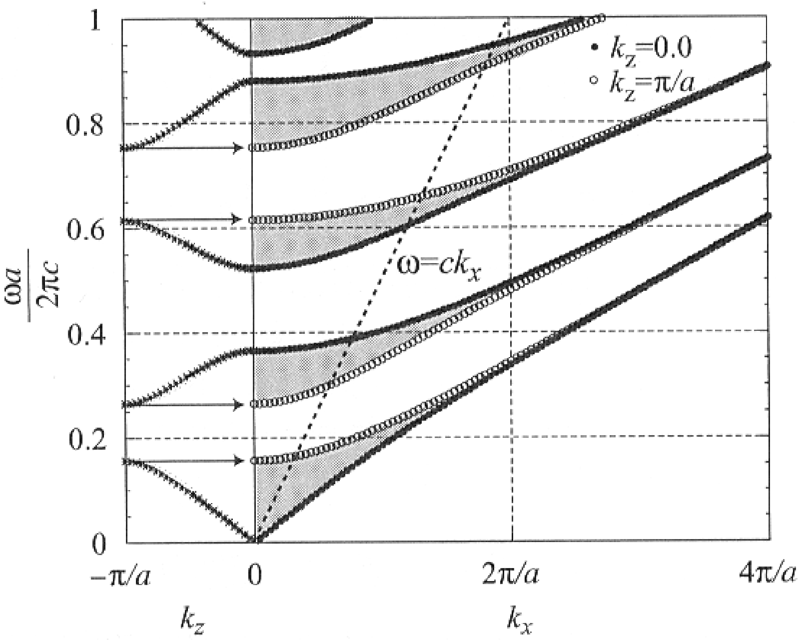
$$\{k_x^2 + (k_z + \frac{2\pi p}{a})^2\} c_p - \sum_{p'=-\infty}^{\infty} (\frac{\omega}{c})^2 \varepsilon_{p-p'} c_{p'} = 0 \qquad (p = 0, \pm 1, \pm 2, \ldots) \qquad (11.4)$$

- To find the band structure this time, we solve the equation:

$$\det\begin{vmatrix} \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & k_x^2 + (k_z - \frac{2\pi}{a})^2 - (\frac{\omega}{c})^2 \varepsilon_0 & -(\frac{\omega}{c})^2 \varepsilon_{-1} & -(\frac{\omega}{c})^2 \varepsilon_{-2} & \cdots \\ \cdots & -(\frac{\omega}{c})^2 \varepsilon_1 & k_x^2 + (k_z)^2 - (\frac{\omega}{c})^2 \varepsilon_0 & -(\frac{\omega}{c})^2 \varepsilon_{-1} & \cdots \\ \cdots & -(\frac{\omega}{c})^2 \varepsilon_2 & -(\frac{\omega}{c})^2 \varepsilon_1 & k_x^2 + (k_z + \frac{2\pi}{a})^2 - (\frac{\omega}{c})^2 \varepsilon_0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{vmatrix} = 0$$

(11.5)

One-Dimensional Photonic Crystal: Off-Axis Modes



- 1D multilayer film with two layers *A* and *B* stacked in the *z*-direction
- Dispersion of TM (s-polarized) guided modes are plotted
- Band structure with k_x=0 is given on left as function of k_z
- Shaded regions of band structure on right show continuum of bands coming from the freedom of k_z values

From: *Photonic Crystals: Physics, Fabrication and Applications*, edited by K. Inoue and K. Ohtaka, 2004

One-Dimensional Photonic Crystal: Off-Axis Modes

•For a multilayer stack of finite thickness, bounded by a surface parallel to the *x*-*y* plane:

-only the modes below the light line (shown by dashed line in figure) are true guided modes confined completely inside the photonic crystal

-those above the light line are leaky modes which can escape from the photonic crystal into air

