OPTI6105/8505

Optical Properties of Materials I

Spring Semester 2005
TH 12:30-1:50, Rm 116 Burson
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Office Hours: 4:00-5:00 T and 3:00-5:00 W

One semester introductory core course for M.S. and Ph.D. programs in Opt. Sci. and Engineering: propagation, absorption, reflection, transmission, scattering, luminescence, birefringence in various materials.

We thank Dr. Angela Davies for providing teaching materials for this course

Welcome to Spring Semester 2005!

Text:

Main: Mark Fox, Optical Properties of Solids, Oxford University Press, 2001
Suppl: B.E.A. Saleh and M.C. Teich, Fundamentals of Photonics, John Wiley&Sons, 1991
Suppl:N.W. Ashcroft and N.D. Mermin, Solid State Physics, Thomson Learning, 1976
Suppl: Charles Kittel, Introduction to Solid State Physics, John Wiley&Sons, 8th Ed., 2005
Suppl: J.H. Simmons, Optical Materials, Acad. Press, 2000
Suppl: E. Hecht, Optics, Addison Wesley 1998

Grading:

Homeworks (~7, assigned occasionally)	25%
Student Presentations	15%
Take Home Midterm Exam	30%
Take Home Final Exam	30%

Grades will be assigned using a 10-point grading scale:
A = 90-100, B=80-89, etc.

Syllabus

Will be posted on the physics webpage, changes are possible!

Course Content

Ist part: Fox: intoduction, opt constants, E&M review, complex refractive index, January 11-25

2nd part: AM: crystal structure, reciprocal lattice, electron band structure, phonons, January 25-Mid February

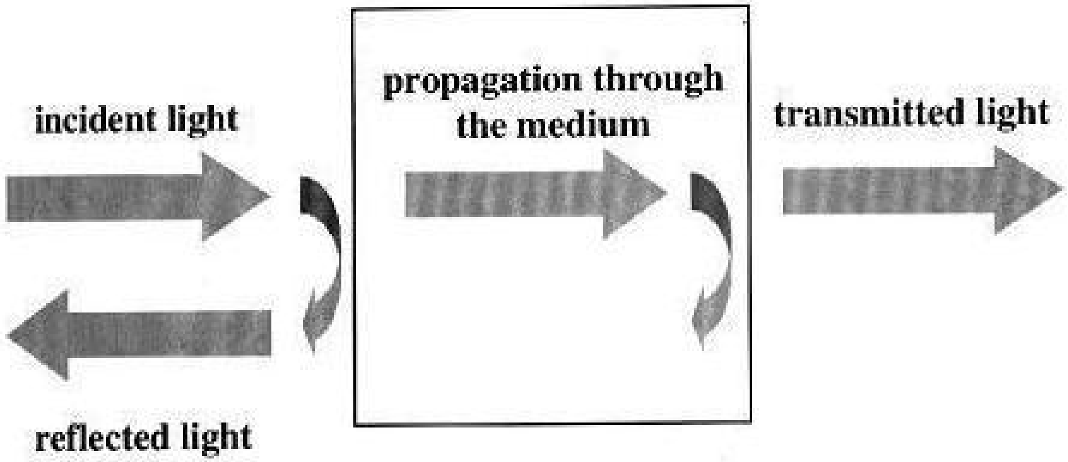
3rd part: Fox: dispersion relations, Kramers-Kroenig relations, free electron model, Mid February- Spring Break (March 8-10)

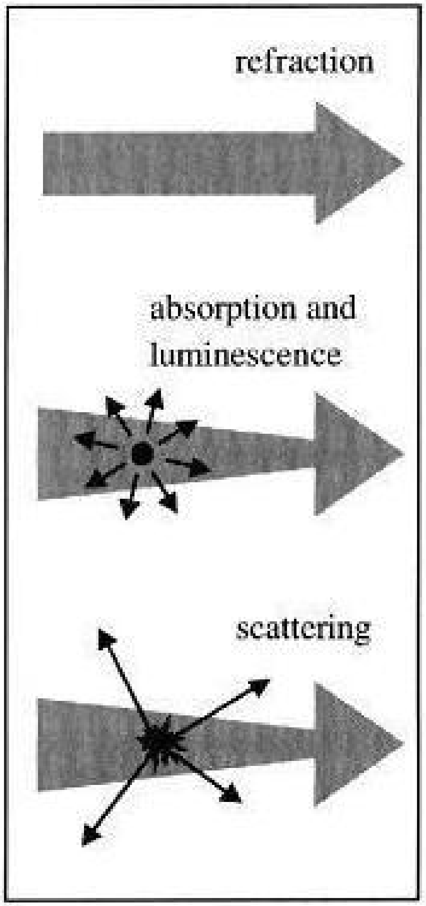
4th part: Fox: interaction of light with phonons, elastic, Raman and Brillouin scattering and glasses, March 15-end of March

5th part: Fox: birefringence, interband absorption, excitons, luminescence, metals, molecular materials, April

Lecture 1: Introduction

Classification of optical processes





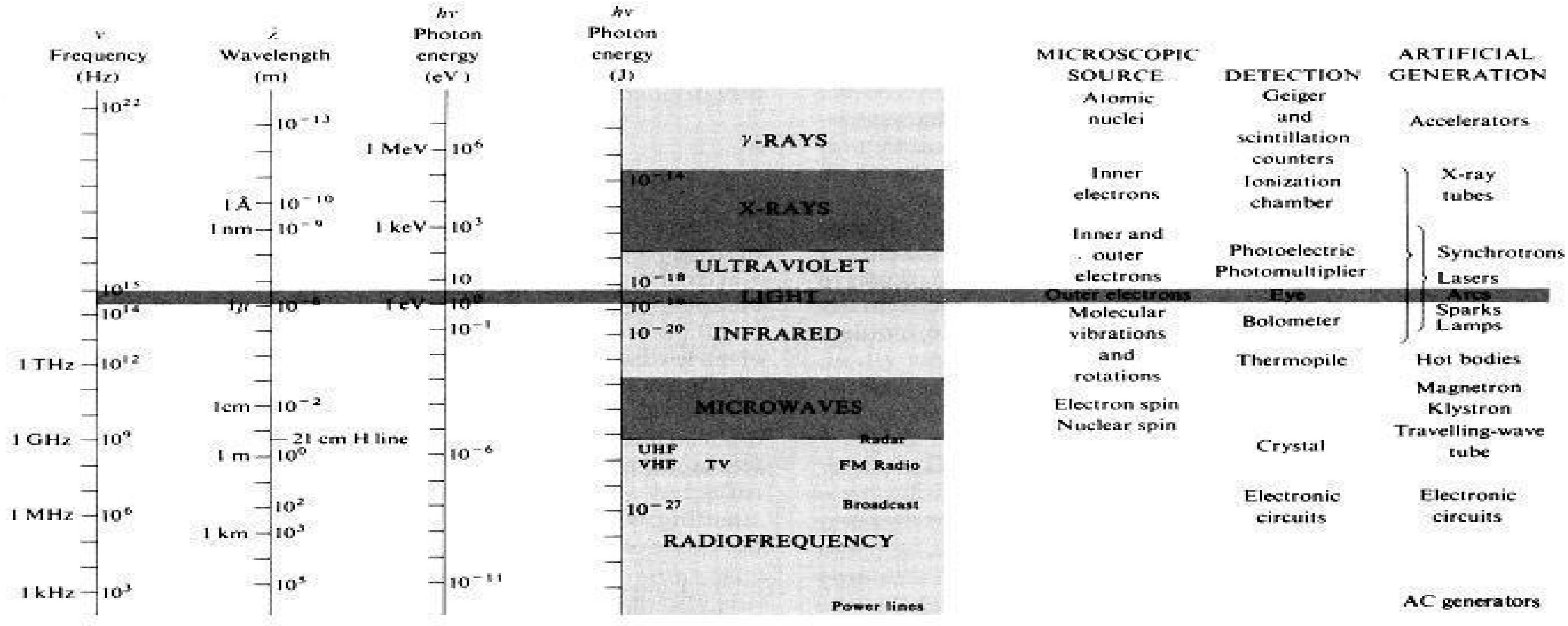
- Refraction causes the light to propagate at smaller velocities

- Absorption occurs if frequency is resonant with electronic transitions

- Luminescence is a spontaneous emission of light by atoms, depends on radiative/nonradiative lifetimes

- Scattering is associated with changing direction, the total number of photons is unchanged:
  Elastic (Example: Rayleigh)
  Inelastic (Example: Raman, Brillouin)

EM Radiation can be any frequency



$$h\nu = \frac{1.240\ \mathrm{eV}\cdot\mu\mathrm{m}}{\lambda}$$

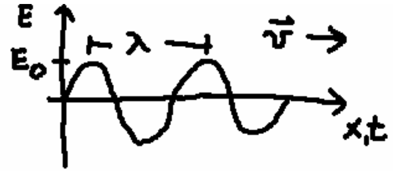
HeNe laser,
λ =633 nm ~2eV

1 eV· photon has
λ of 1.24 μ (in near IR)

$$\tilde{E} = E_0 e^{i(kx-\omega t)}$$

$$\tilde{E} = E_0[\cos(kx-\omega t) + i\sin(kx-\omega t)]$$

$$E = \mathrm{Im}[\tilde{E}] = E_0\sin(kx-\omega t)$$



$k = 2\pi/\lambda$ $\omega = 2\pi\nu$ $v = \lambda\nu$

Note: Frequency rarely if ever changes. Would need to change the energy of the photons to do that.

Velocity set by properties of material. This then sets the wavelength

Optical coefficients

- Will be using a simple plane wave propagaton
- Will be normal incidence
- Will restrict ourselves to non-magnetic materials

- Reflectivity at a surface is described by the **coefficient of reflectivity**

$$R = \frac{I_r}{I_0}$$

Ratio of Reflected to incident power

- **Coefficient of transmission or Transmissivity**

$$T = \frac{I_T \leftarrow \text{Transmitted Power}}{I_0 \leftarrow \text{Incident Power}}$$

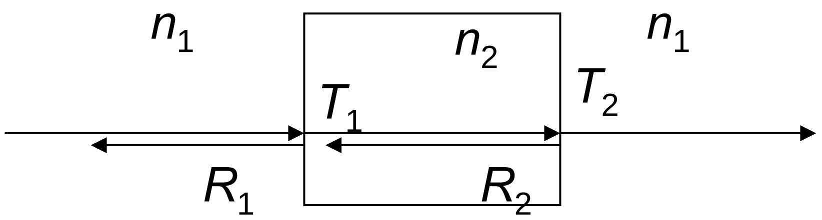
In the absence of scattering or absorption at the interface,

$$R + T = 1$$

- The power reflection (R) and transmission (T) on each interface:

$$R = (\frac{n_1 - n_2}{n_1 + n_2})^2$$

$$R + T = 1$$



- The absorption of light by the medium is quantified by its **absorption coefficient**, α

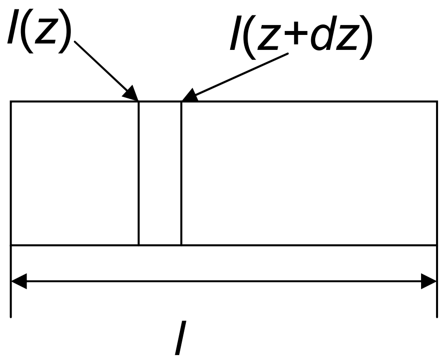
$$dI = -\alpha dz \times I(z)$$

Beer’s Law:

$$I(z) = I_0 e^{-\alpha z}$$

Attenuation due to total thickness *l*:

$$I(l) = I_0 e^{-\alpha l}$$



- The refractive index depends on frequency, **dispersion**
- The absorption coefficient is also a function frequency

Responsible for the distinct color of some materials.

Transmission through absorbing medium:

$$T = (1-R_1)e^{-\alpha l}(1-R_2)$$

usually $R_1 = R_2$

so $T = (1-R)^2 e^{-\alpha l}$

The absorption can be described in terms of the optical density, **O.D.** Called the **absorbance**.

$$O.D. = -\log_{10}\left(\frac{I(l)}{I_0}\right)$$

This can be written in terms of α

$$OD = -\log(e^{-\alpha l}) = \alpha l \log e = 0.434\,\alpha l$$

Will see OD as a specification for filters but not very useful as a general characterization of a material because the value depends on thickness.

Scattering causes attenuation in the same way as absorption and can be described similarly:

$$I(z) = I_0 e^{-N\sigma_s z}$$

$N\sigma_s$ plays role of α

scattering sites/vol.

"scattering cross-section"

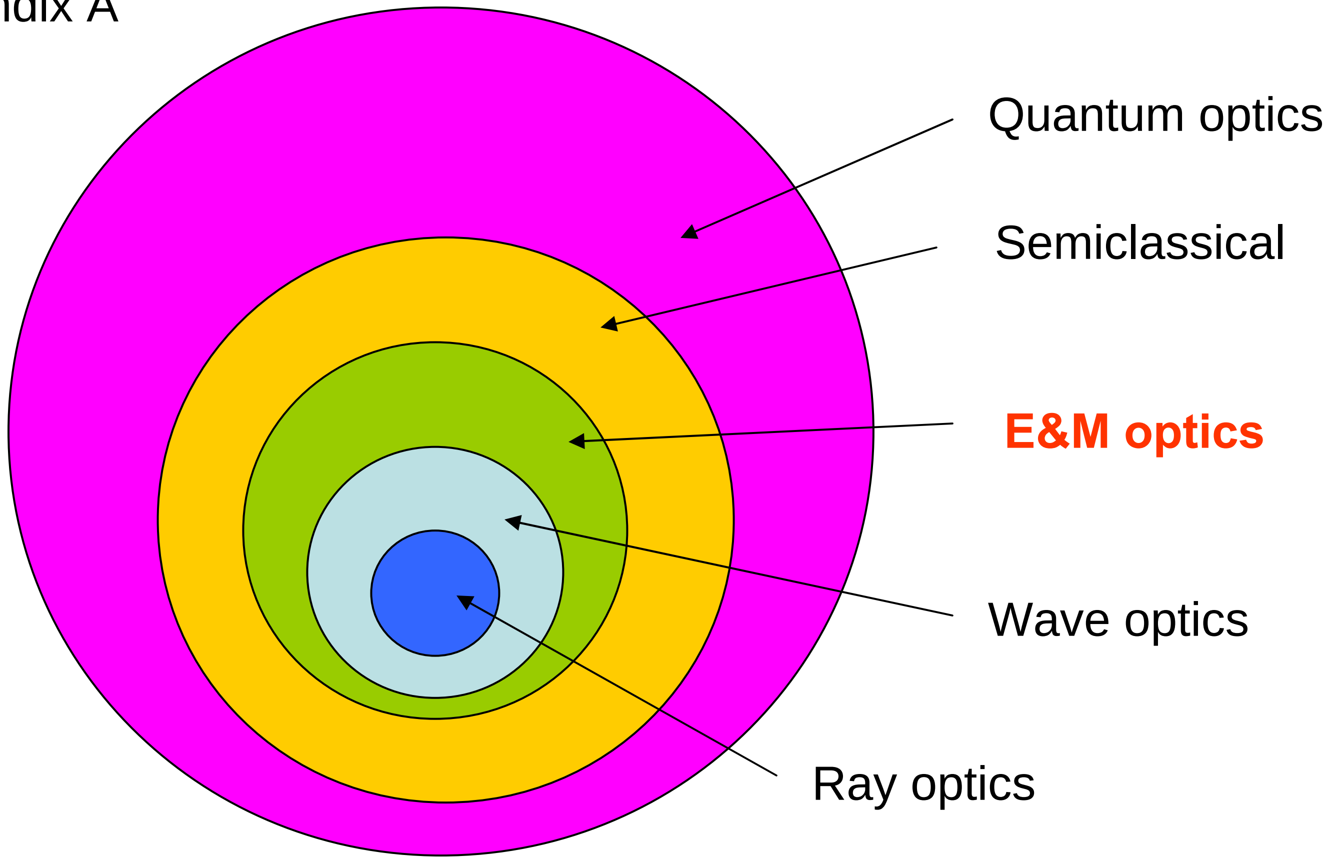
units of area $[m^2]$

Rayleigh scattering:

$$\sigma_s(\lambda) \propto \frac{1}{\lambda^4}$$

Lecture 2: E&M Review

B.E.A. Saleh & M.C. Teich, Fundamentals of Photonics, John Wiley & Sons (1991)
Fox: Appendix A



Quantum optics treats light and matter quantum mechanically
Semiclassical – treat light classically, but apply QM to atoms
E&M optics – treats both light and material classically
Wave optics is the scalar approximation of E&M
Ray optics is the limit of wave optics when λ is very short

Goals: Maxwell’s Equations
What determines phase velocity?

