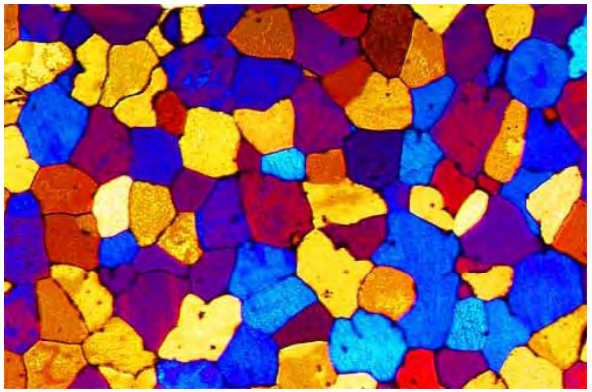
Acknowledge

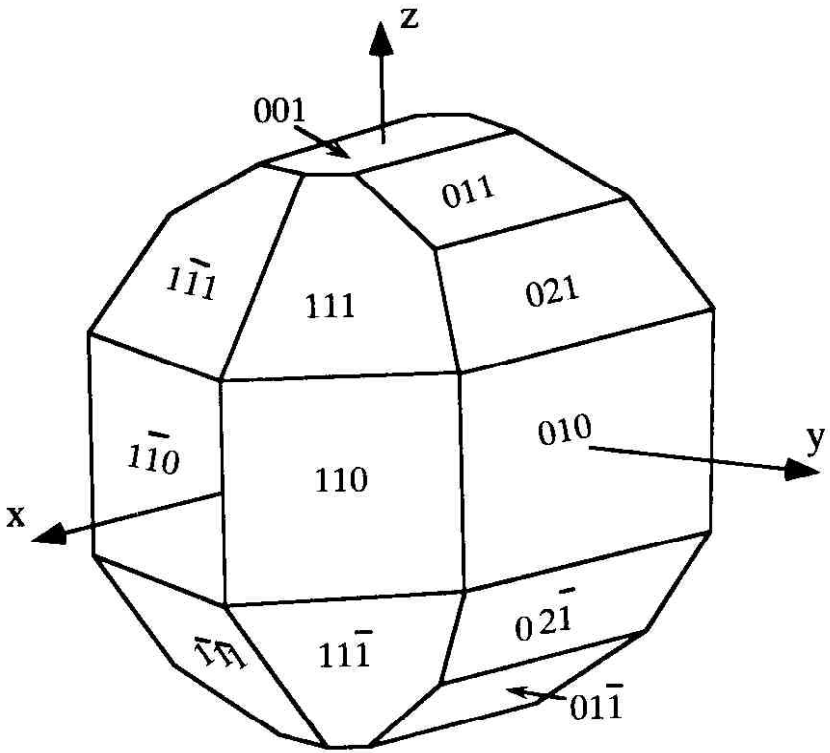
- Pengcheng's slides
- Profs in condensed matter physics
- internet