Bloch Theorem

- In periodic dielectric media, the electric ***E(r)*** and magnetic ***H(r)*** fields are given by:

$$\boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}_{\boldsymbol{k}n}(\boldsymbol{r}) = \boldsymbol{u}_{\boldsymbol{k}n}(\boldsymbol{r})e^{j\boldsymbol{k}\cdot\boldsymbol{r}} \qquad (11.6a)$$

$$\boldsymbol{H}(\boldsymbol{r}) = \boldsymbol{H}_{\boldsymbol{k}n}(\boldsymbol{r}) = \boldsymbol{v}_{\boldsymbol{k}n}(\boldsymbol{r})e^{j\boldsymbol{k}\cdot\boldsymbol{r}} \qquad (11.6b)$$

where $\boldsymbol{u}_{\boldsymbol{k}n}(\boldsymbol{r})$ and $\boldsymbol{v}_{\boldsymbol{k}n}(\boldsymbol{r})$ are periodic vectorial functions that satisfy:

$$\boldsymbol{u}_{\boldsymbol{k}n}(\boldsymbol{r}+\boldsymbol{a}_i) = \boldsymbol{u}_{\boldsymbol{k}n}(\boldsymbol{r}) \qquad (11.7a)$$

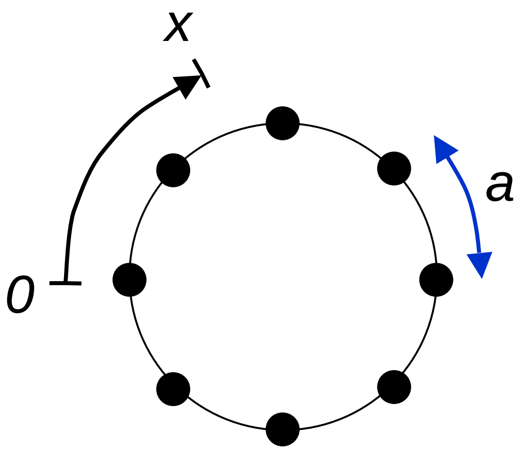
$$\boldsymbol{v}_{\boldsymbol{k}n}(\boldsymbol{r}+\boldsymbol{a}_i) = \boldsymbol{v}_{\boldsymbol{k}n}(\boldsymbol{r}) \qquad \text{for} \quad i=1,2,3 \qquad (11.7b)$$

- Note that the periodicity of the medium may be expressed as:

$$\varepsilon(\boldsymbol{r}+\boldsymbol{a}_i) = \varepsilon(\boldsymbol{r}) \qquad \text{where} \quad i=1,2,3 \qquad (11.8)$$

Proof of Bloch Theorem in 1D

- Consider *N* identical lattice points on a ring of length *Na*



- The dielectric function is periodic in *a:*

$$\varepsilon(x) = \varepsilon(x+a) \qquad (11.9)$$

- We expect solutions to obey the relation:

$$\frac{\boldsymbol{E}(x+a)}{\boldsymbol{E}(x)} = C \qquad (11.10)$$

where *C* is a constant

- Going once around the ring, we have:

$$\begin{aligned} E(x+Na) &= C^N E(x) \\ &= E(x) \qquad (11.11) \end{aligned}$$

Proof of Bloch Theorem in 1D

- Then, we have:

$$C = e^{j2\pi s/N} \quad \text{where} \;\; s = 0,\ 1,\ 2,\ 3,\ \ldots,\ N-1 \qquad (11.12)$$

- The following form for ***E****(x)* will satisfy (11.10) and (11.11):

$$\begin{aligned} \boldsymbol{E}(x) &= \boldsymbol{u}_k(x)\, e^{j\frac{2\pi s x}{Na}} \\ &= \boldsymbol{u}_k(x)\, e^{jkx} \qquad (11.13) \end{aligned}$$

- where $\boldsymbol{u}_k(x)$ is a vectorial function periodic in *a*:

$$\boldsymbol{u}_k(x+a) = \boldsymbol{u}_k(x) \qquad (11.14)$$

- This is the Bloch Theorem in 1D

The Reciprocal Lattice

- Suppose function *f(**r**)* is periodic on a lattice:

$$f(\boldsymbol{r}) = f(\boldsymbol{r} + \boldsymbol{R}) \qquad (11.14)$$

for all vectors ***R*** that translate the lattice into itself

- The set of vectors ***R*** is called the lattice vectors

- Build *f(**r**)* out of plane waves using the Fourier Transform:

$$f(\boldsymbol{r}) = \int g(\boldsymbol{q})\, e^{j\boldsymbol{q}\cdot\boldsymbol{r}}\, d\boldsymbol{q} \qquad (11.15)$$