Waves on strings

$$v = \sqrt{\frac{\tau}{\mu}} = \sqrt{\frac{elastic}{inertial}}$$

Sound Waves

$$v = \sqrt{\frac{B}{\rho}}$$

Require medium
For “tight” and “light” media *v* is higher

EM wave doesn’t require medium!

Maxwell’s Equations in Free Space

$$\overline{\nabla} \times \overline{H} = \varepsilon_0 \frac{\partial \overline{E}}{\partial t} \qquad (1)$$

Displacement current in a capacitor

$$\overline{\nabla} \times \overline{E} = -\mu_0 \frac{\partial \overline{H}}{\partial t} \qquad (2)$$

Faraday Law+Lenz’s Rule

$$\overline{\nabla} \cdot \overline{E} = 0 \qquad (3)$$

No electric charges

$$\overline{\nabla} \cdot \overline{H} = 0 \qquad (4)$$

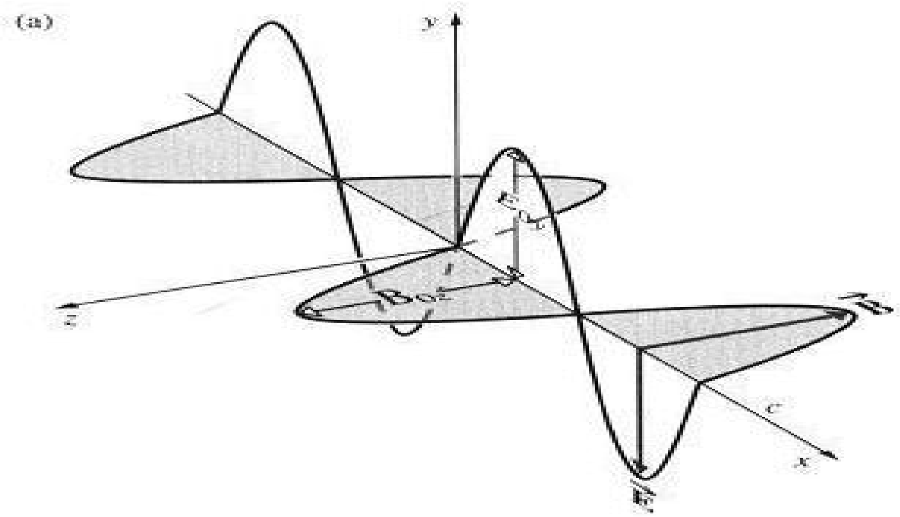
No magnetic charges

$\varepsilon_0 = 8.85\ 10^{-12}$ F/m, $\mu_0 = 1.26\ 10^{-6}$ Tm/A

The Wave Equation:

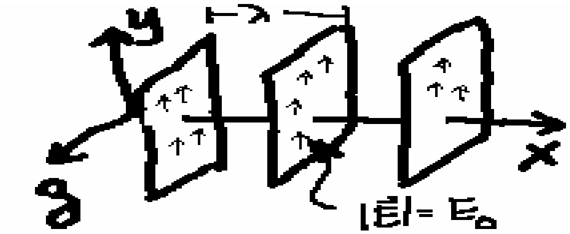
$$\nabla^2 u - \frac{1}{c_0^2}\frac{\partial^2 u}{\partial t^2} = 0$$

Where: $$c_0 = \frac{1}{(\varepsilon_0 \mu_0)^{1/2}} = 3\times 10^8 m/s$$



$$\vec{E} = E_0 \hat{y} e^{i(kx-\omega t)}$$

$$\vec{B} = B_0 \hat{z} e^{i(kx-\omega t)}$$



- EM waves are **transverse waves** (like string waves).

$$\vec{E} = \vec{E}_0 e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

Polarization information

$$\vec{k} = \frac{2\pi}{\lambda}\hat{k}$$

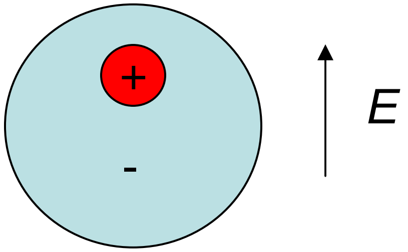
Unit vector in propagation direction

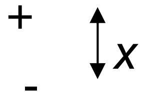
- For isotropic materials we can ignore the polarization and use scalar wave theory:

$$E = E_0 e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

What is different in the medium? (Microscopic picture of polarization)

Simplistic model of an atom in an electric field:

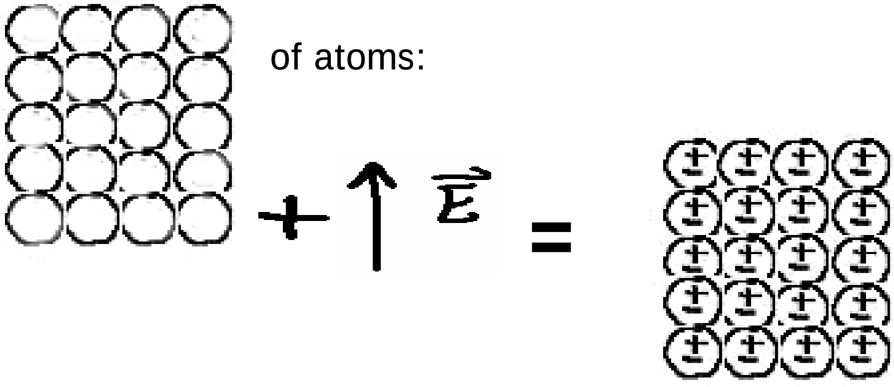




$p=qx$, $x \sim E$

$\bar{p} = \alpha \bar{E}$ α - atomic polarizability

of atoms:



$\Rightarrow \vec{P} = n\vec{p}$

“The dipole moment per unit volume”

atoms/vol.

So, $P \sim E$

$\vec{P} = \epsilon_0 \chi \vec{E}$

Electric permittivity of free space

Electric susceptibility of the material

Continuing macroscopic discussion…

$$\overline{D} = \varepsilon_0 \overline{E} + \overline{P}$$

$$\overline{B} = \mu_0 \overline{H} + \mu_0 \overline{M}$$

D – electric displacement
P – polarization density
B – magnetic flux density
M – magnetization density

$$\overline{\nabla} \times \overline{H} = \frac{\partial \overline{D}}{\partial t}$$

$$\overline{\nabla} \times \overline{E} = -\frac{\partial \overline{B}}{\partial t}$$

$$\overline{\nabla} \cdot \overline{D} = 0$$

$$\overline{\nabla} \cdot \overline{B} = 0$$

In free space, $\boldsymbol{P}=\boldsymbol{M}=0$, so that $\boldsymbol{D}=\varepsilon_0\boldsymbol{E}$ and $\boldsymbol{B}=\mu_0\boldsymbol{H}$, and (1-4) recovers

Intensity and Power

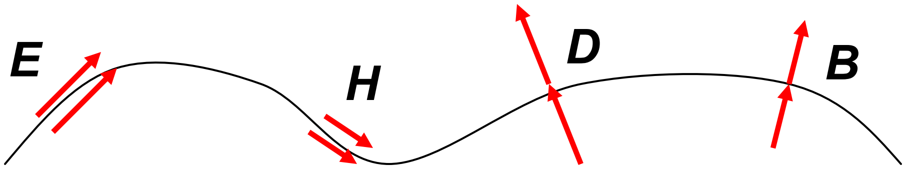
Poynting vector: $\boldsymbol{S} = \boldsymbol{E} \times \boldsymbol{H}$ represents the flow of EM power. The optical intensity (power flow across a unit area): $\boldsymbol{I} = \langle \boldsymbol{S} \rangle$

Boundary Conditions

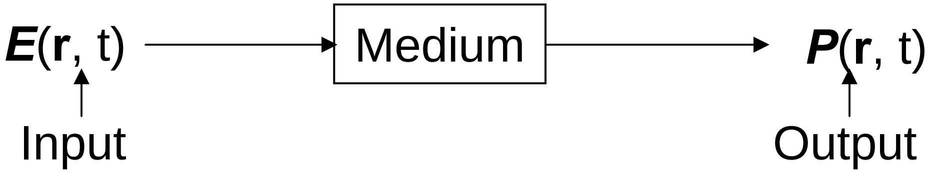
At the boundary between two dielectric media and in the *absence of free charges and currents*:

- Tangential components of ***E*** and ***H***
- Normal components of ***D*** and ***B***

Must be continuous



Dielectric Media



$\boldsymbol{E}(\mathbf{r}, t)$ → Medium → $\boldsymbol{P}(\mathbf{r}, t)$

Input

Output

Linear:

$\boldsymbol{P}(\mathbf{r}, t)$ is linearly related to $\boldsymbol{E}(\mathbf{r}, t)$

Nondispersive:

$\boldsymbol{P}(\mathbf{r}, t)$ is determined by $\boldsymbol{E}(\mathbf{r}, t)$ at the same time ‘t’, instantaneous response

Homogeneous:

Relation between $\boldsymbol{P}(\mathbf{r}, t)$ and $\boldsymbol{E}(\mathbf{r}, t)$ is independent of $\mathbf{r}$.

Isotropic:

Relation between $\boldsymbol{P}(\mathbf{r}, t)$ and $\boldsymbol{E}(\mathbf{r}, t)$ is independent of the direction of $\boldsymbol{E}$.

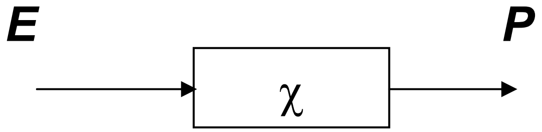
Spatially nondispersive:

Relation between $\boldsymbol{P}(\mathbf{r}, t)$ and $\boldsymbol{E}(\mathbf{r}, t)$ is local.

Lecture 3: Complex Index, K-vector and ε

Linear, Nondispersive, Homogeneous, and Isotropic Media

$P = \varepsilon_0 \chi E$, χ - electric susceptibility



Under these conditions:

$$\overline{\nabla} \times \overline{H} = \varepsilon \frac{\partial \overline{E}}{\partial t}$$

$$\overline{\nabla} \times \overline{E} = -\mu_0 \frac{\partial \overline{H}}{\partial t}$$

$$\overline{\nabla} \cdot \overline{E} = 0$$

$$\overline{\nabla} \cdot \overline{H} = 0$$

Since ***D*** and ***E*** are parallel:

$D = \varepsilon E$, where $\varepsilon = \varepsilon_0(1 + \chi) = \varepsilon_0 \, \varepsilon_r$ - electric permittivity of the medium,

$\varepsilon_r = \varepsilon/\varepsilon_0 = (1 + \chi)$ – relative dielectr. constant

By analogy with the free space case:

$$\nabla^2 u - \frac{1}{v^2} \frac{\partial^2 u}{\partial t^2} = 0 \qquad c_0 = \frac{1}{(\varepsilon_0 \mu_0)^{1/2}} = 3 \times 10^8 \, m/s$$

Where $v = c/n$ – speed of light in a Medium

$$n = \left(\frac{\varepsilon}{\varepsilon_0} \right)^{1/2} = \varepsilon_r^{1/2} = (1 + \chi)^{1/2}$$ - Refractive Index

Magnetic phenomena were neglected

$\boldsymbol{B} = \mu_0\boldsymbol{H} + \mu_0\boldsymbol{M}$, $\boldsymbol{M} = \chi_m\boldsymbol{H}$
$\boldsymbol{B} = \mu\boldsymbol{H}$, where $\mu = \mu_0(1+\chi_m)$, χ_m - magnetic susceptibility

Magnitization can be classified as:

•Diagmagnetic (due to interaction of external
Field with orbital motion of electrons, causes B to decrease)

•Paramagnetism (due to interactions of spin of unpaired
electrons with field, causes B to increase

•Ferromagnitism: Material with a large internal
magnetization (e.g. Iron, cobalt, nickel)

Will not be dealing with ferromagnetic material in this class. For most materials, paramagnetic and diagmetic affects lead to:

$\chi_m \sim 10^{-8} – 10^{-5}$, hence $\mu_r \cong 1$, $\mu \cong \mu_0$

Complex Refractive Index and Conductivity

The origin of imaginary part can be traced down to the conductivity of material. In a conductor: ***j*** = σ***E***.