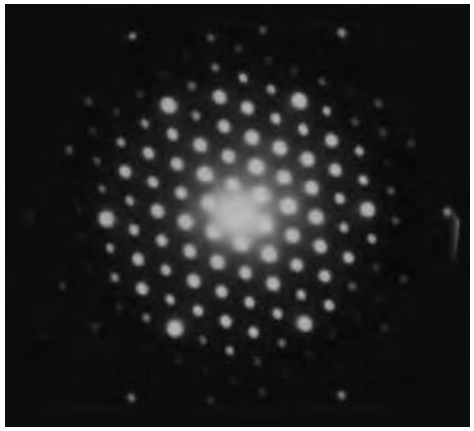


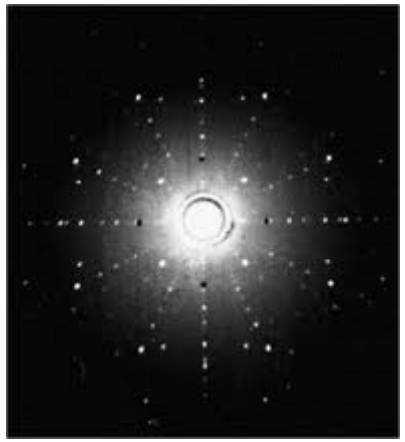

Nicelce.com

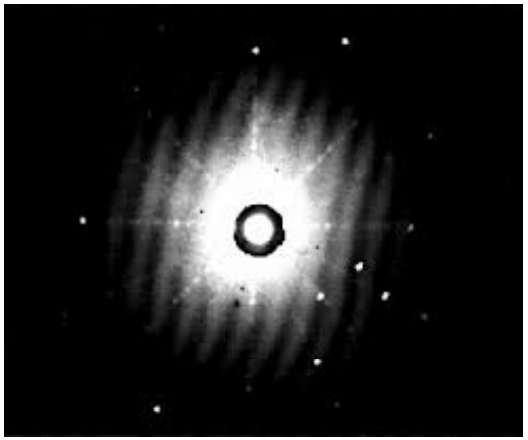

Skullis.com

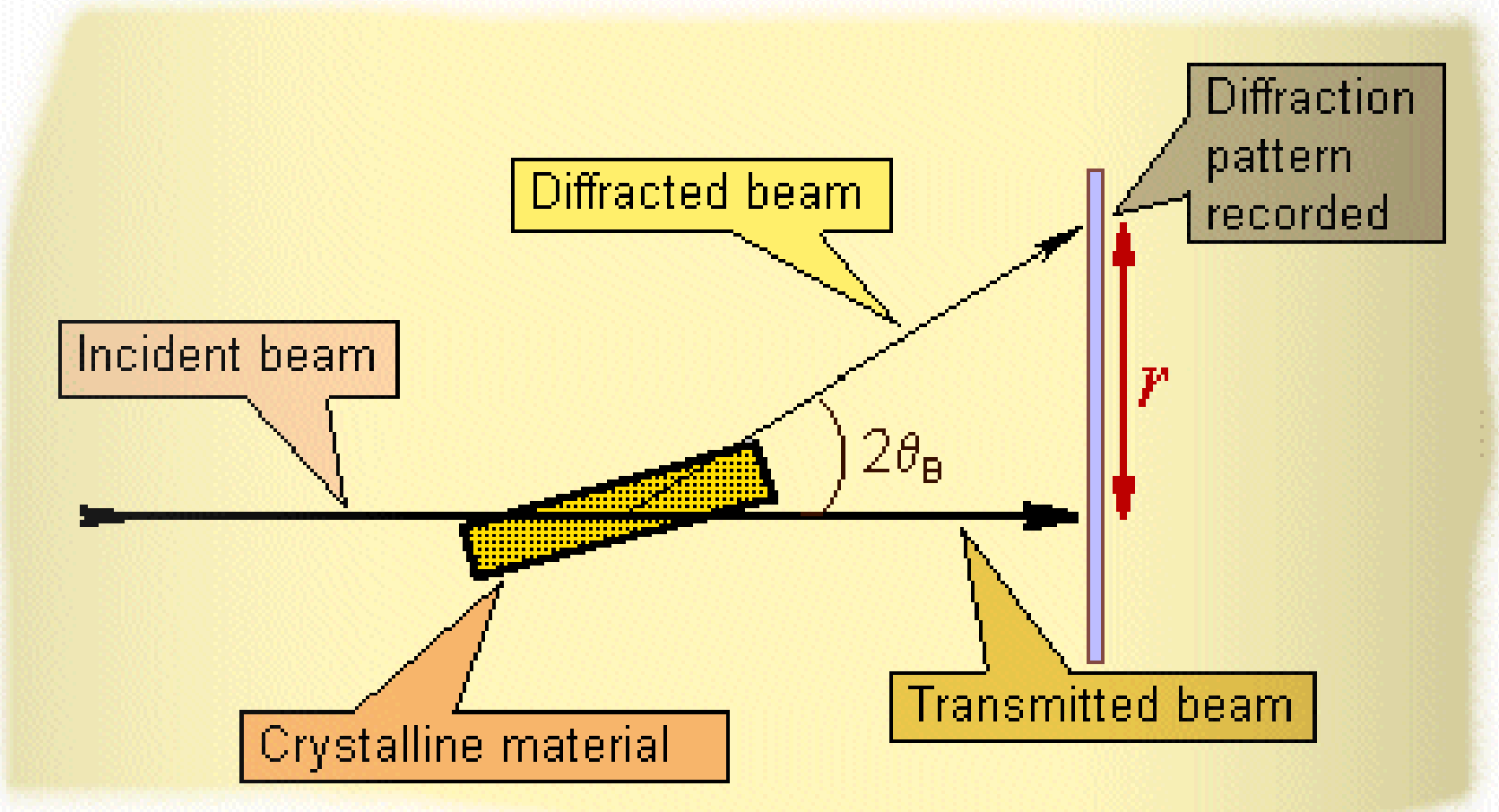
Miller indices










Diffraction pattern recorded
Diffracted beam
Incident beam
$2\theta_B$
Y
Crystalline material
Transmitted beam

Don’t get lost in Matrix

$$\mathbf{K} \cdot \mathbf{R} = 2\pi(k_1 n_1 + k_2 n_2 + k_3 n_3)$$

$$\left[\mathbf{b}_1 \mathbf{b}_2 \mathbf{b}_3\right]^T = 2\pi \left[\mathbf{a}_1 \mathbf{a}_2 \mathbf{a}_3\right]^{-1}.$$

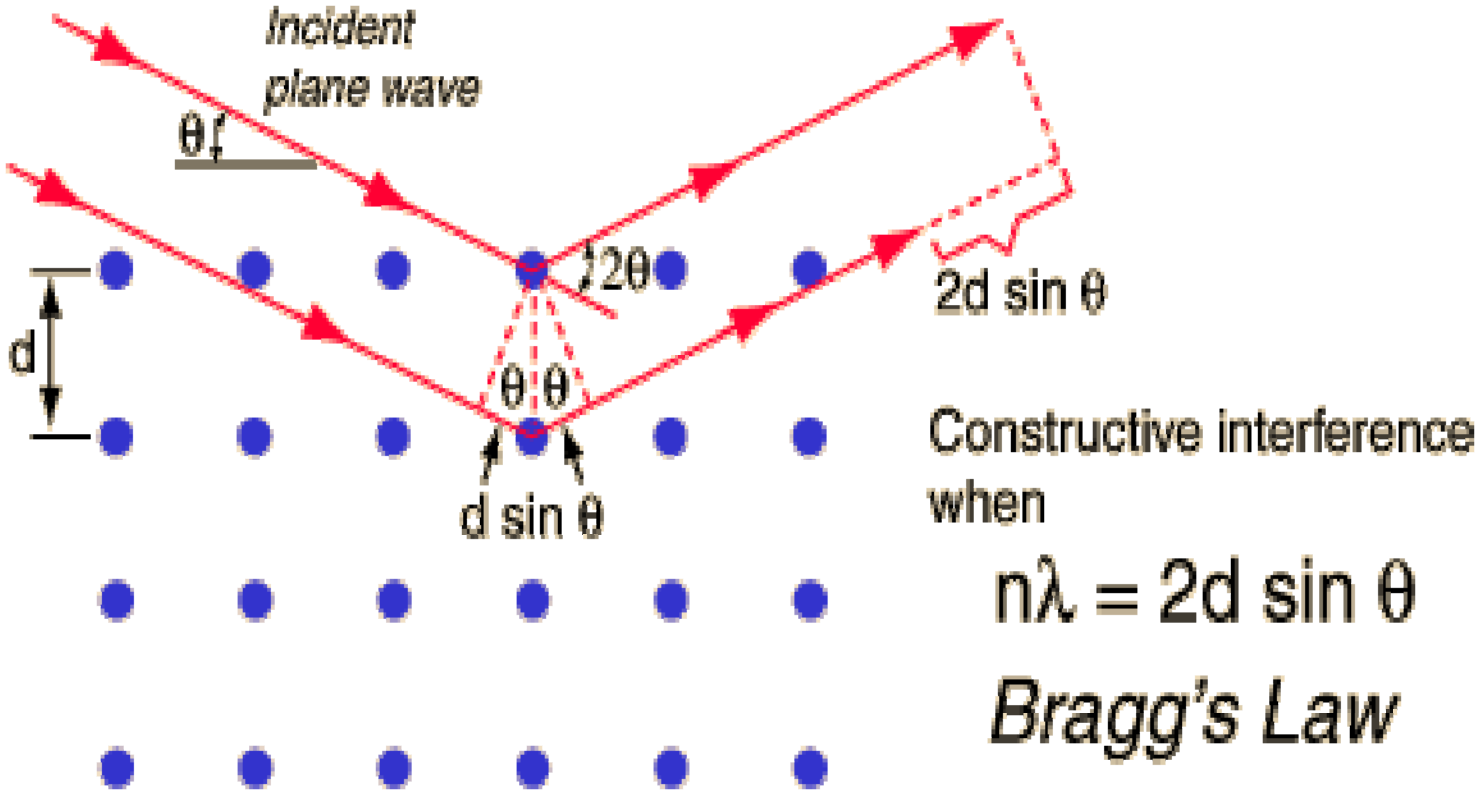
Where is the atom?

Diffraction Methods

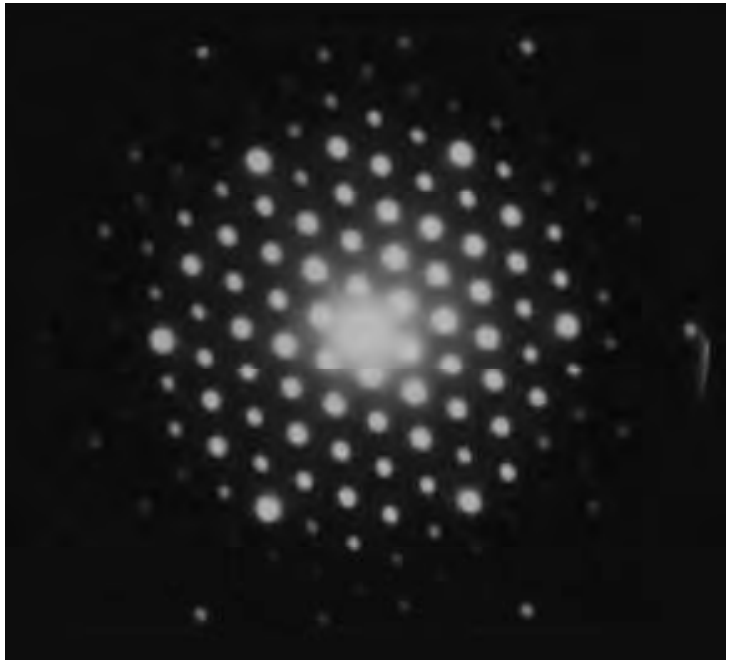
Diffraction

X-Rays	Neutrons	Electrons
λ ~ 1 Å E ~ 10^4 eV interact with electrons, penetrating	λ ~ 1 Å E ~ 0.08 eV interact with nuclei, highly penetrating	λ ~ 1 Å E ~ 150 eV interact with electrons, less penetrating