where *g(**q**)* is the coefficient of plane waves with wave vector ***q***

- This can be performed on any well-behaved function

The Reciprocal Lattice

- Our function *f(**r**)* is periodic on the lattice, so we have:

$$\begin{aligned} f(\boldsymbol{r}+\boldsymbol{R}) &= \int g(\boldsymbol{q}) e^{j\boldsymbol{q}\cdot\boldsymbol{r}} e^{j\boldsymbol{q}\cdot\boldsymbol{R}}\, d\boldsymbol{q} \\ &= f(\boldsymbol{r}) \\ &= \int g(\boldsymbol{q}) e^{j\boldsymbol{q}\cdot\boldsymbol{r}}\, d\boldsymbol{q} \end{aligned} \qquad (11.16)$$

- Therefore, we have:

$$g(\boldsymbol{q}) = g(\boldsymbol{q}) e^{j\boldsymbol{q}\cdot\boldsymbol{R}} \qquad (11.17)$$

- Therefore, we must have:

$$g(\boldsymbol{q}) = 0 \qquad (11.18a)$$

or

$$e^{j\boldsymbol{q}\cdot\boldsymbol{R}} = 1 \qquad (11.18b)$$

The Reciprocal Lattice

- Therefore, *g(**q**)* is zero except for spikes at values of ***q*** such that:

$$e^{j\boldsymbol{q}\cdot\boldsymbol{R}} = 1 \qquad \text{for all values of } \boldsymbol{R} \qquad (11.19)$$

- So, in building a periodic function *f(**r**)* out of plane waves, we only need to use those plane waves with vectors ***q*** that satisfy (11.19)

- These vectors ***q*** satisfying (11.19) are called the reciprocal lattice vectors

- They are usually designated by ***G***

- We can build the function ***f(r)*** with an appropriate weighted sum of reciprocal lattice vectors:

$$f(\boldsymbol{r}) = \sum_{\boldsymbol{G}} f_{\boldsymbol{G}}\, e^{j\boldsymbol{G}\cdot\boldsymbol{r}} \qquad (11.20)$$

The Reciprocal Lattice

Constructing Reciprocal Lattice Vectors

- Given a lattice with a set of lattice vectors {***R***}, how do we find reciprocal lattice vectors {***G***} ?

- Need to find all ***G*** such that ***G·R*** is an integral multiple of 2π for all ***R***

- Every lattice vector ***R*** can be written in terms of the primitive lattice vectors ($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$)

- These are the smallest vectors pointing from one lattice point to another

- For a simple cubic lattice with spacing *a*, the vectors ***R*** are of the form:

$$\boldsymbol{R} = la\hat{\mathbf{x}} + ma\hat{\mathbf{y}} + na\hat{\mathbf{z}} \qquad (11.21)$$

where *(l, m, n)* are integers

The Reciprocal Lattice

- In general, we have:

$$\boldsymbol{R} = l\,\boldsymbol{a}_1 + m\,\boldsymbol{a}_2 + n\,\boldsymbol{a}_3 \qquad (11.21)$$

- The reciprocal lattice also has a set of primitive vectors (b_1, b_2, b_3) :

$$\boldsymbol{G} = l'\boldsymbol{b}_1 + m'\boldsymbol{b}_2 + n'\boldsymbol{b}_3 \qquad (11.22)$$

- So we have the requirement:

$$\boldsymbol{G}\cdot\boldsymbol{R} = (l\boldsymbol{a}_1 + m\boldsymbol{a}_2 + n\boldsymbol{a}_3)\cdot(l'\boldsymbol{b}_1 + m'\boldsymbol{b}_2 + n'\boldsymbol{b}_3) = N2\pi \qquad (11.23)$$

- We can satisfy this by choosing $\boldsymbol{b}_i$ such that:

$$\boldsymbol{a}_i\cdot\boldsymbol{b}_j = \begin{cases} 2\pi & \text{if } i = j \\ 0 & \text{otherwise} \end{cases} \qquad (11.24)$$

The Reciprocal Lattice

- Now we have the vector identity:

$$\boldsymbol{x} \cdot (\boldsymbol{x} \times \boldsymbol{y}) = 0$$ for any vectors ***x*** and ***y*** (11.25)