Real current is included in a full Ampere-Maxwell law:

$$\overline{\nabla}\times\overline{H}=\boxed{\overline{j}}+\frac{\partial\overline{D}}{\partial t}$$

By substituting ***j*** and eliminating ***D***, ***B***, and ***H*** we have:

$$\nabla^2\overline{E}-\boxed{\sigma\mu_0\frac{\partial\overline{E}}{\partial t}}-\frac{1}{v^2}\frac{\partial^2\overline{E}}{\partial t^2}=0$$

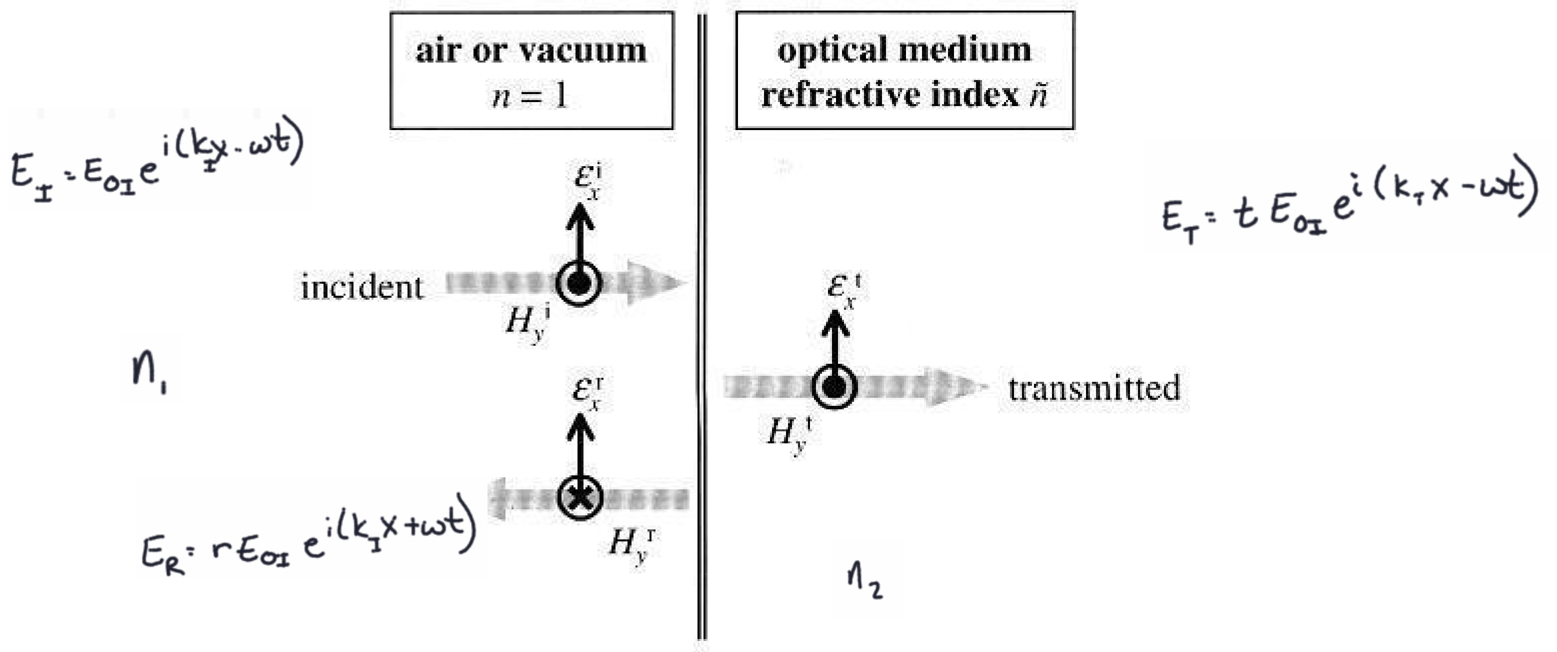
Substituting $\overline{E}(z,t)=\overline{E}_0e^{i(kz-\omega t)}$ gives:

$$k^2=\boxed{i\sigma\mu_0\omega}+(\omega/v)^2$$

On the other hand: $k = n\omega/c$. If *k*-complex, why don't we introduce complex *n*?

$$n^2=\boxed{i\sigma/(\varepsilon_0\omega)}+\varepsilon_r$$

Behavior at a boundary: Reflection and Transmission



Boundary Conditions:

$$E_x^i + E_x^r = E_x^t \qquad (1)$$

$$H_y^i - H_y^r = H_y^t \qquad (2)$$

i,*r*,*t* – incident, reflected and transmitted beams. The sign “-” for reflected *H* component is due to opposite directions of $\boldsymbol{S}_i = \boldsymbol{E} \times \boldsymbol{H}$ and $\boldsymbol{S}_r$.

Taking into account the relationship between the magnitudes of ***E*** and ***H*** vectors:

$$H_y^i = c\varepsilon_0 n_1 E_x^i \qquad H_y^t = c\varepsilon_0 n_2 E_x^t \qquad H_y^r = c\varepsilon_0 n_1 E_x^r$$

Assuming n_1 = 1, and n_2 = *n* we can represent (2):

$$E_x^i - E_x^r = \tilde{n} E_x^t \qquad (3)$$

By soliving (1) and (3) together we obtain:

$$\frac{E_x^r}{E_x^i} = \frac{\tilde{n} - 1}{\tilde{n} + 1}$$

That can be rearranged to obtain the result:

$$R = \left| \frac{E_x^r}{E_x^i} \right|^2 = \left| \frac{\tilde{n} - 1}{\tilde{n} + 1} \right|^2$$

Complex Refractive Index and Dielectric Constant

$$\tilde{n} = n + iK$$

K - extinction coefficient. Since n=$\sqrt{\varepsilon_r}$ and n – complex we can introduce

$\boldsymbol{\varepsilon_r} = \varepsilon_1 + i\varepsilon_2$

The link between ε_1, $i\varepsilon_2$ from one side and *n*, *K* from another side:

$$\varepsilon_1 = n^2 - K^2$$

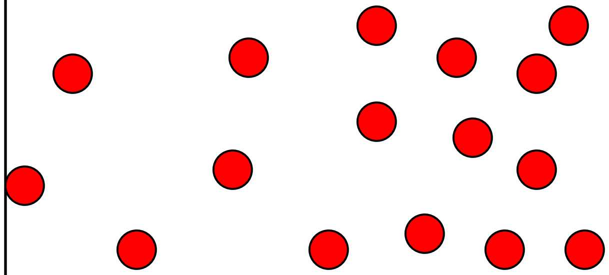
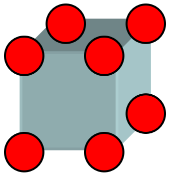
$$n = \frac{1}{\sqrt{2}}(\varepsilon_1 + (\varepsilon_1^2 + \varepsilon_2^2)^{\frac{1}{2}})^{\frac{1}{2}}$$

$$\varepsilon_2 = 2nK$$

$$K = \frac{1}{\sqrt{2}}(-\varepsilon_1 + (\varepsilon_1^2 + \varepsilon_2^2)^{\frac{1}{2}})^{\frac{1}{2}}$$

Lecture 4: Crystal Structure

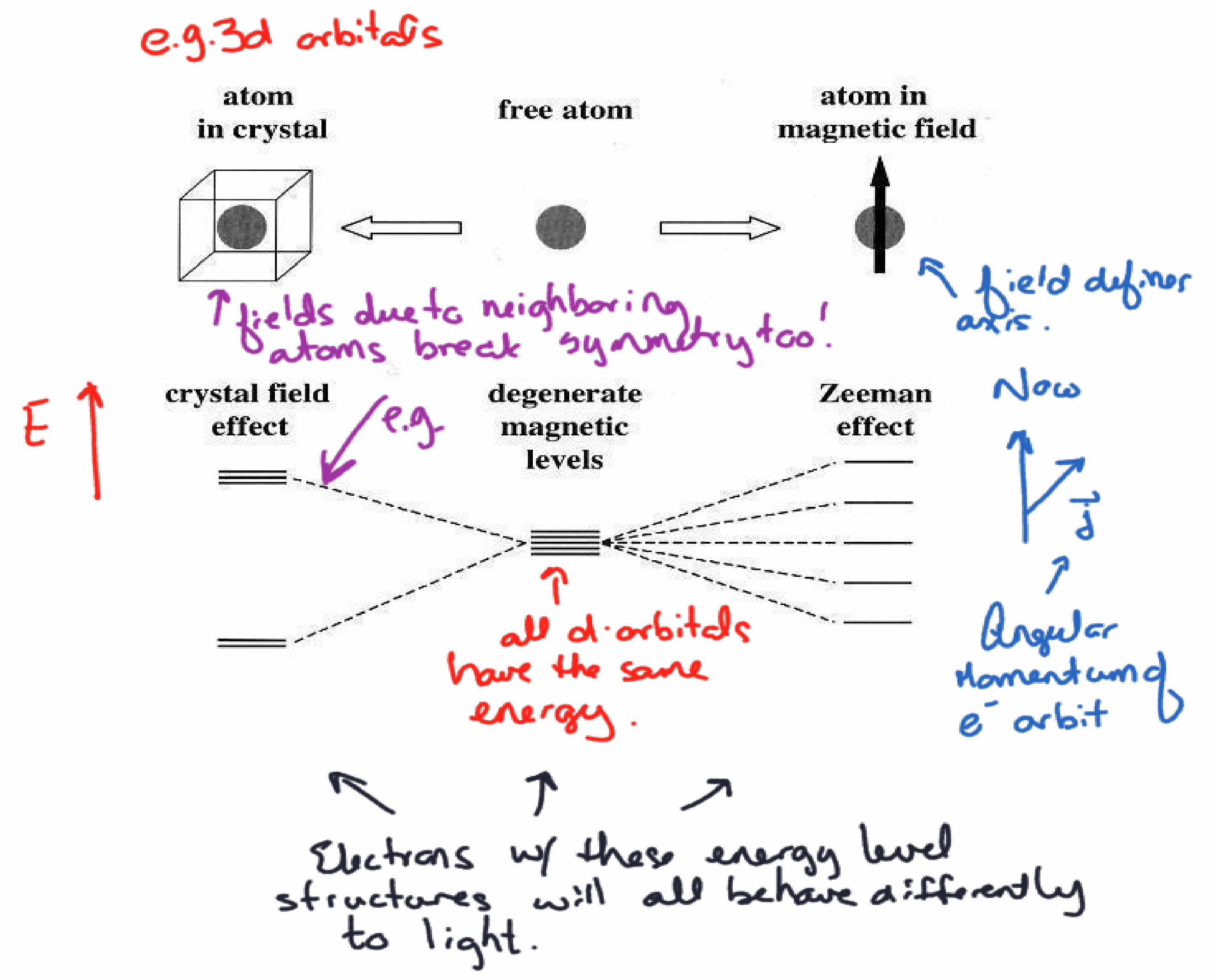
Features of Optical Physics in Solid State

Free Atoms	Gases, Liquids, Glasses	Solids
		
Atomic or Molecular Physics Spherically symmetric	No translational symmetry Weak interaction High density	Translational symmetry Stronger interaction

Aspects of the solid particularly relevant to the optical properties:

- crystal symmetry
- electronic bands (conservation of *E* and *k*-vector will dictate allowed transitions).
- Vibronic bands, phonons. Small energy, play a critical role in scattering and in k-vector conservation.
- The density of states (directly related to the absorption coefficient).
- Delocalized states and collective states: excitons, plasmon, polaritons.

Crystal Symmetry



↑ fields due to neighboring atoms break symmetry too!

↖ field defines axis.

↑ all d-orbitals have the same energy.

↗ Angular Momentum of e^- orbit

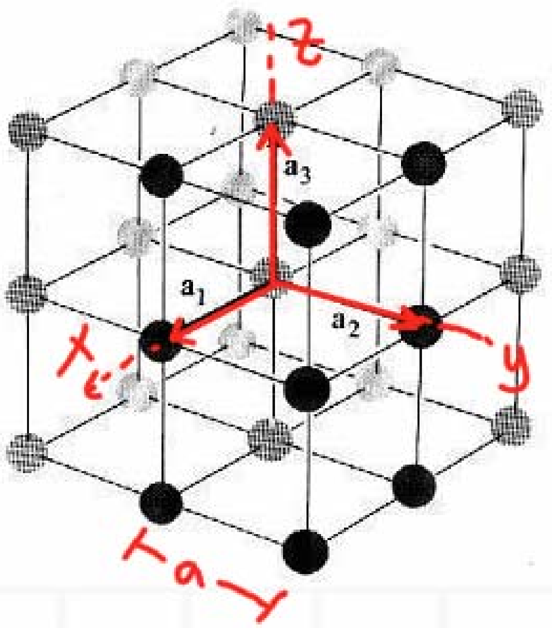
Electrons w/ these energy level structures will all behave differently to light.

Lifting of degeneracies by reduction of the symmetry.
Optical anisotropy (Neumann's Principle):
Macroscopic physical properties must have at least the symmetry of the crystal structure

Bravais Lattice

Bravais Lattice, Unit Cell and Basis

A 3-D Bravais lattice consists of all points with position vectors ***R*** of the form:
$\boldsymbol{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$

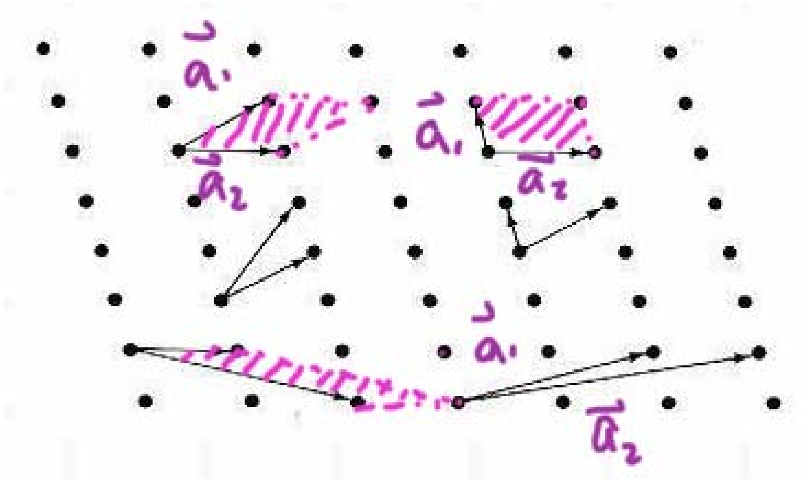


Definition Holds in 3D.
← Simple Cubic Bravais Lattice.
w/ generators $\vec{a}_1, \vec{a}_2, \vec{a}_3$
$\vec{a}_1 = a\hat{x}$ $\vec{a}_2 = a\hat{y}$ $\vec{a}_3 = a\hat{z}$

Coordination #: Number of nearest neighbors
e.g. for S.C. structure, c# is 6

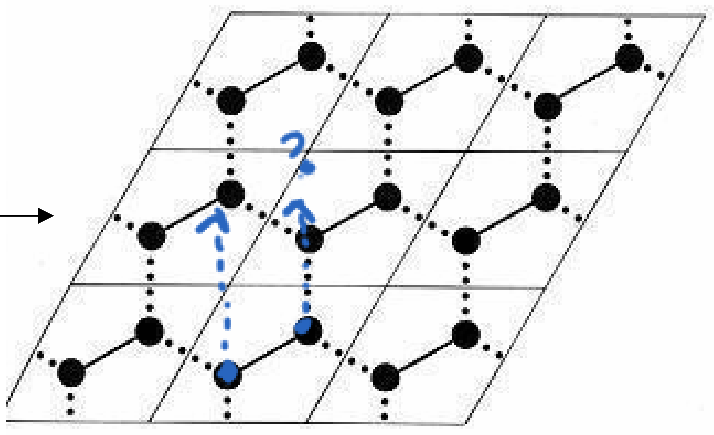
What defines a legitimate pair?