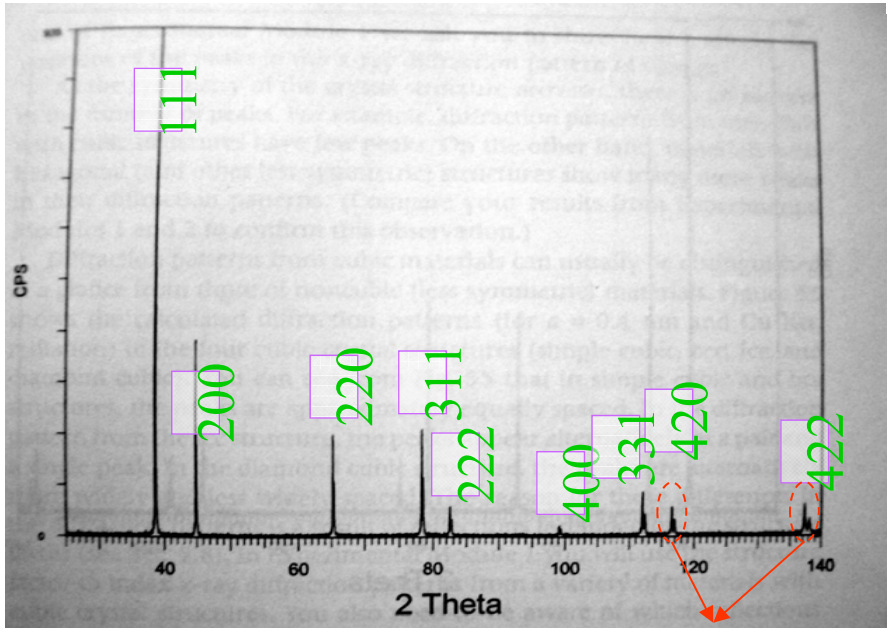
Bragg's law


Incident
plane wave
θ
2θ
2d sin θ
d
θ θ
d sin θ
Constructive interference
when
nλ = 2d sin θ
Bragg's Law