- Therefore, we will satisfy (11.24) if we construct primitive reciprocal lattice vectors such:

$$\boldsymbol{b}_1 = 2\pi \frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 \times \boldsymbol{a}_3} \qquad (11.26a)$$

$$\boldsymbol{b}_2 = 2\pi \frac{\boldsymbol{a}_3 \times \boldsymbol{a}_1}{\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 \times \boldsymbol{a}_3} \qquad (11.26b)$$

$$\boldsymbol{b}_3 = 2\pi \frac{\boldsymbol{a}_1 \times \boldsymbol{a}_2}{\boldsymbol{a}_1 \cdot \boldsymbol{a}_2 \times \boldsymbol{a}_3} \qquad (11.26c)$$

The Brillouin Zone

Bloch Form of the Electromagnetic Modes

$$\boldsymbol{H}_k(\boldsymbol{r}) = e^{j\boldsymbol{k}\cdot\boldsymbol{r}}\,\boldsymbol{u}_k(\boldsymbol{r}) = e^{j\boldsymbol{k}\cdot\boldsymbol{r}}\,\boldsymbol{u}_k(\boldsymbol{r}+\boldsymbol{R}) \qquad (11.27)$$

•Mode consists of a plane wave modulated by a function that shares the periodicity of the lattice

•Important feature of Bloch states: mode with wave vector ***k*** and ***k+G*** are the same mode if ***G*** is a reciprocal lattice vector

-Wave vector ***k*** serves to specify phase difference between cells that are described by ***u***

-If ***k*** is incremented by ***G***, then phase between cells is incremented by ***G·R***, which is $n2\pi$ and not really a phase difference at all

-Incrementing ***k*** by ***G*** results in the same physical mode

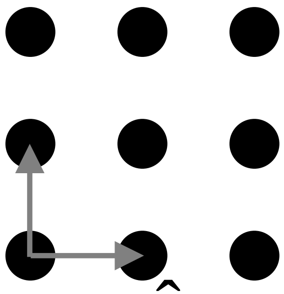
The Brillouin Zone

- We can restrict our attention to a finite zone in reciprocal space in which we cannot get from one part of the volume to another by adding ***G***

- This is called the Brillouin Zone. It is the volume around a lattice point closer to that lattice point than any other lattice point