2-D Examples:



The parallelogram (primitive unit cell) defined by the pair must enclose only 1 lattice site…

Homeycomb lattice
Not a Bravais Lattice

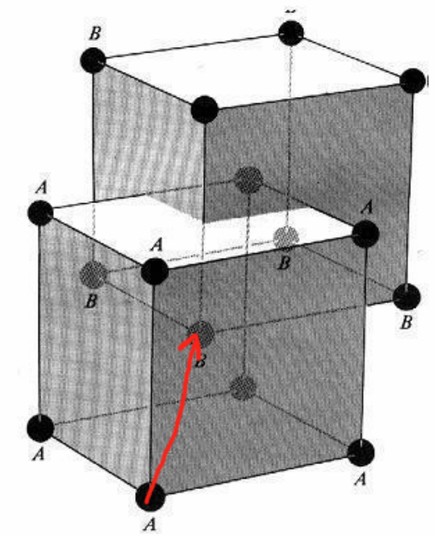


Need to define this as a lattice with a basis

Body-Centered Cubic (BCC) Lattice

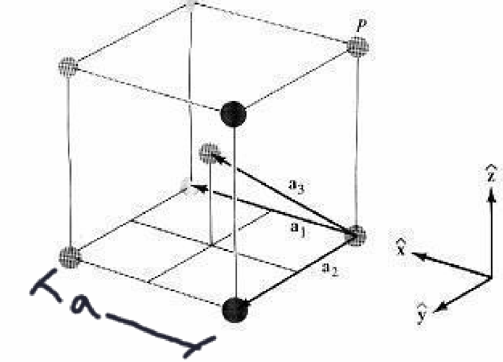
BCC Lattice: e.g. Fe, Cr, Cs, …

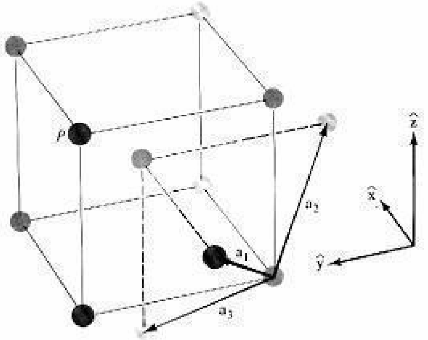
Is it Bravais Lattice?
What is the coordination number?



2nd S.C. Bravais lattice offset by ½ along cube diagonal

Examples of Primitive Vectors





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

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

$$\vec{a}_3 = \frac{1}{2}a(\hat{x}+\hat{y}+\hat{z})$$

a better, symmetric choice.

$$\vec{a}_1 = \frac{1}{2}a(-\hat{x}+\hat{z})$$

$$\vec{a}_2 = \frac{1}{2}a(\hat{x}-\hat{y})$$

$$\vec{a}_3 = \frac{1}{2}a(\hat{x}-\hat{z})$$

Face-Centered Cubic (FCC) Lattice

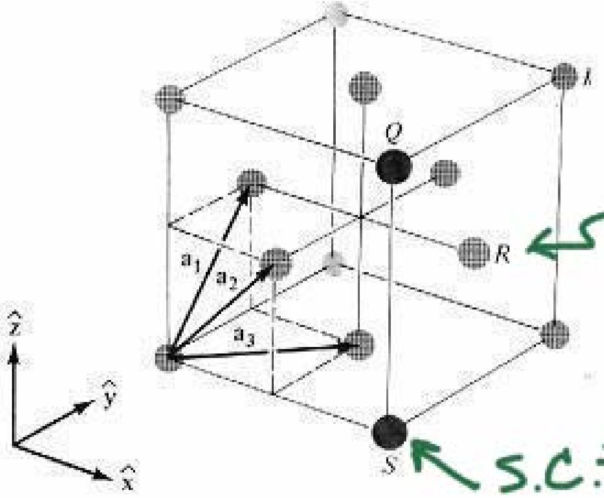
FCC Lattice: e.g. Au, Ag, Al, Cu…

Is it Bravais Lattice?
What is the coordination number?

$R = \mathbf{a}_2 + \mathbf{a}_3$

$L = \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$

$Q = 2\mathbf{a}_2$



sc #2, translated by $a/2\,\hat{x}$, $a/2\,\hat{z}$

s.c. #1

Coord # = 12

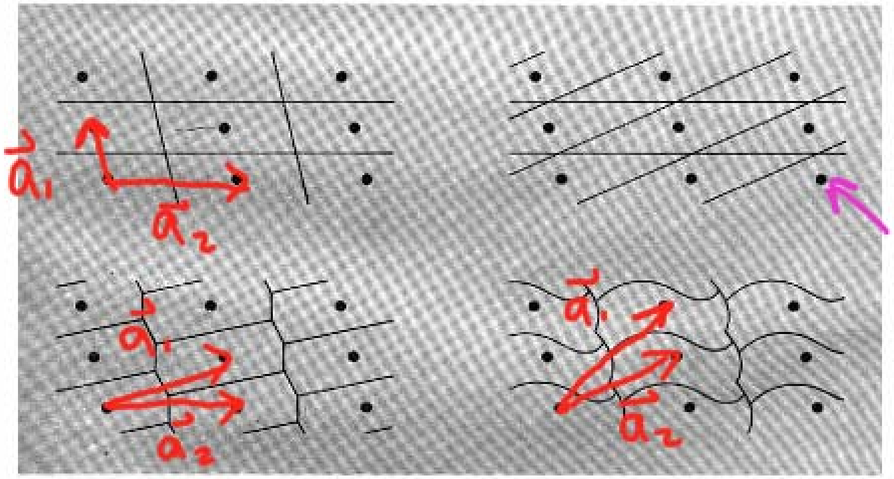
Symetric Primitive Vectors:

$\vec{a}_1 = \frac{a}{2}\hat{y} + a/2\,\hat{z}$ $\vec{a}_2 = a/2\,\hat{x} + a/2\,\hat{z}$ $\vec{a}_3 = a/2\,\hat{x} + \frac{a}{2}\hat{y}$

Primitive Unit Cell

A volume that, when translated in a Bravais lattice, fills all of space without overlapping itself or leaving voids.

Ex 2D structure. Different shaped cells, but each is periodic



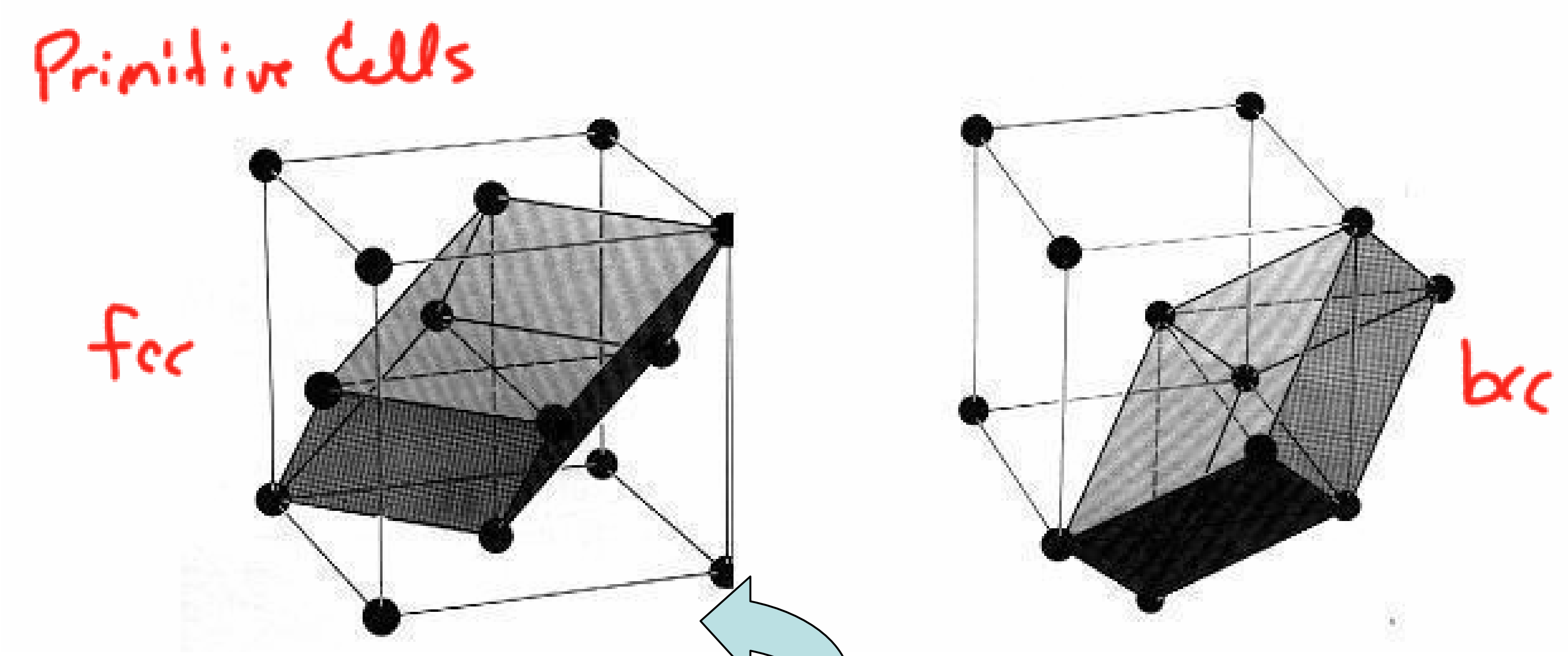
lattice Point

Translate by lattice Pts to repeat in space

A primitive cell must contain precisely one lattice point: *nv* = 1 where *n* – density of points, *v* – volume of the primitive cell.

Primitive Unit Cell (Continued)

Obvious primitive cell:
$\mathbf{r} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + x_3\mathbf{a}_3$, where $0 < x_i < 1$

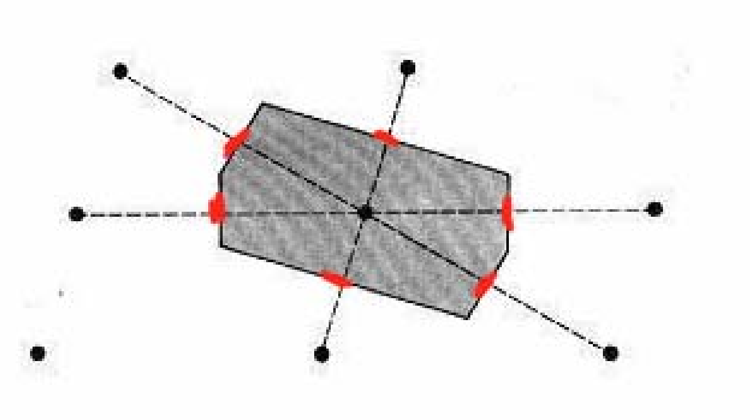


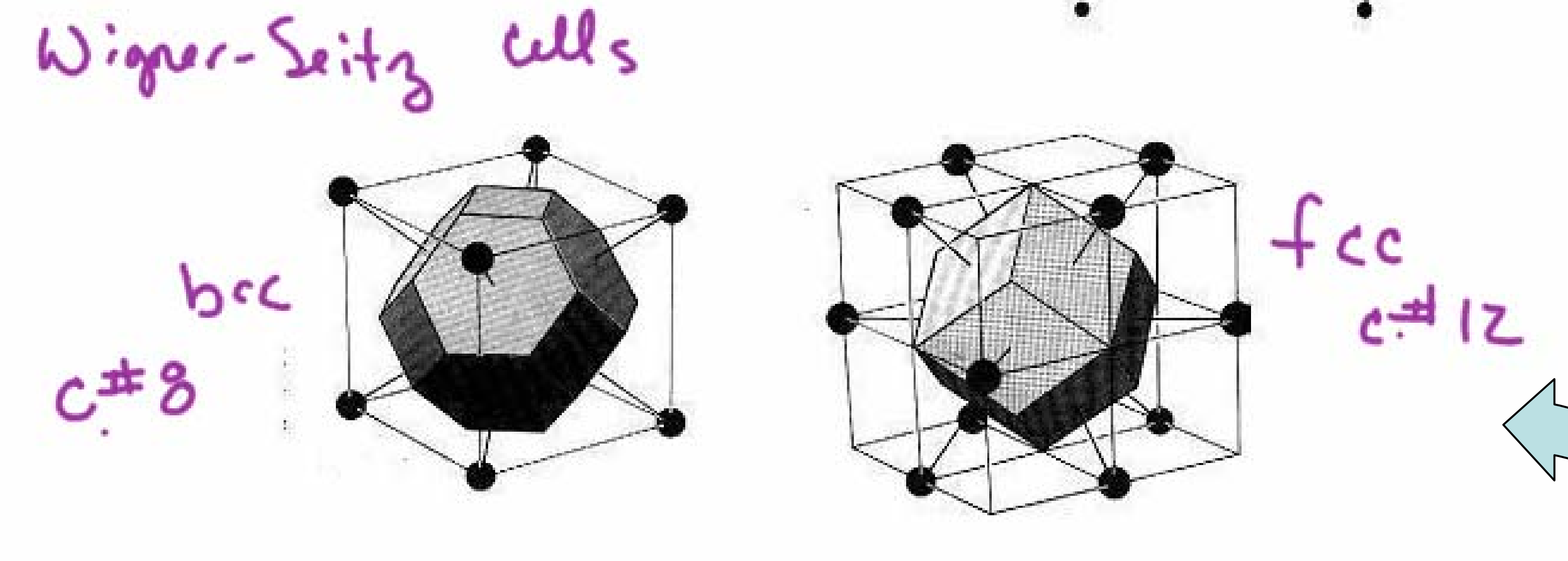
Conventional unit cell – large cube
Primitive cell – figure with six parallelogram faces, ¼ *v* and less symmetry

Disadvantage: doesn't display the full symmetry of the Bravais lattices.

Wigner-Seitz Primitive Cell

Region around a lattice point such that the area enclosed is closest the enclosed point than to any other lattice point.