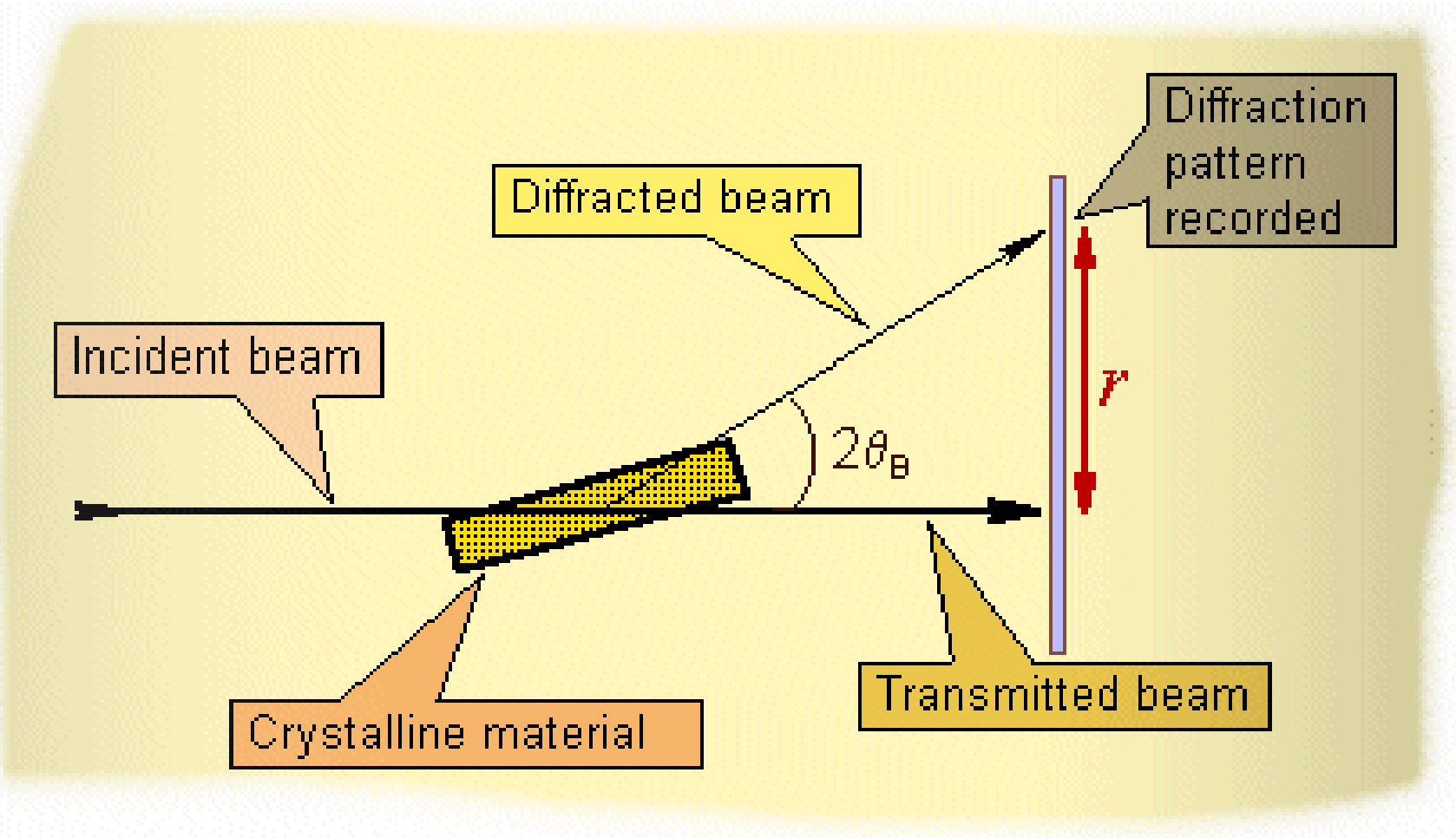
Laue



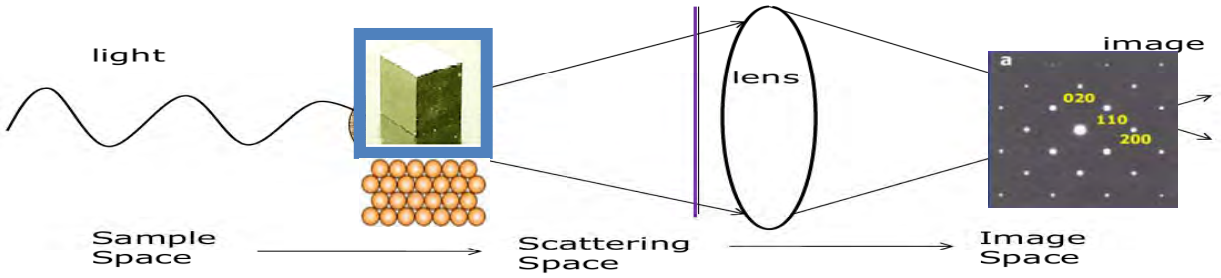
X-ray pattern

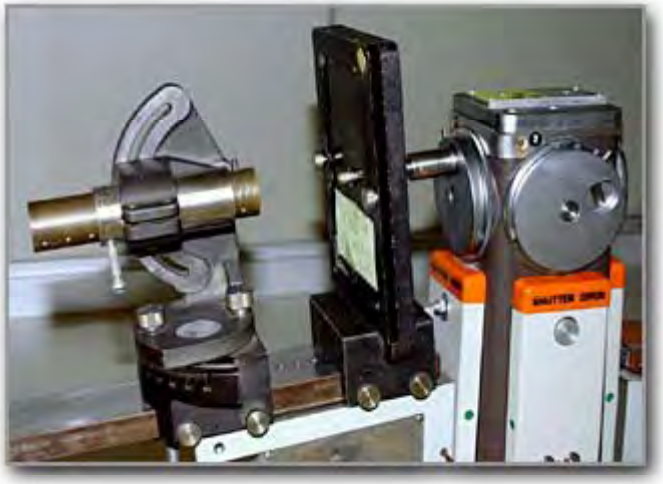


How many ways?
$n\lambda=2d_{hkl}\sin\theta$

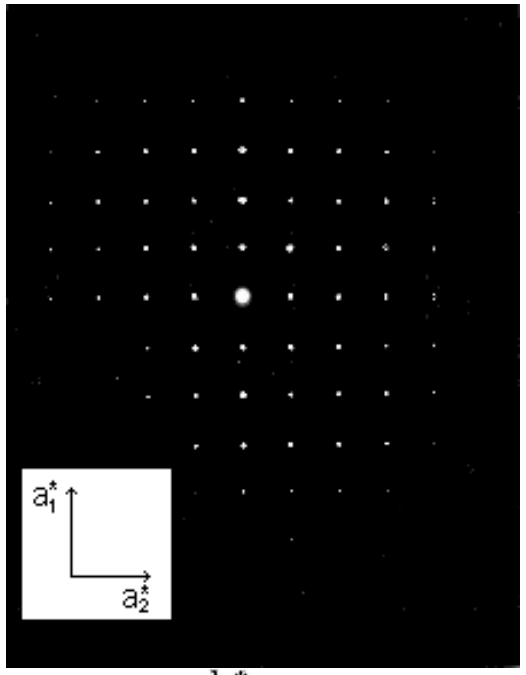


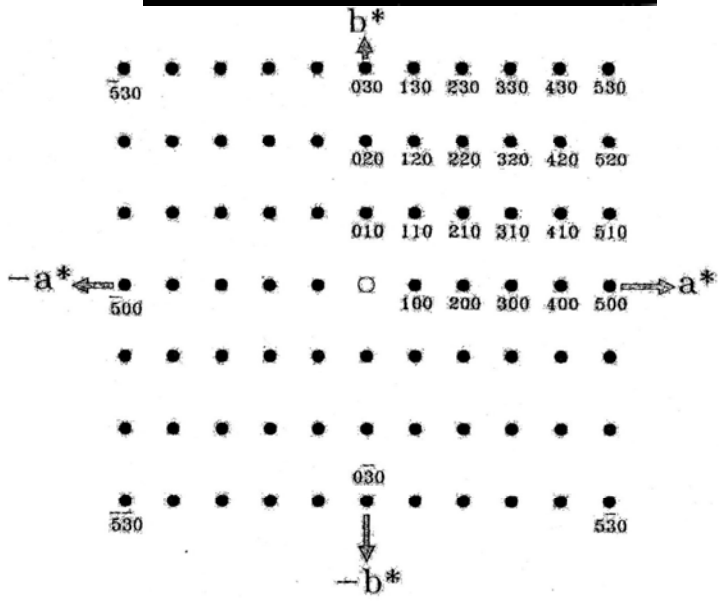
$$n\lambda = 2d_{hkl}\sin\theta$$





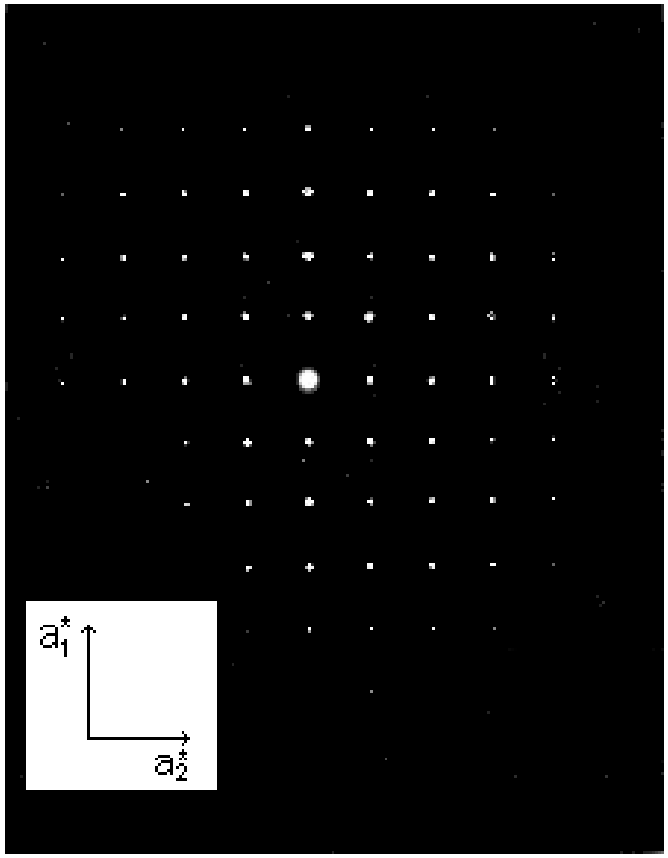
fixed θ, variable λ



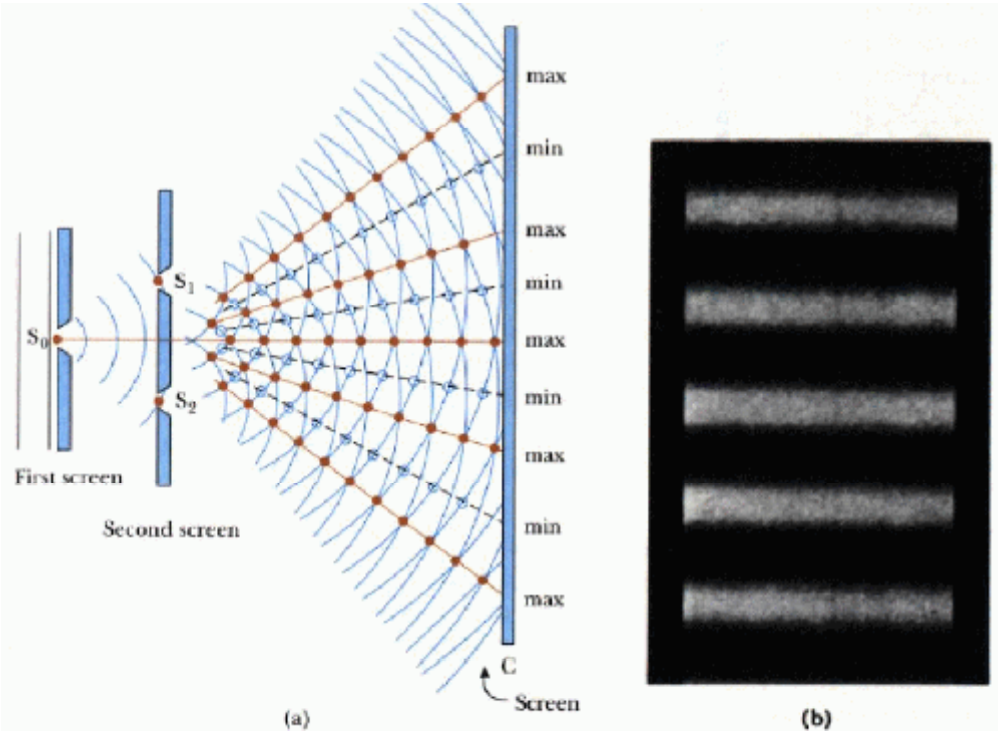


Why can different planes be observed?