2D Square Lattice

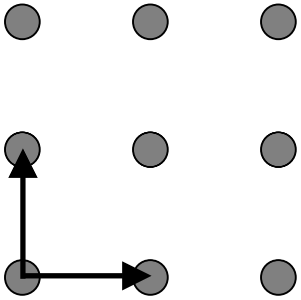
Real Lattice



$\boldsymbol{a}_1 = a\hat{x}$

$\boldsymbol{a}_2 = a\hat{y}$

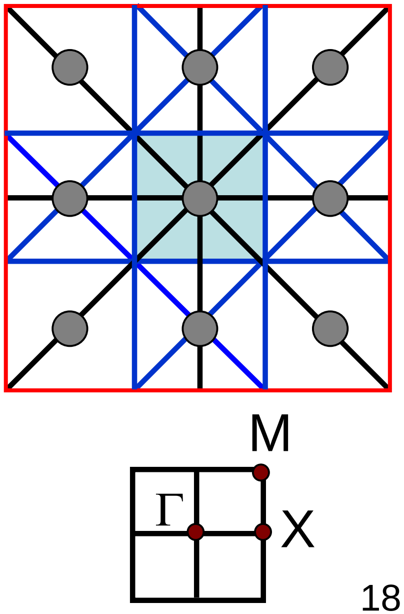
Reciprocal Lattice



$\boldsymbol{b}_1 = \frac{2\pi}{a}\hat{y}$

$\boldsymbol{b}_2 = \frac{2\pi}{a}\hat{x}$

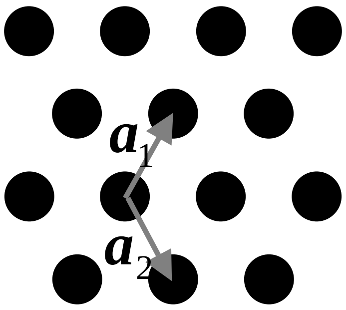
Brillouin Zone



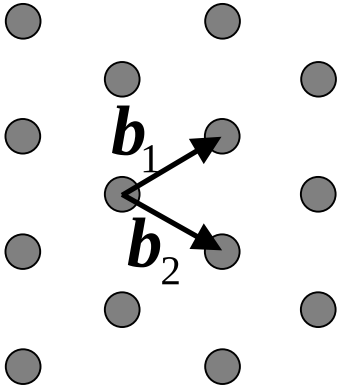
The Brillouin Zone

2D Triangular Lattice

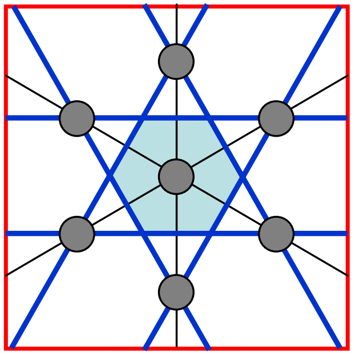
Real Lattice

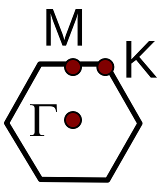


Reciprocal Lattice



Brillouin Zone





$$\boldsymbol{a}_1 = a(\hat{x}\sqrt{3}+\hat{y})/2$$

$$\boldsymbol{a}_2 = a(-\hat{x}\sqrt{3}+\hat{y})/2$$

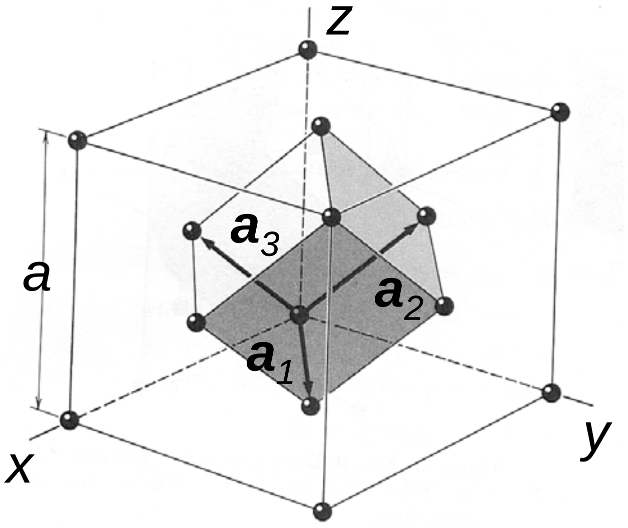
$$\boldsymbol{b}_1 = \frac{2\pi}{a}(\hat{x}\sqrt{3}+\hat{y})/2$$

$$\boldsymbol{b}_2 = \frac{2\pi}{a}(\hat{x}\sqrt{3}-\hat{y})/2$$

The Brillouin Zone

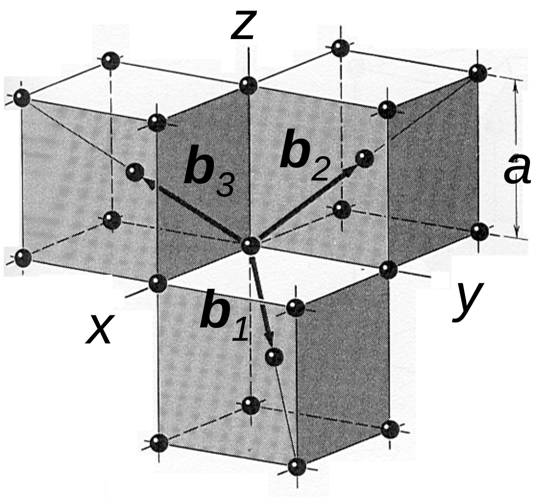
Real Lattice

Face-Centered Cubic (FCC)



Reciprocal Lattice

Body-Centered Cubic (BCC)



$$\boldsymbol{a}_1 = a(\hat{x} + \hat{y})/2$$
$$\boldsymbol{a}_2 = a(\hat{y} + \hat{z})/2$$
$$\boldsymbol{a}_3 = a(\hat{x} + \hat{z})/2$$

$$\boldsymbol{b}_1 = (2\pi/a)(\hat{x} + \hat{y} - \hat{z})$$
$$\boldsymbol{b}_2 = (2\pi/a)(-\hat{x} + \hat{y} + \hat{z})$$
$$\boldsymbol{b}_3 = (2\pi/a)(\hat{x} - \hat{y} + \hat{z})$$