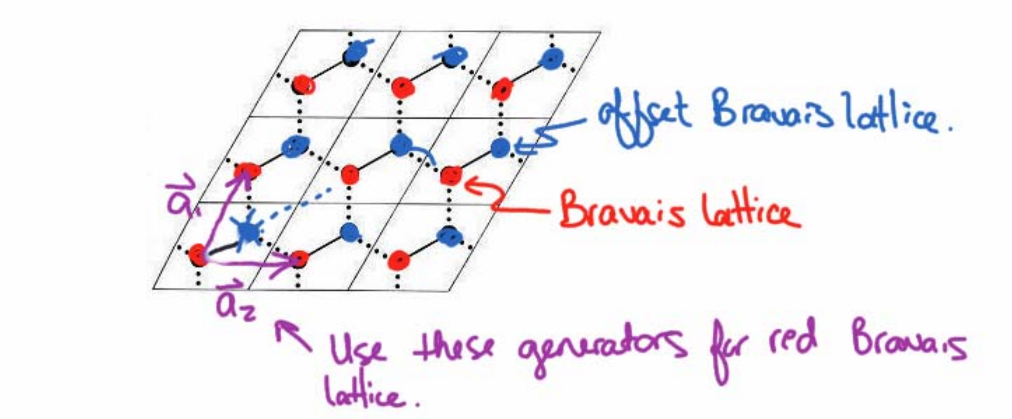


Wigner-Seitz cells

The surrounding cube in not the conventional FCC cell, but a shifted one

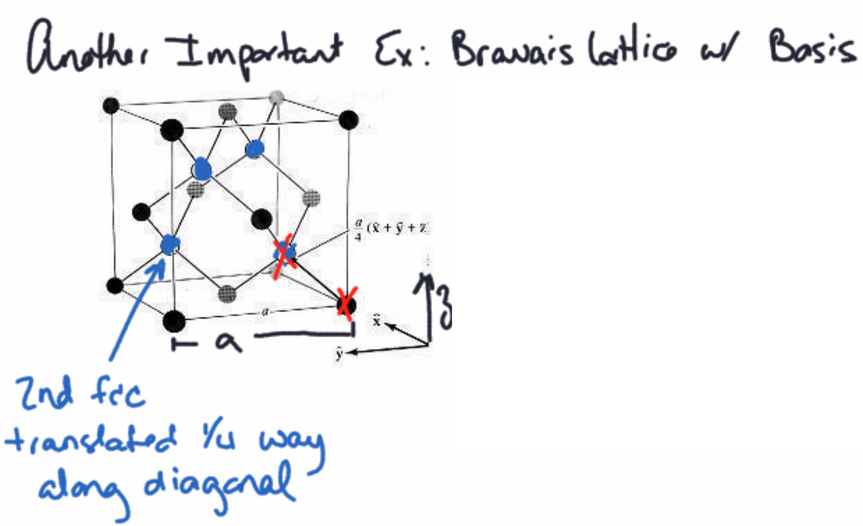
Not all periodic structures are equivalent to a Bravais Lattice with a single-point basis

Honeycomb lattice in 2-D:



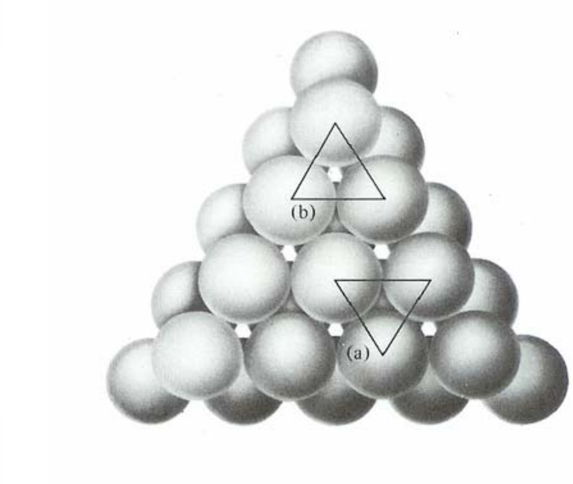
Can be considered as a 2-D triangular Bravais lattice with a ***two-point basis***

Diamond structure in 3-D:



Can be regarded as a FCC lattice with the two-point basis 0 and (a/4)(**x**+**y**+**z**)

Hexagonal Close-Packed (HCP):



Can be regarded as a hexagonal lattice with the two-point basis

Lecture 5: The Reciprocal Lattice

This is an important concept:

- Theory of crystal diffraction
- *Study of functions with the periodicity of Bravais lattice*
- Laws of momentum conservation in periodic structures

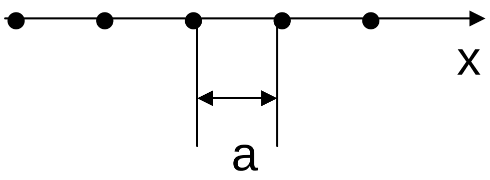
Definition:

Consider Bravais lattice with points represented by $\mathbf{R}(n_1, n_2, n_3)$ and a plane wave, $e^{i\mathbf{kr}}$.
For certain ***K*** the plane waves will have the periodicity of a given Bravais lattice:

$$e^{i\bar{K}(\bar{r}+\bar{R})} = e^{i\bar{K}\bar{r}} \quad \Longrightarrow \quad e^{i\bar{K}\bar{R}} = 1$$

Should be held for all **R**'s

Simplest example 1-D:



The direct lattice: $\mathbf{R} = n\mathbf{a}$, the reciprocal lattice: $\boldsymbol{k} = k\mathbf{b}$.
Let us require $\mathbf{ba} = 2\pi$, then $\boldsymbol{k}\mathbf{R} = 2\pi k_1 n$ which means that $k_1 = 0,1,2,\ldots$
Thus the reciprocal lattice is a Bravais lattice where ***b*** can be taken as a primitive vector.

Reciprocal Lattice in a 3-D case

Can be generated by the three primitive vectors:

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

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

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

This leads to $\mathbf{b}_i\, \mathbf{a}_j = 2\pi\delta_{ij}$, where δ_{ij} is the Kronecker delta symbol

For any $\mathbf{k} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3$ and

$\mathbf{R}=n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ we have:

$\mathbf{kR} = 2\pi(k_1n_1 + k_2n_2 + k_3n_3)$

Thus $e^{i\overline{K}\,\overline{R}} = 1$ is satisfied by those **k**-vectors, and the reciprocal lattice as a Bravais lattice and $\mathbf{b}_i$ – are primitive vectors.

Important Examples

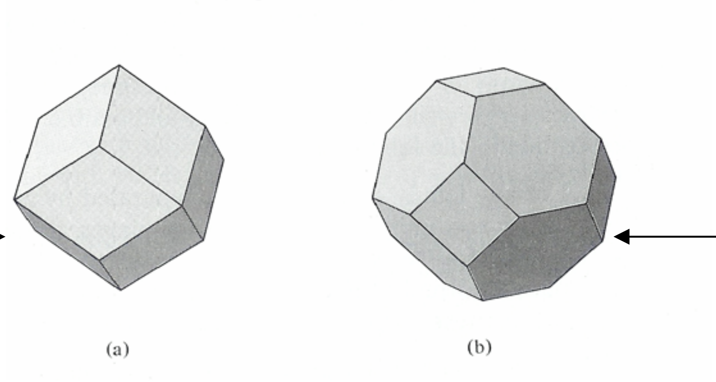
Direct Lattice	**Corresponding Reciprocal**
Simple Cubic (SC): $\mathbf{a}_1=a\mathbf{x}$, $\mathbf{a}_2=a\mathbf{y}$, $\mathbf{a}_3=a\mathbf{z}$	SC with $\mathbf{b}_1 = (2\pi/a)\mathbf{x}$, …
FCC with a cubic cell of side *a*	BCC with a cubic cell of side $4\pi/a$
BCC with a cubic cell of side *a*	FCC with a cubic cell of $4\pi/a$
Simple Hexagonal (SH) with lattice constants *a* and *c*	SH with $2\pi/c$ and $4\pi/(\sqrt{3}a)$

- The reciprocal of reciprocal lattice is nothing but the original direct lattice.

- If *v* is the volume of a primitive cell in the direct lattice, then the primitive cell of the reciprocal lattice has volume $(2\pi)^3/v$

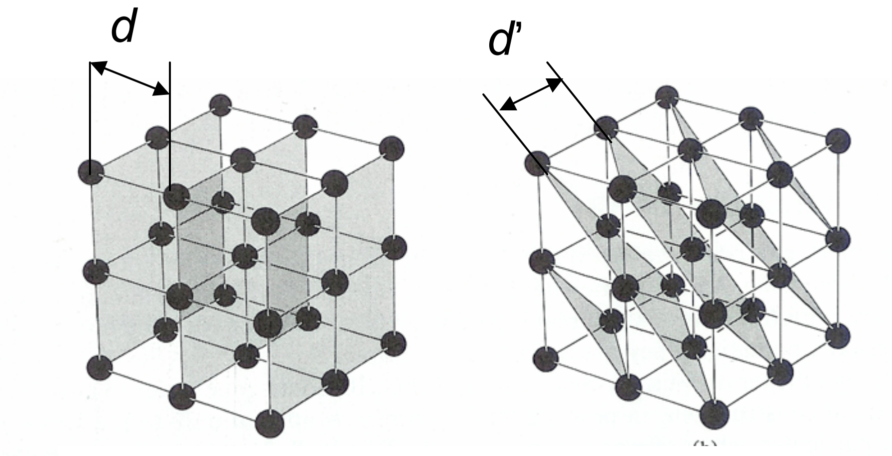
- The Wigner-Seitz primitive cell of the reciprocal lattice is known as the first Brillouin zone.

The first Brillouin zone for the BCC lattice



The first Brillouin zone for the FCC lattice

Lattice Planes and their Miller Indices



- For any *family of lattice planes* separated by d there are perpendicular lattice vectors, with the shortest of which have a length of $2\pi/d$.

- The Miller indices of a lattice plane (h, k, l) are the coordinates of the shortest reciprocal lattice vector normal to that plane

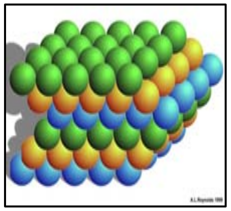
- Miller indices depend on the particular choice of primitive vectors. Plane with indices h, k, l, is normal to the reciprocal lattice vector $h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$.

- FCC and BCC Bravais lattices are described in terms of a conventional cubic cell, SC with bases. In crystallography to determine the orientation of lattice planes in real space: How to find Miller indices from the real space analysis?
$\underset{\text{recipr.}}{h : k : l} = \underset{\text{direct}}{(1/x_1) : (1/x_2) : (1/x_3)}$, where x_i- intercepts of the plane along the crystal axes.

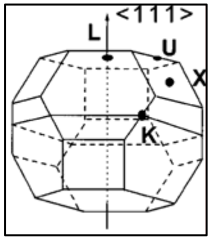
- Directions in a direct lattice can be specified by $[n_1\ n_2\ n_3]$ indices (not to be confused with Miller indices): $n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$