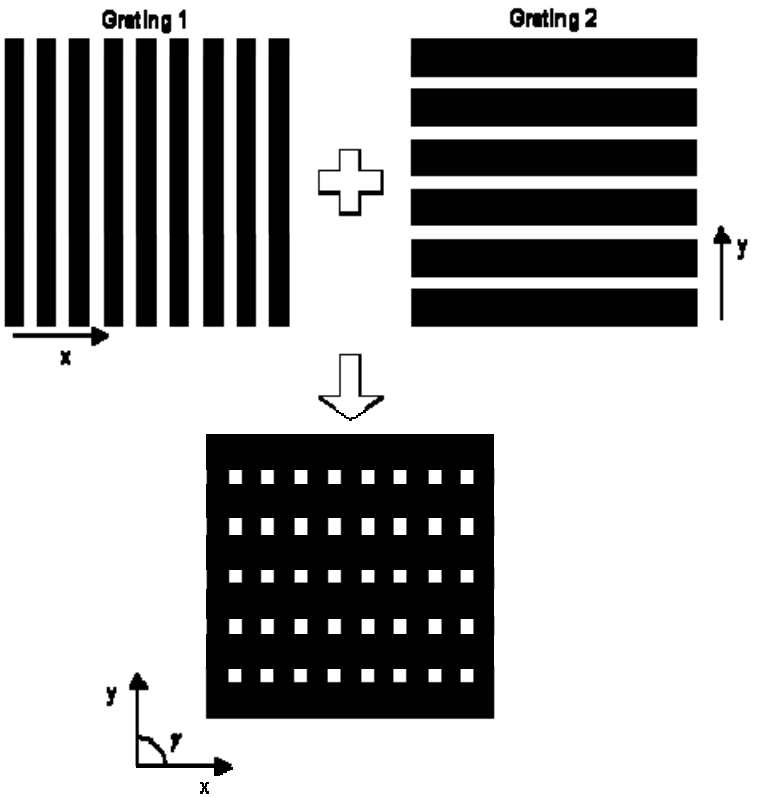
Why are there bright and dark area?



1D grating


max
min
max
min
max
min
max
min
max
S_0
S_1
S_2
First screen
Second screen
C
Screen
(a)
(b)

2D grating



http://www.youtube.com/watch?v=ACjr66v4gyo

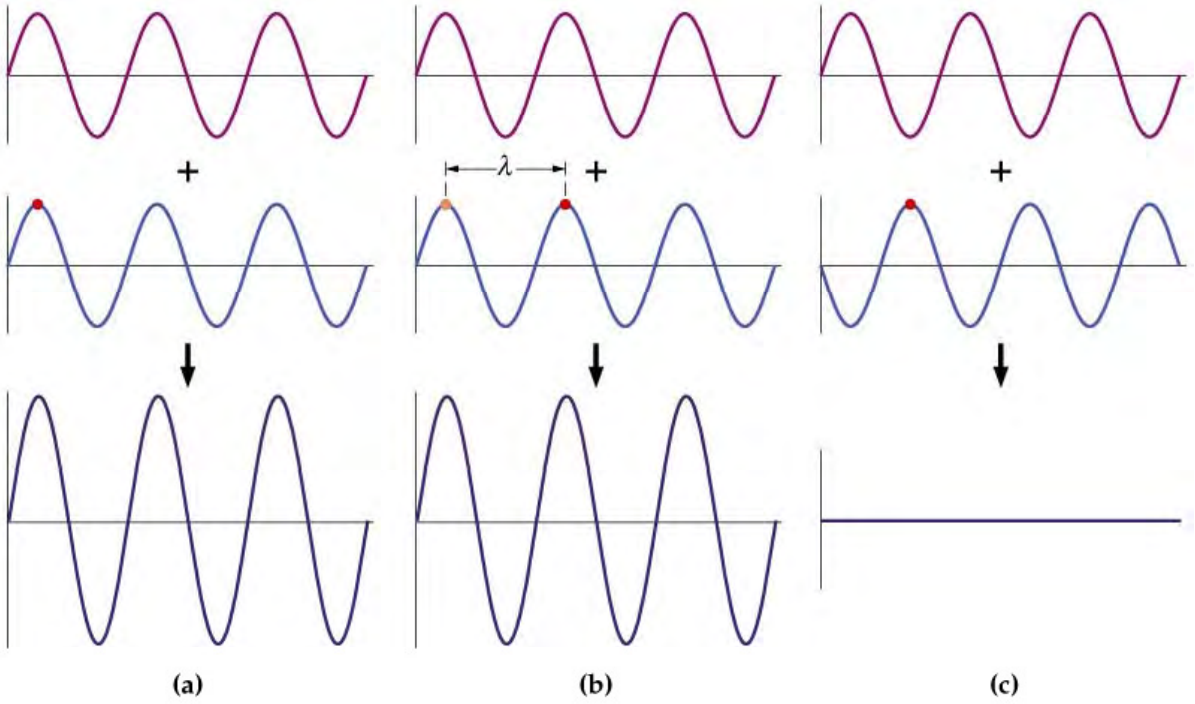
Constructive and destructive interference

Cases (a) & (b): constructive interference

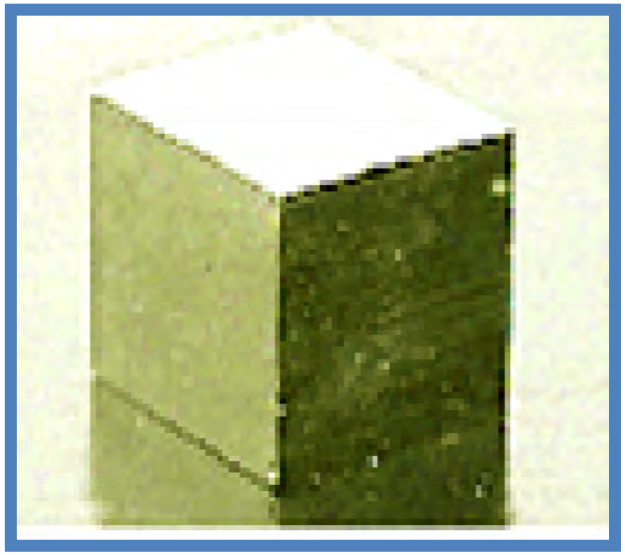
$d \sin\theta = m\lambda \qquad m = 0, \pm 1, \pm 2..$

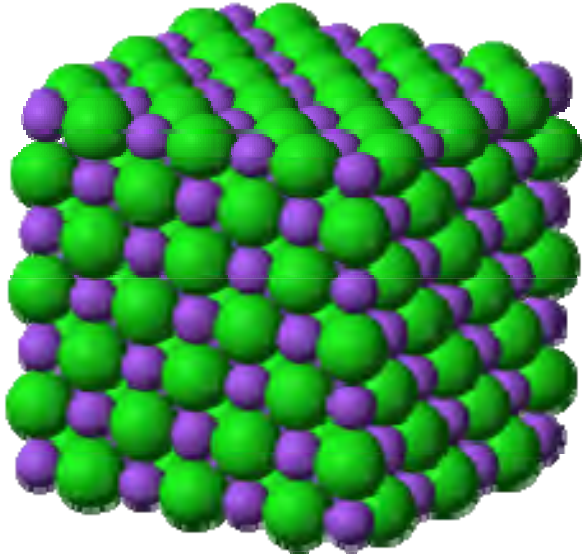
Case (c): destructive interference

$d \sin\theta = (m + 1/2)\lambda \quad m = 0, \pm 1, \pm 2, ..$

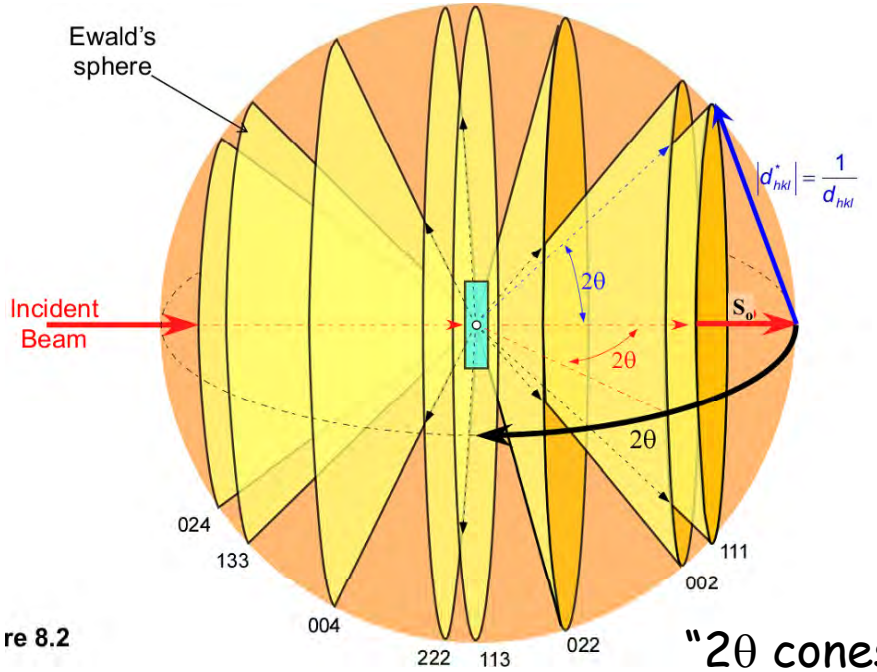


3D grating



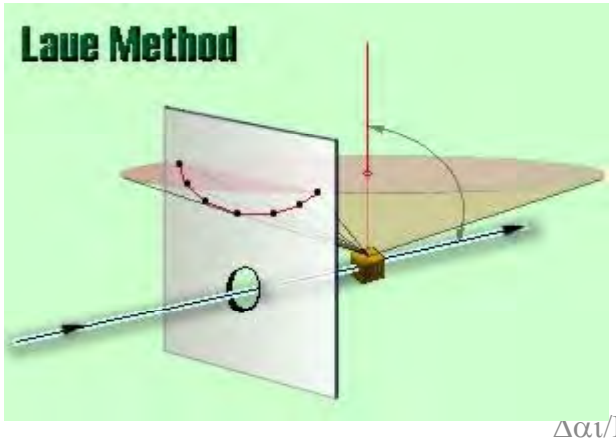


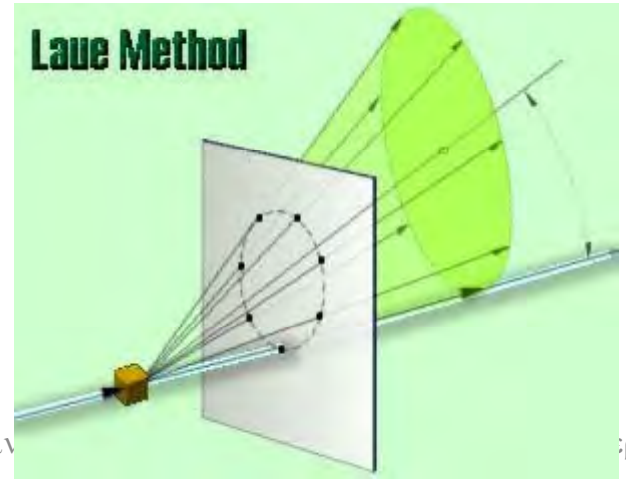
Where should we posit detector



re 8.2

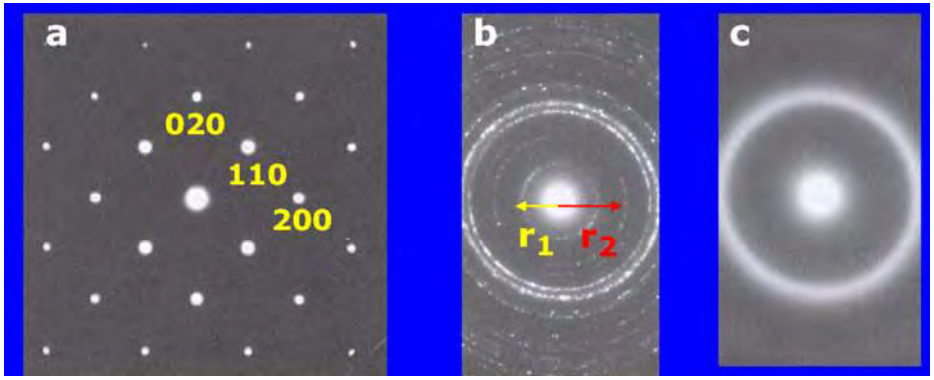
"2θ cones" or diffracted rays