Crystallography of Photonic Crystals – Opals

3-D FCC

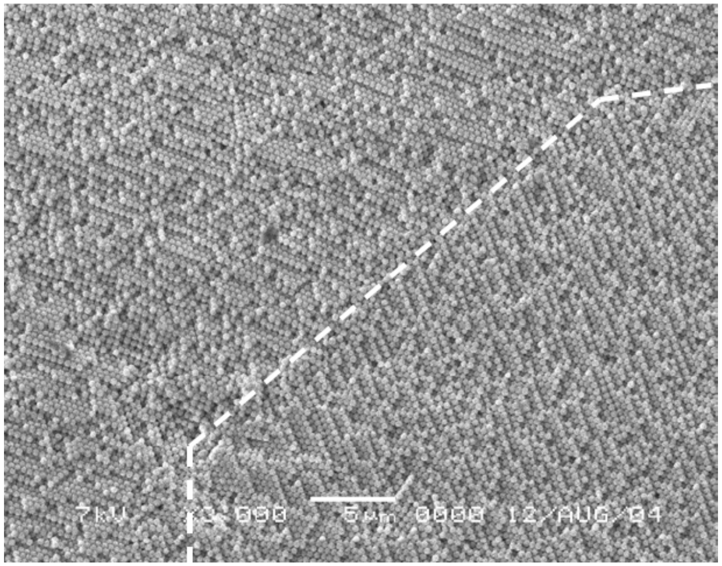


K-space

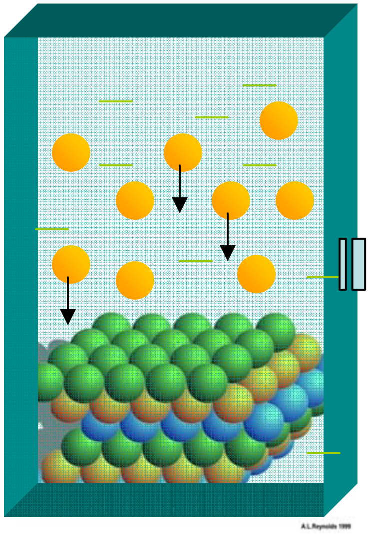


Size of the spheres 0.2-0.5 micron ~ λ

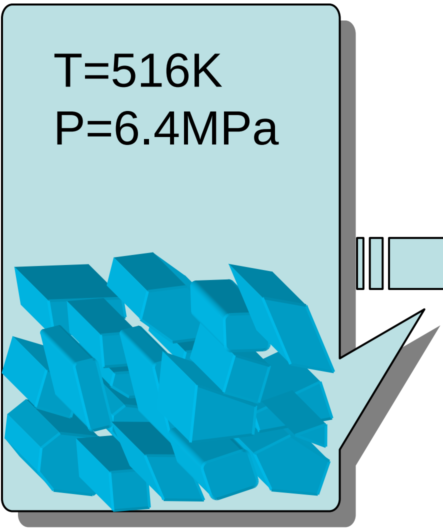
SEM of polished surface



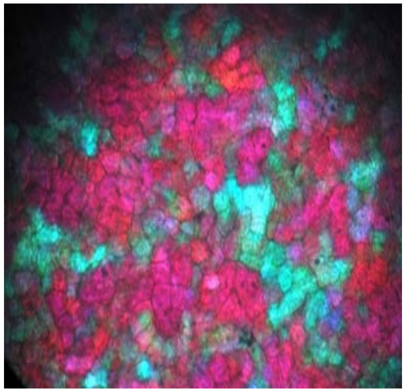
Sedimentation



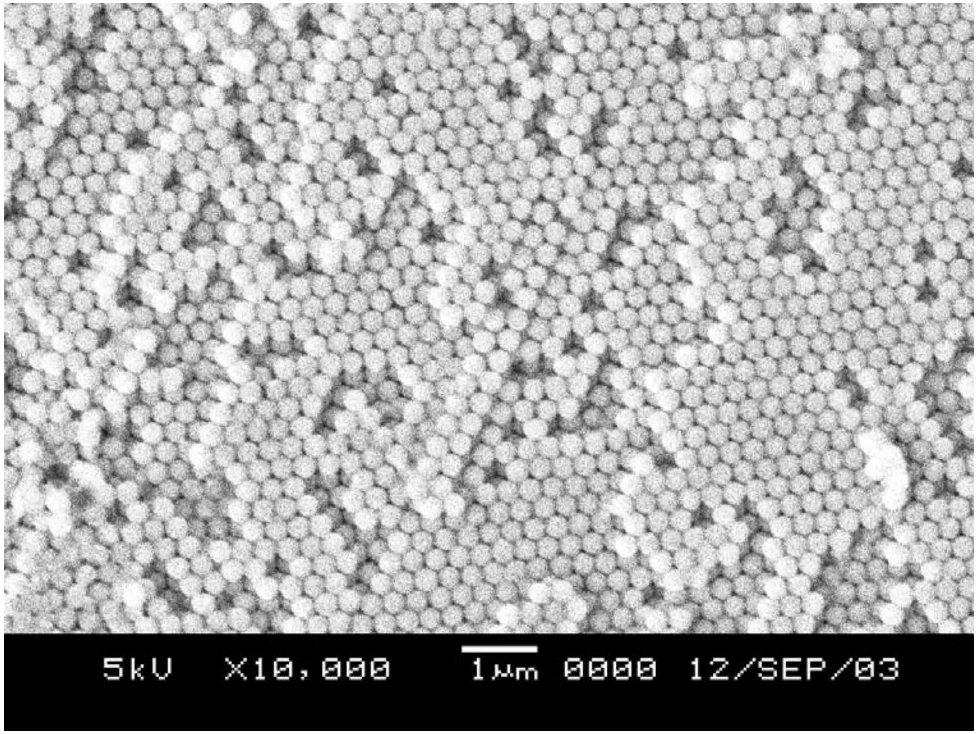
Structural collapse



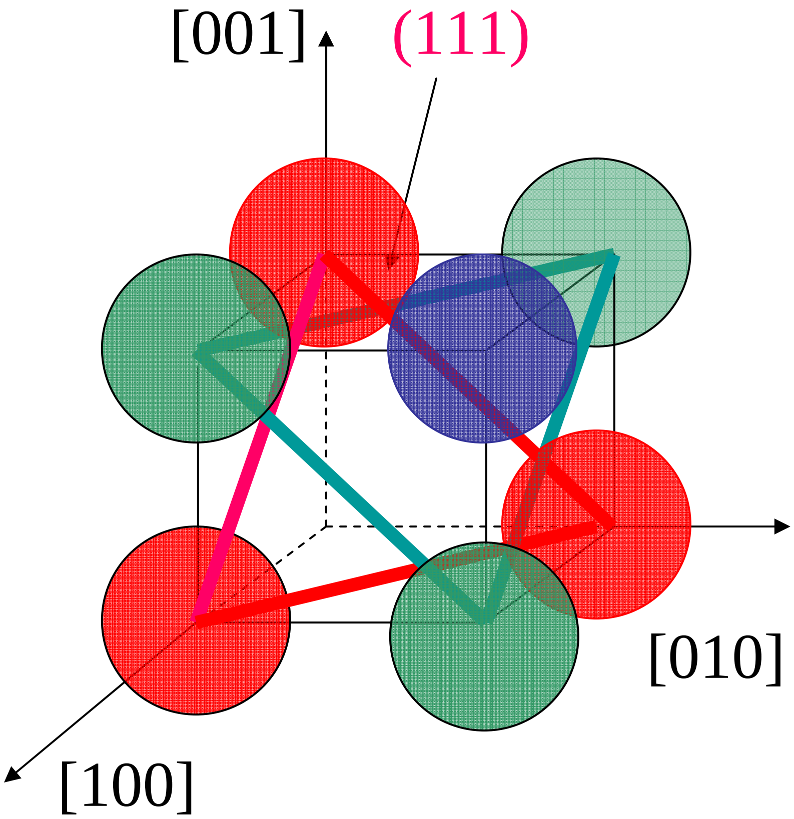
T=516K
P=6.4MPa



Triangular packing for (111) planes – *L* point



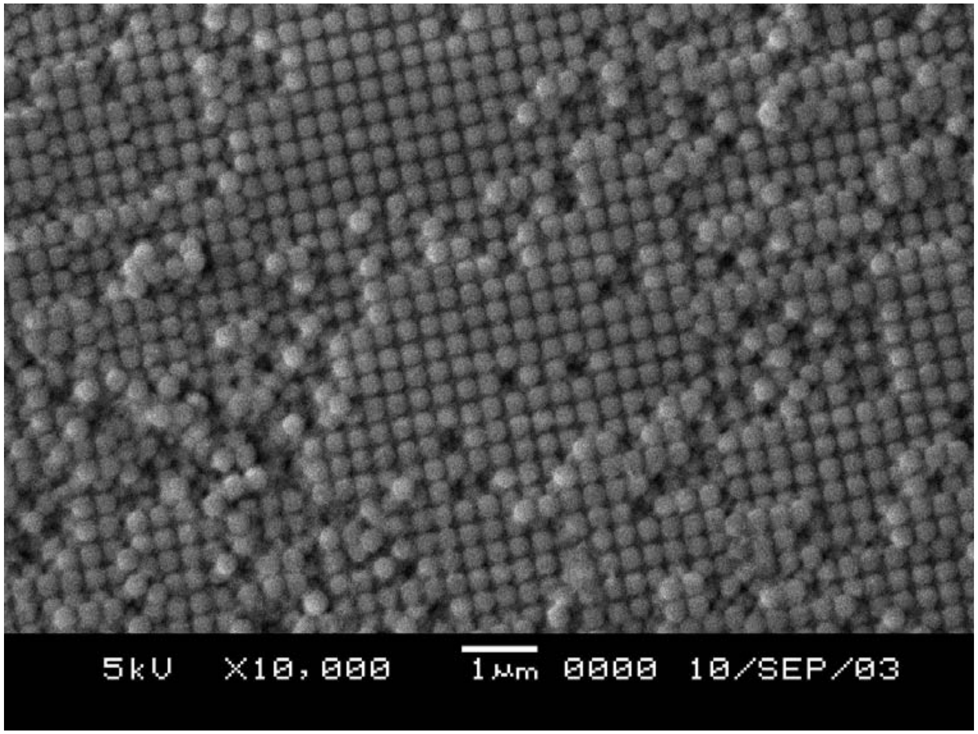
Conventional cubic cell:

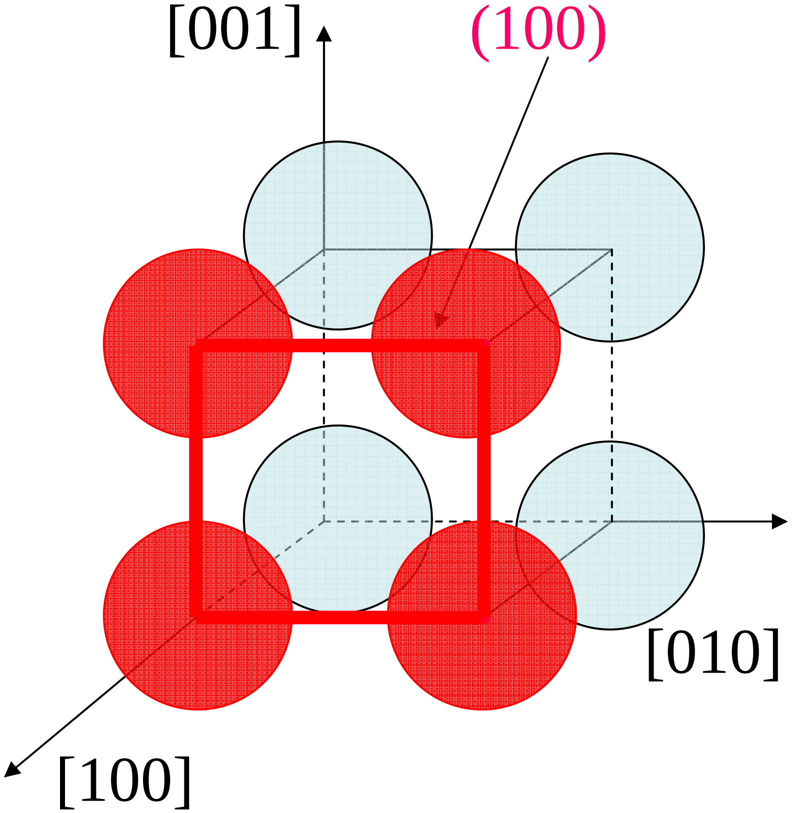


- Represented ~10% of the total surface area of the samples

Square Packing for (100) planes – *X* point

SEM

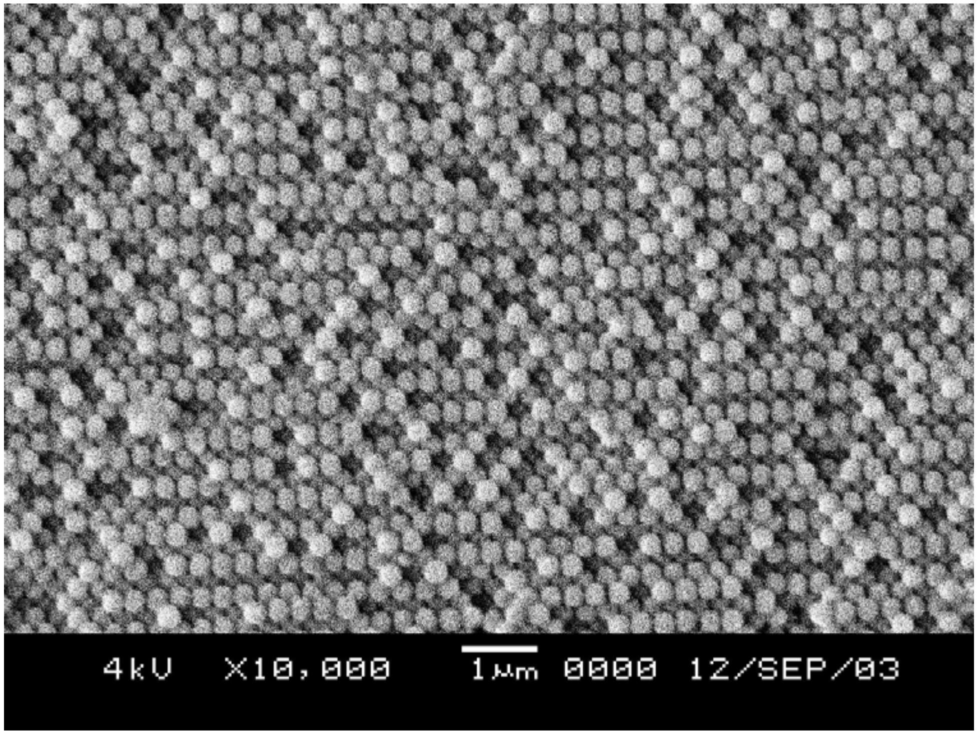


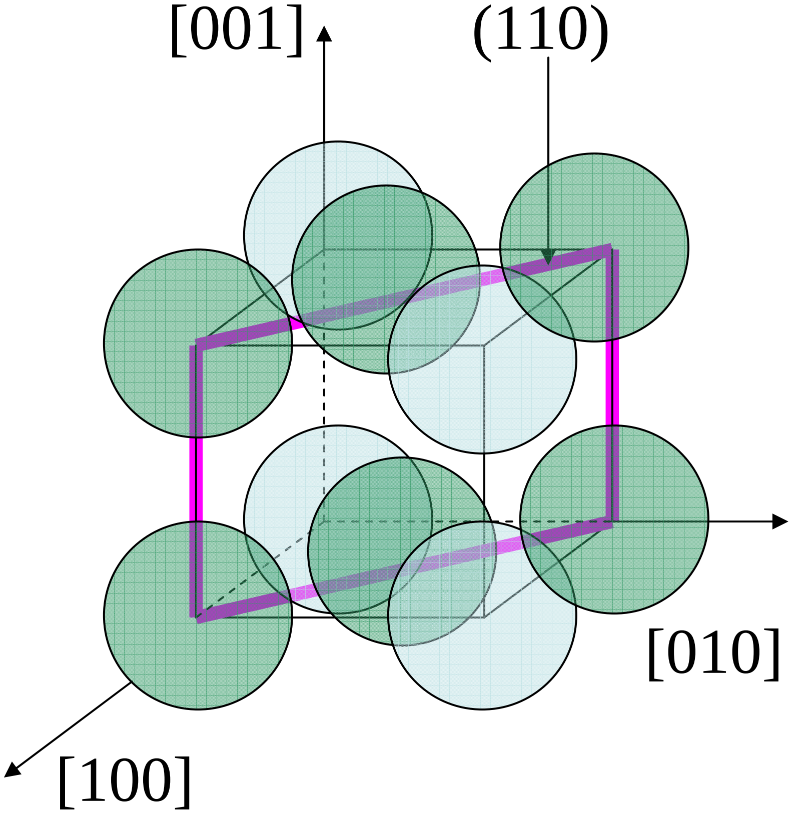


- Represented at ~70% of the total surface area of the samples

Rectangular packing for (110) – *K* point

SEM





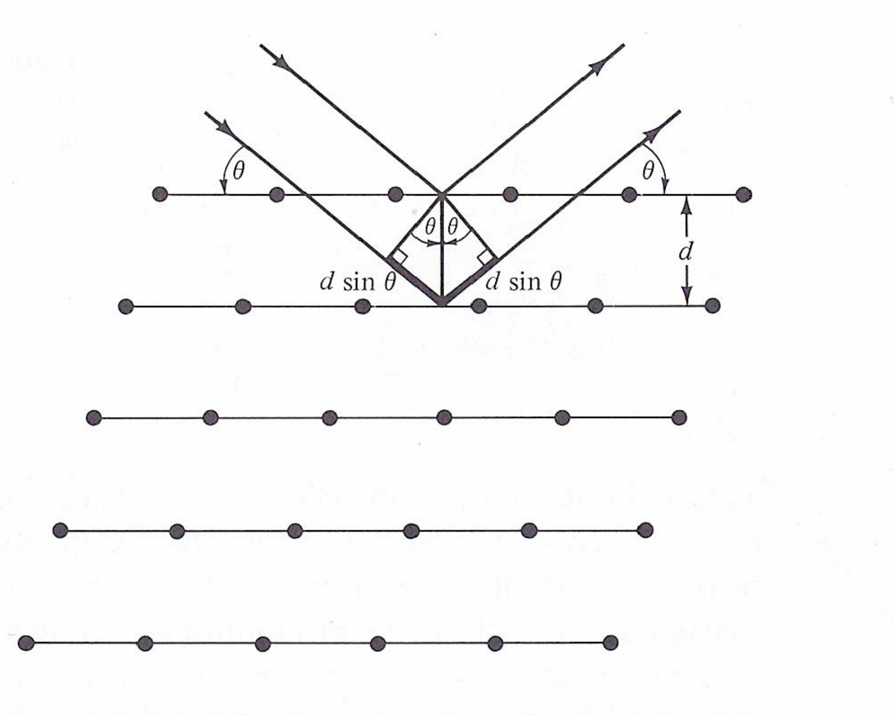
- Represented at ~20% of the total surface area of the samples

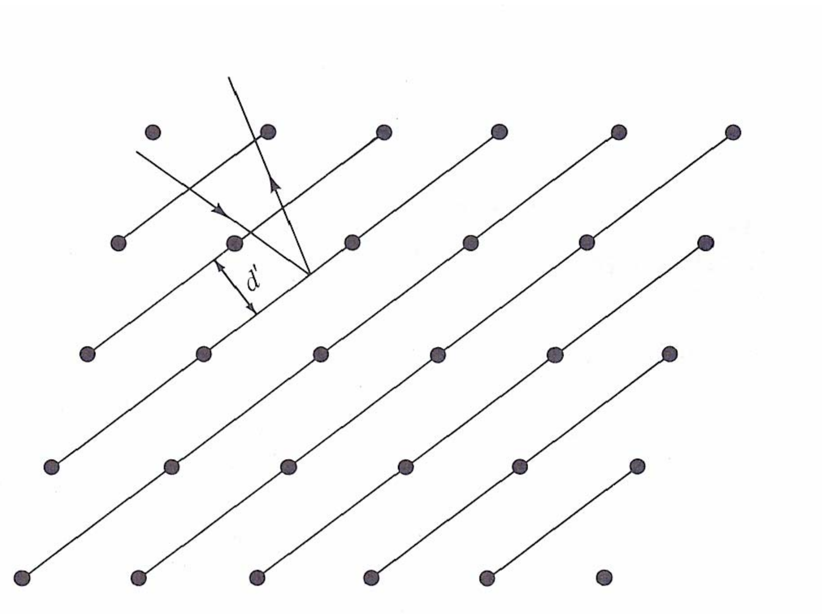
Lecture 6: Determination of Crystal Structures by X-ray or Optical Diffraction

Formulation of Bragg and von Laue
Ewald’s Construction
Experimental methods: Laue, Rotating Crystal, Powder
Geometrical Structure Factor and Atomic Form Factor
Fascinating Example of Photonic Crystals

Bragg Formulation

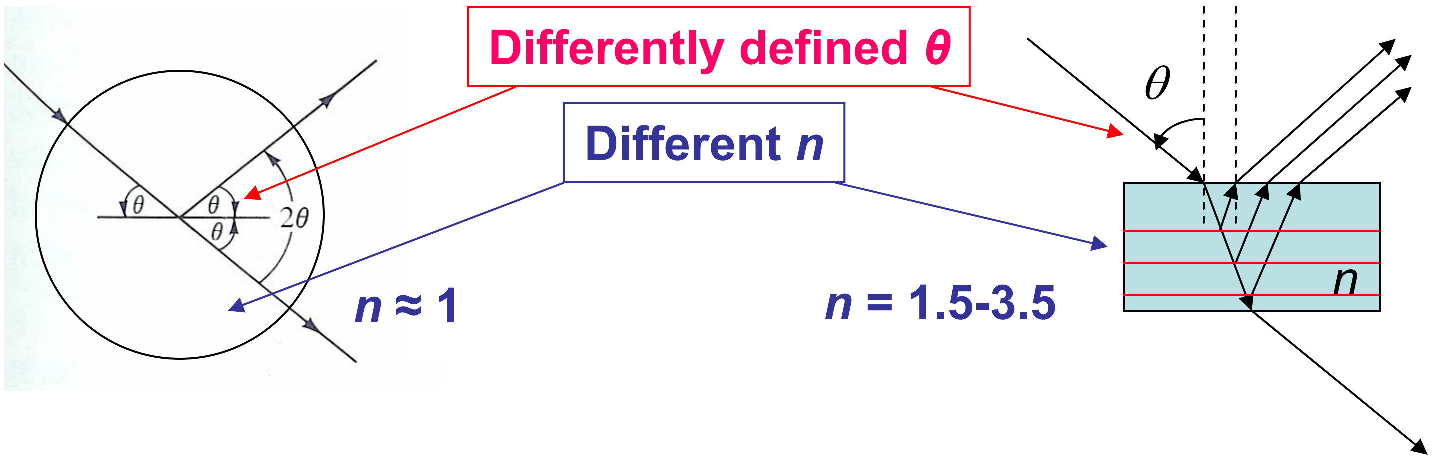
Assumption: diffraction is produced by specular reflections produced by lattice planes.