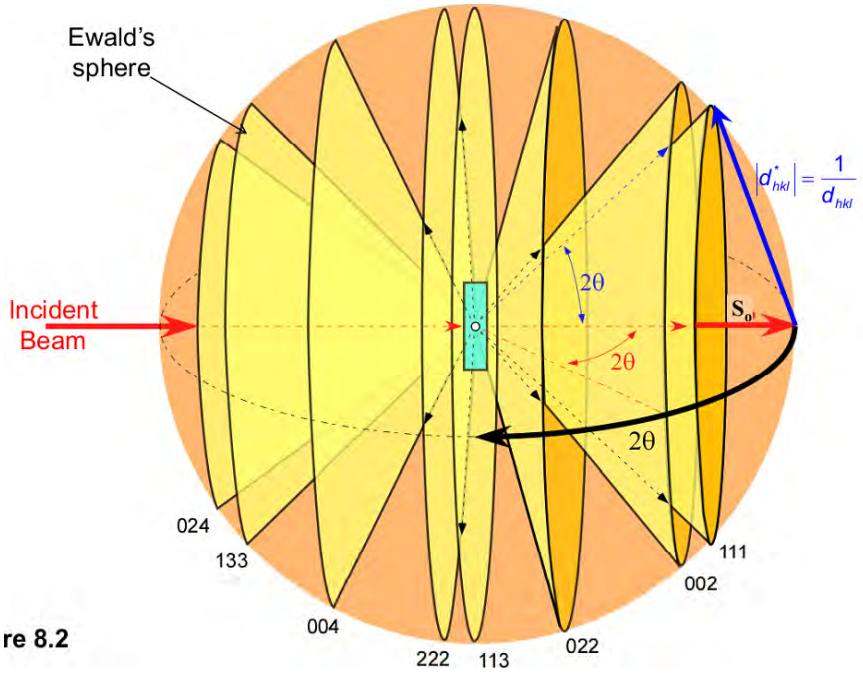


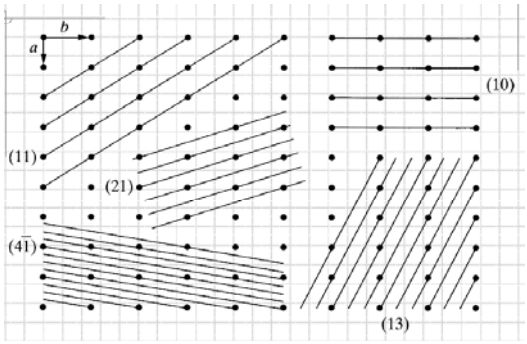


What is meaning of one ring (Powder)

$n\lambda=2d_{hkl}\sin\theta$

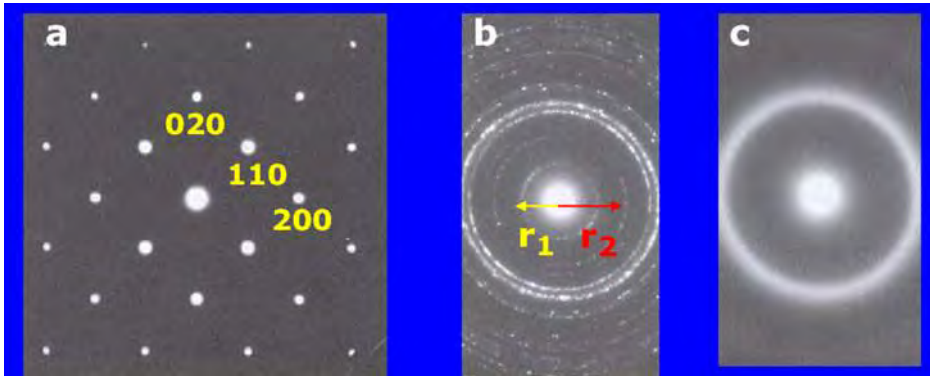


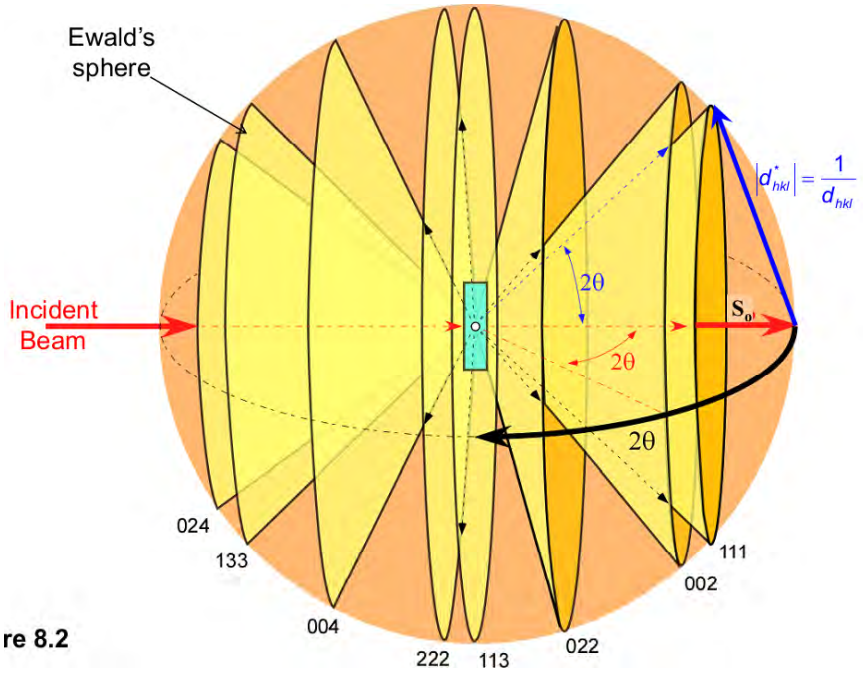




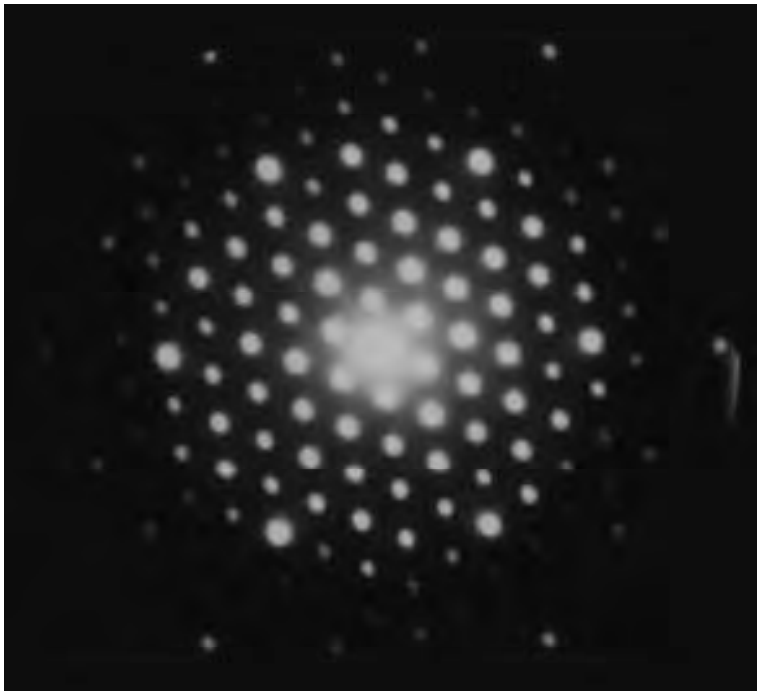
What is meaning of one spot (crystal)?

$n\lambda=2d_{hkl}\sin\theta$





Why are spots denser near the center?