X-rays: Atomic Lattices

Visible: Photonic Crystals



Differently defined *θ*

Different *n*

***n* ≈ 1**

***n* = 1.5-3.5**

Bragg Formula

$m\lambda = 2d \sin\theta$, $m=1, 2, \ldots$

Wavelength

Longest for $m = 1$, $\theta = 90^0$

$\lambda = 2d$, $d \sim 1$Å $= 10^{-8}$ cm $\Rightarrow \lambda \sim 10^{-8}$ cm

or $E = h\nu = hc/\lambda \sim 10^3\text{-}10^4$ eV

Linewidth

$\Delta\nu/\nu \sim \Delta n/n$

$\Delta n/n \sim 10^{-5} \Rightarrow \Delta\nu/\nu \sim 10^{-5}$

Bragg Formula

$m\lambda = 2nd \cos\theta$, $m=1, 2, \ldots$

Wavelength

Longest for $m = 1$, $\theta = 0^0$

$\lambda = 2nd$, d $\sim 0.1\text{-}1\ \mu$m $\Rightarrow \lambda \sim 0.3\text{-}3\ \mu$m

or $E = h\nu = hc/\lambda \sim 1$ eV

Linewidth

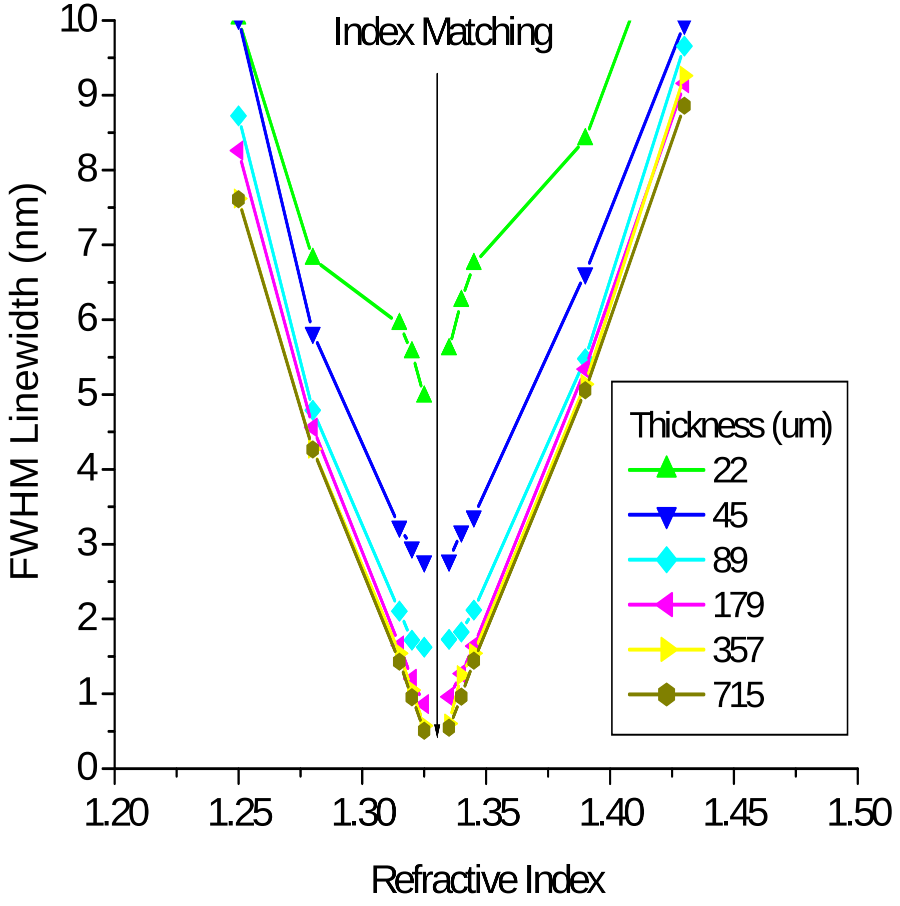
$\Delta\nu/\nu \sim \Delta n/n$

$\Delta n/n \sim 0.1\text{-}3.5 \Rightarrow \Delta\nu/\nu \sim 1$

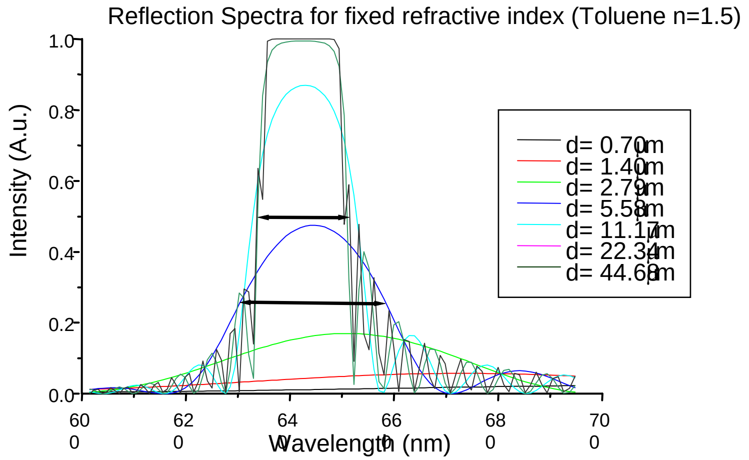
More on Linewidths in Opals (FCC)

$\Delta\nu = (2/\pi)\,\nu\Delta n/n$ – in 1-D case

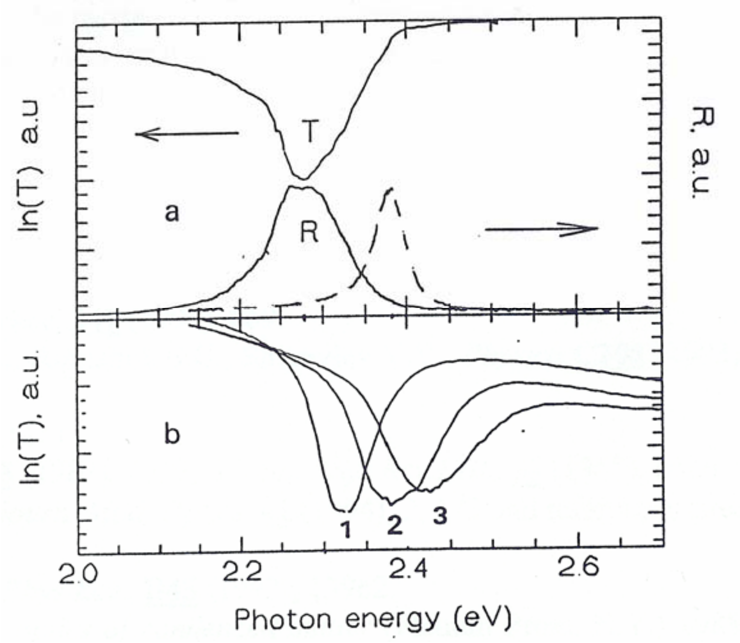
In 3-D FCC opal structure:



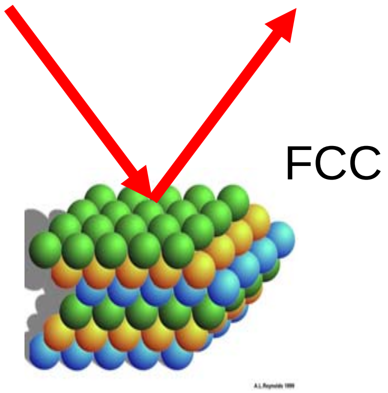
Thickness dependency

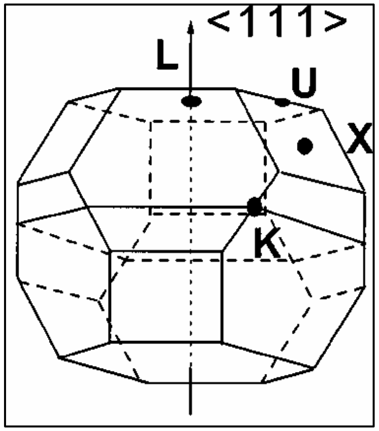


Experiment: V.N. Astratov et al., Nuovo Cimento **17**, 1349 (1995)

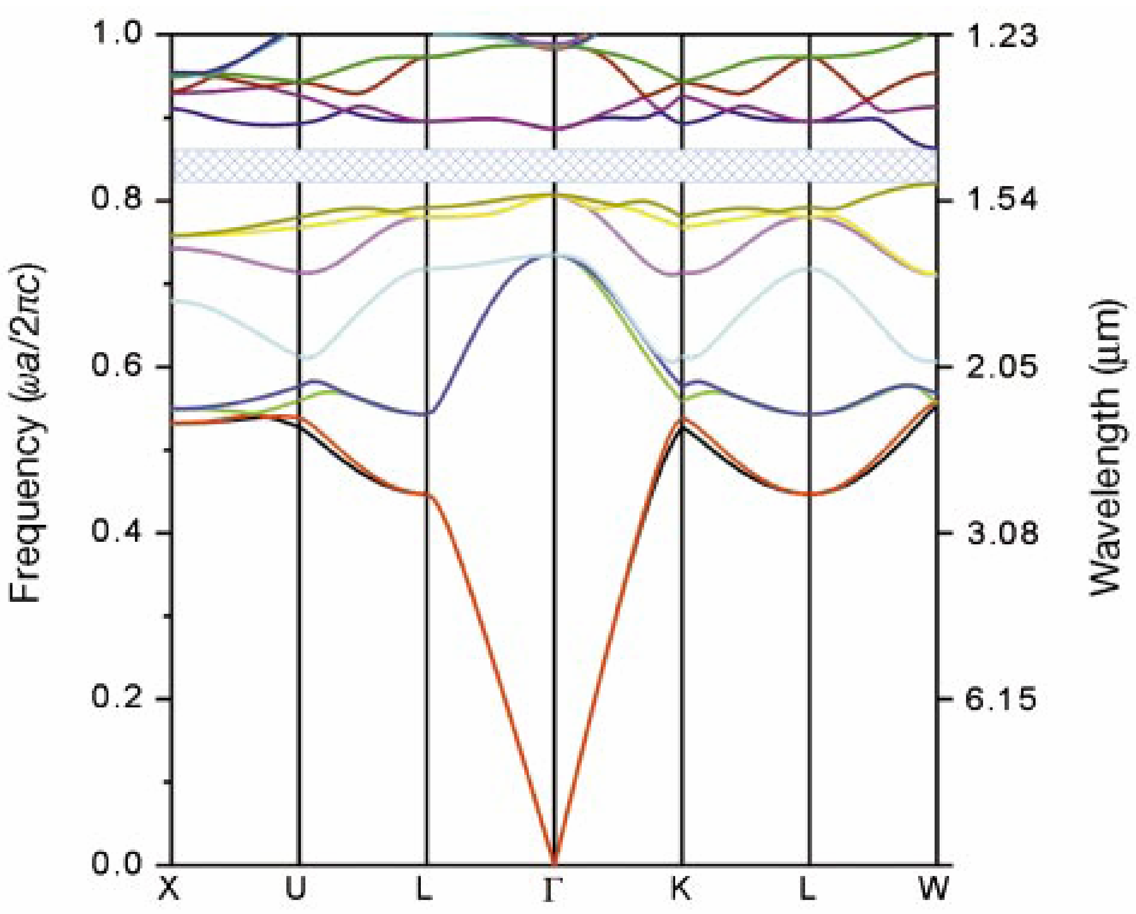


Real Space Measurements can be Related to Directions in k-Space





Photonic Band Structure



A.Blanko et al., Nature 405, 437 (2000)

Complete Photonic Band Gap and Control of Spontaneous Emission

Pioneering Idea of Eli Yablonovitch, PRL58, 2059 (1987)

Complete photonic band gap is an overlap of partial stop bands for ALL directions in space

Stop band frequency: $\omega = (c/n_{av})k$,
where $k_{hkl} = 2\pi / d_{hkl}$,
FCC lattice spacings d_{hkl} are given:

$d_{100} = a/2,\ d_{111} = a/\sqrt{3} \Rightarrow$

$k_{100} = 4\pi/a,\ k_{111} = 2\pi\sqrt{3}/a \Rightarrow$

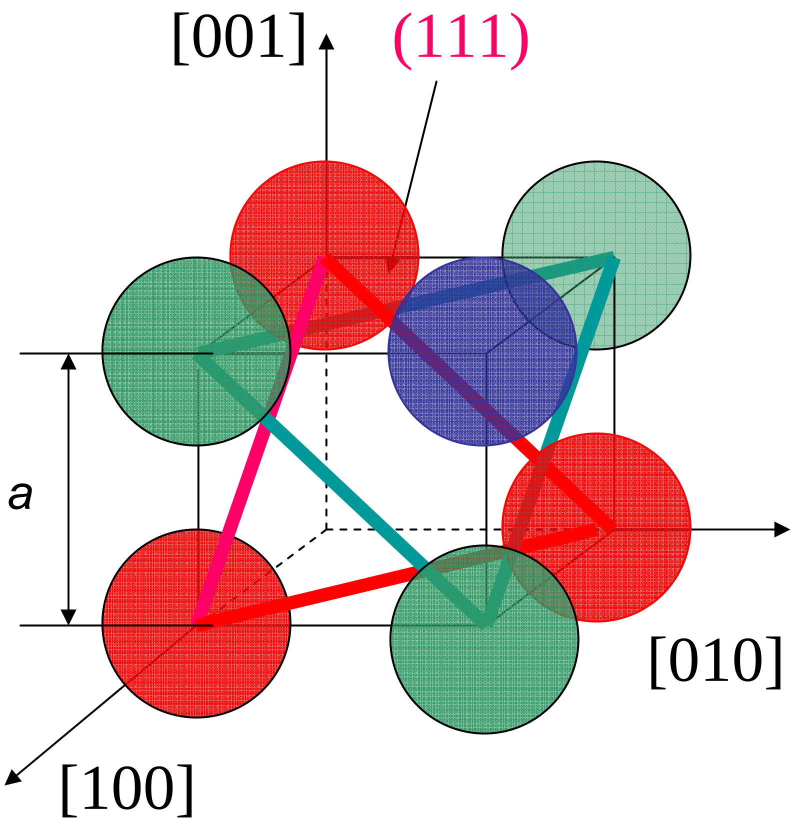
$\nu_{100} = (c/2\pi n_{av})k_{100} = 2c/(an_{av})$

$\nu_{111} = (c/2\pi n_{av})k_{111} = \sqrt{3}c/(an_{av})$

$(\nu_{100} - \nu_{111})/\nu_{100} = 1 - (\sqrt{3})/2$

$\Delta\nu/\nu = (2/\pi)\,\Delta n/n$ – in 1-D case

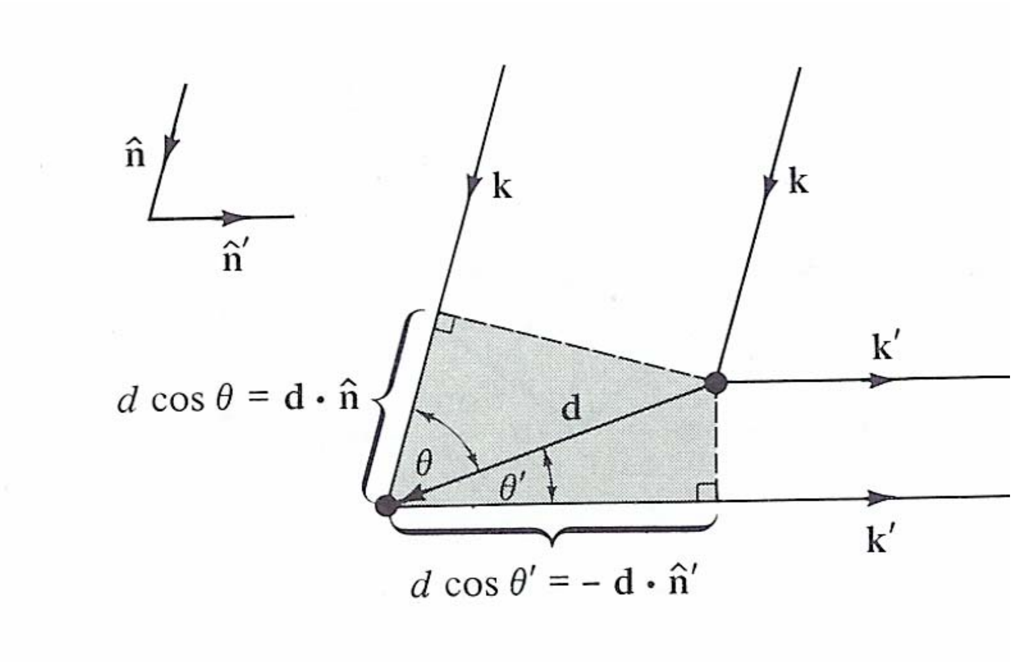
$\Delta n/n = 0.21$ – **Historical Interest**



Spheres at the centers of the faces are removed for clarity

Von Laue Formulation of X-ray Diffraction

No assumption of specular reflection by planes, but reradiation the incident radiation by individual atoms in all directions. Sharp peaks appear as a result of constructive interference.



Path difference:

$d\cos\theta + d\cos\theta' = \boldsymbol{d}\,(\mathbf{n} - \mathbf{n}')$

Constructive interference:

$\boldsymbol{d}\,(\mathbf{n} - \mathbf{n}') = m\,\lambda$, m = 0,1,2,…

Multiplying by $2\pi/\lambda$:

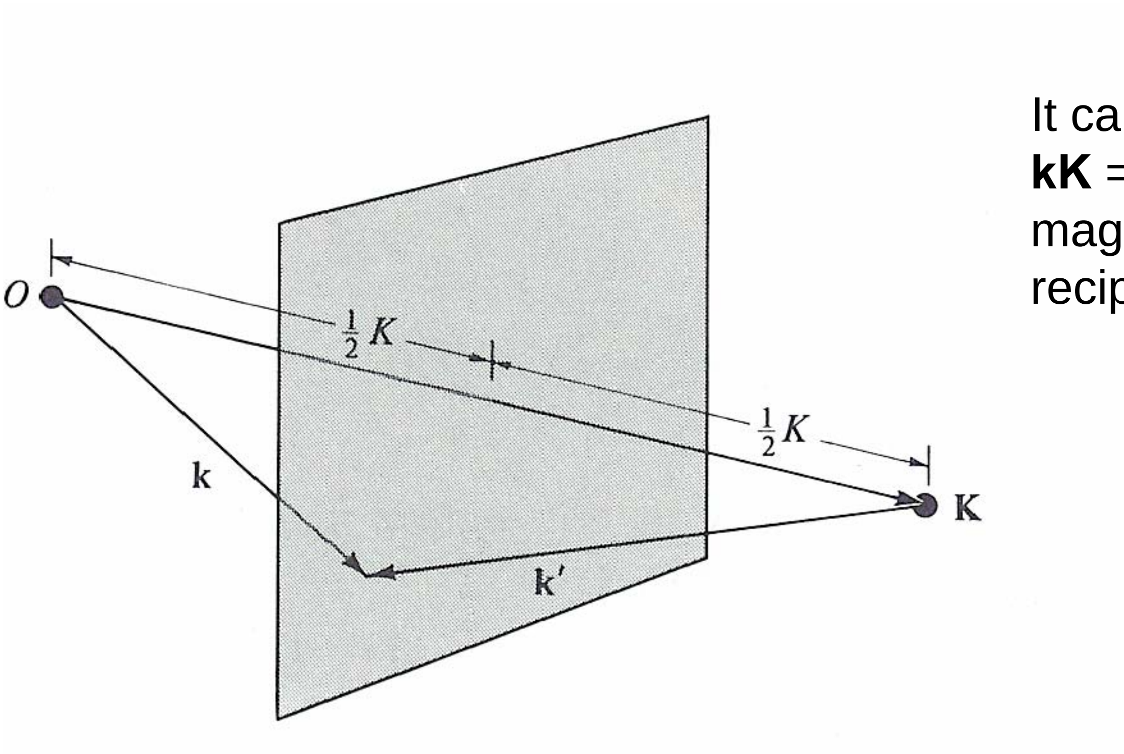
$\boldsymbol{d}\,(\mathbf{k} - \mathbf{k}') = 2\pi m$

For a Brave lattice:

$\mathbf{R}\,(\mathbf{k} - \mathbf{k}') = 2\pi m$

Laue condition: constructive interference occurs provided that the change in k-vector, **K** = **k** - **k**’, is a vector of the reciprocal lattice

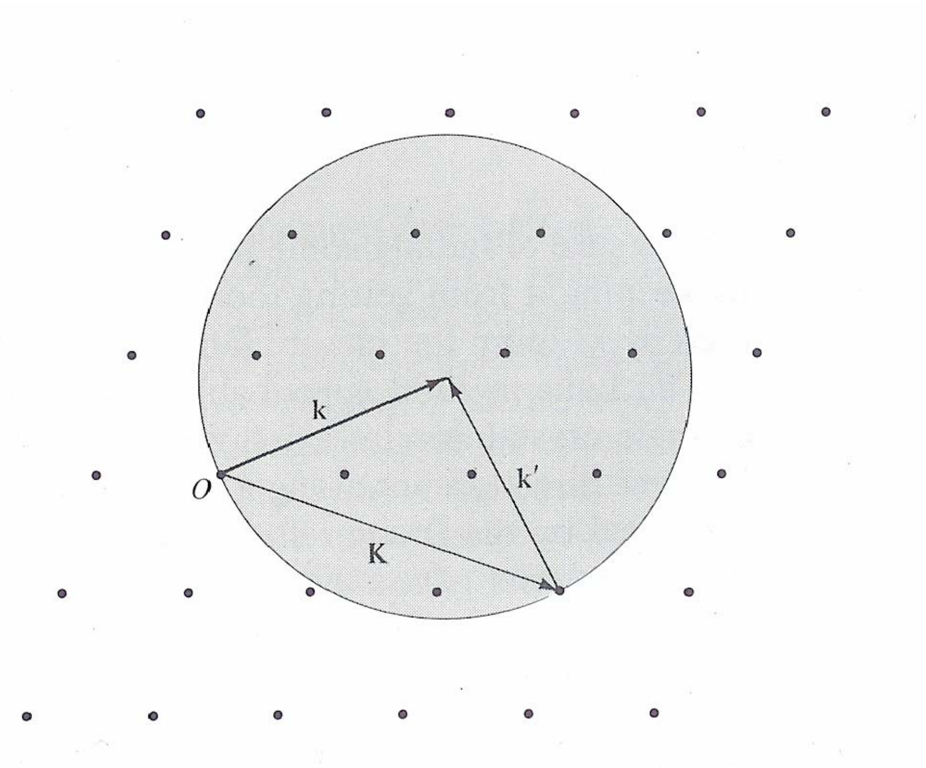
Equivalence of the Bragg and Von Laue Formulations



It can be shown:
kK = (1/2)K, where K – magnitude of the vector of the reciprocal lattice

Equivalence of the von Laue and Bragg approaches means that the k-space lattice plane associated with a diffraction peak in the Laue formulation is parallel to the family of direct lattice planes responsible for peak in the Bragg formulation.

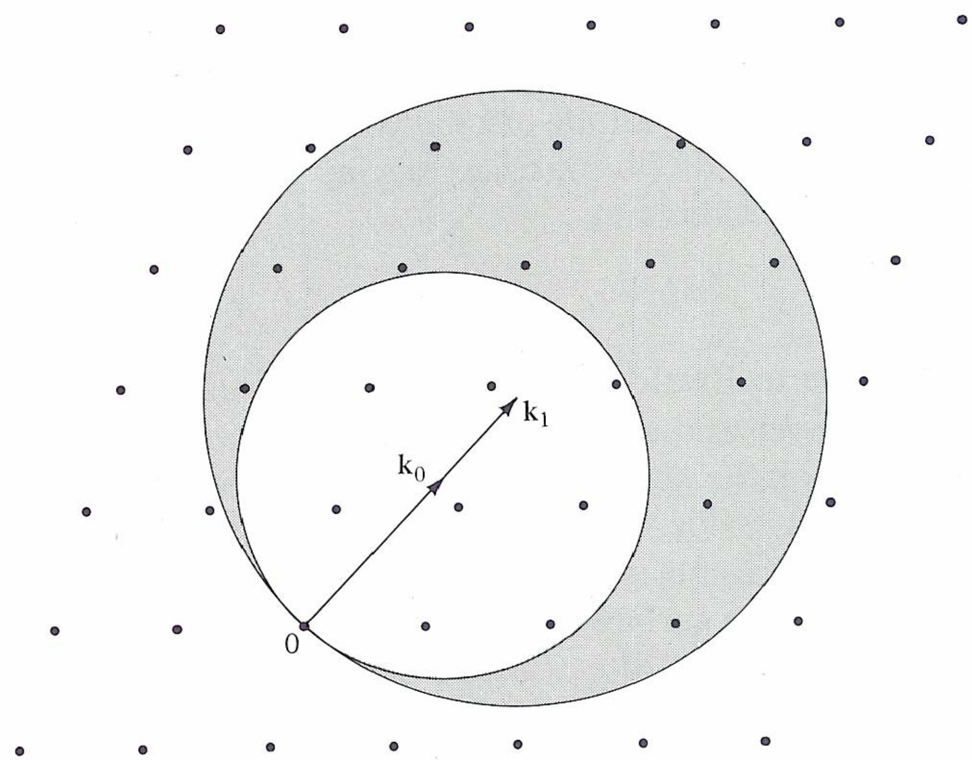
Ewald Construction



Given the incident **k**, a sphere of radius *k* is drawn about the point **k**. Diffraction peaks corresponding to reciprocal lattice vectors **K** will be observed only if the sphere intersects lattice points different from point *O*.

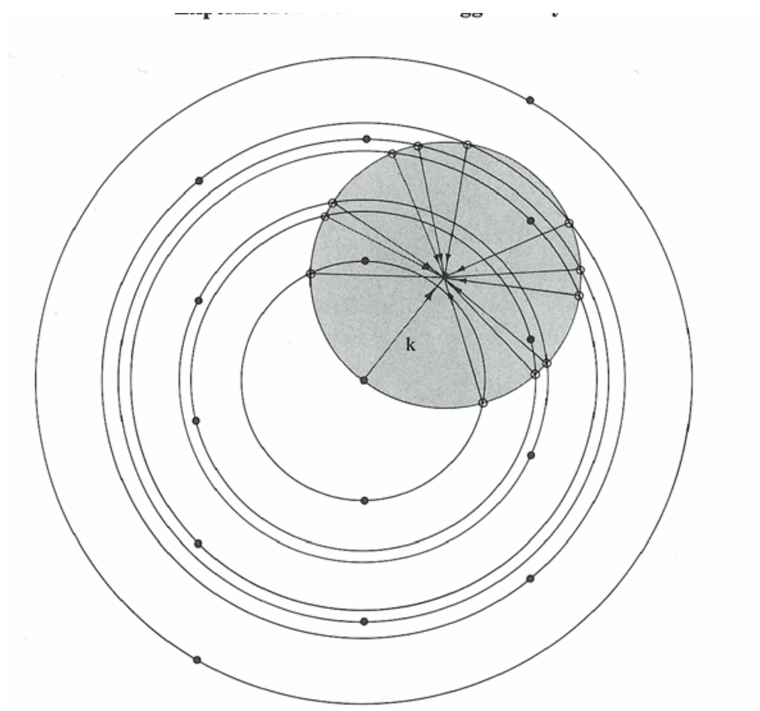
Need to vary parameters (λ, direction of propagation) to observe diffraction.

The Laue Method



By varying k from k_0 to k_1 we can expand Ewald sphere to fill the shaded region. Bragg peaks will be observed corresponding to all reciprocal lattice points in the shaded region.

The Rotating-Crystal Method



Evald sphere determined by the incident k-vector is fixed in k-space, while the entire reciprocal lattice rotates about the axis of rotation of the crystal. The Bragg reflection occur whenever these circles intersect the Ewald sphere.

Similarly we can introduce **The Rotating-Crystal Method.**

Topics for reading: Geometrical Structure Factor and Atomic Form Factor