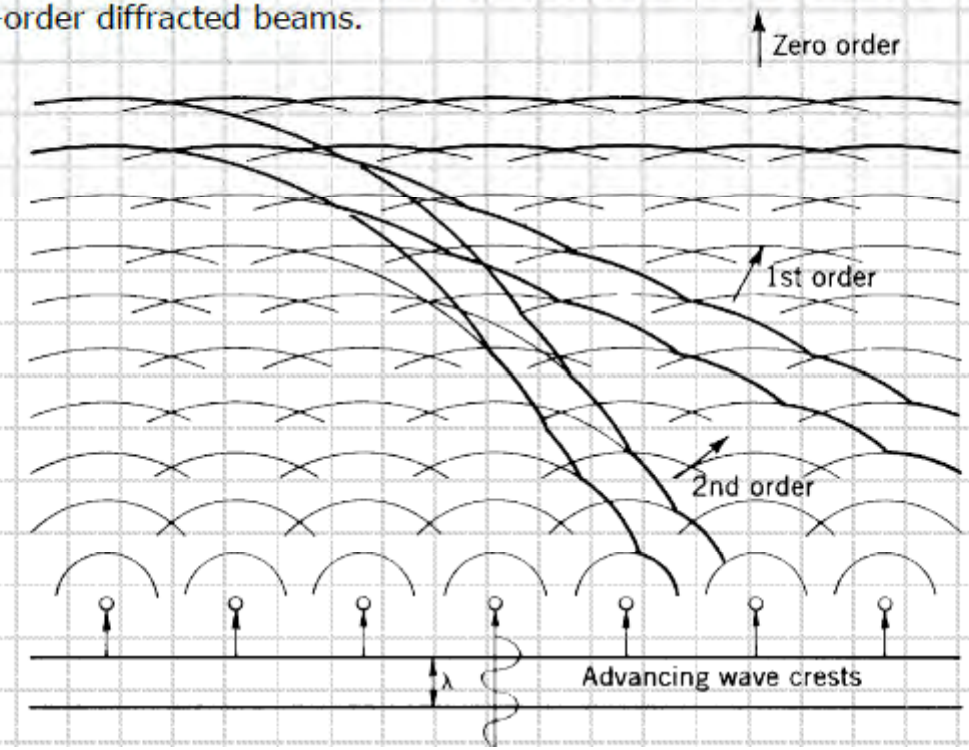


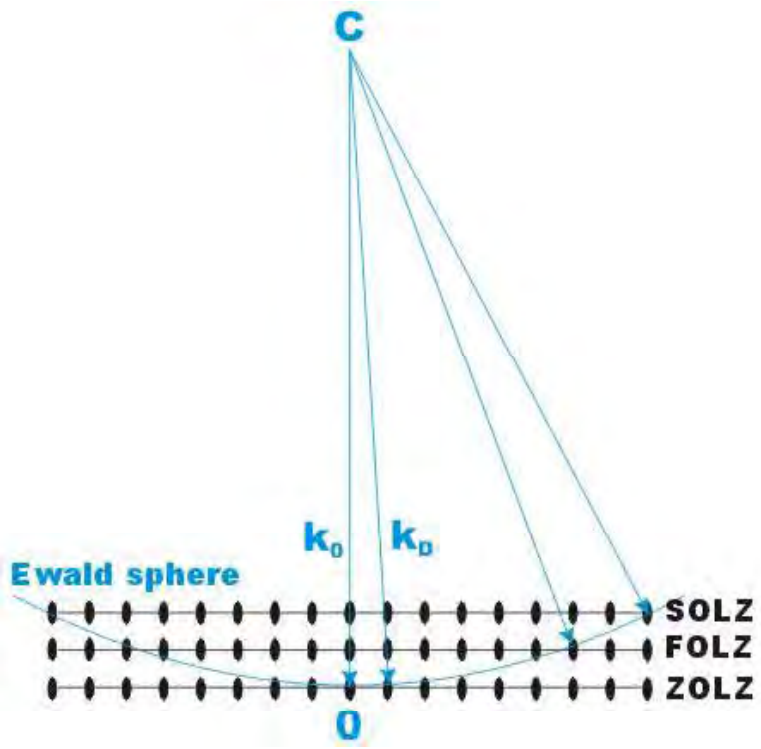
$$n\lambda = 2d_{hkl}\sin\theta$$

The Laue Equations

$n = ?$

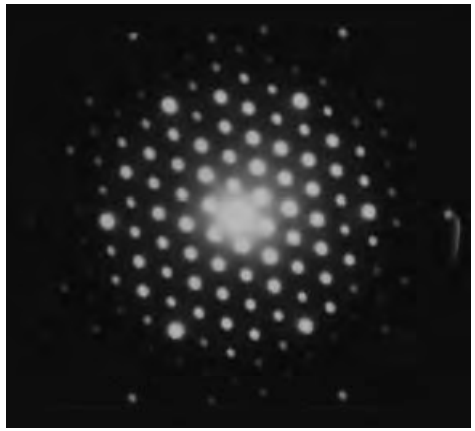
- If an X-ray beam impinges on a row of atoms, each atom can serve as a source of scattered X-rays.
- The scattered X-rays will reinforce in certain directions to produce zero-, first-, and higher-order diffracted beams.

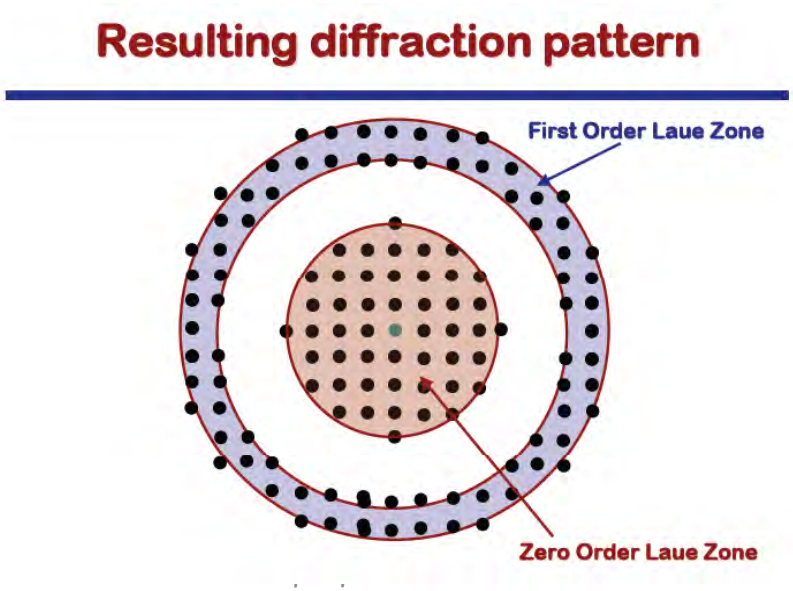


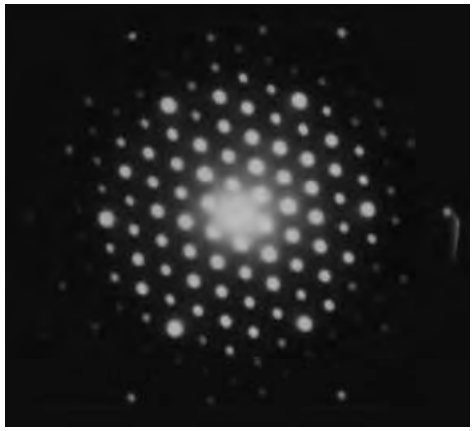


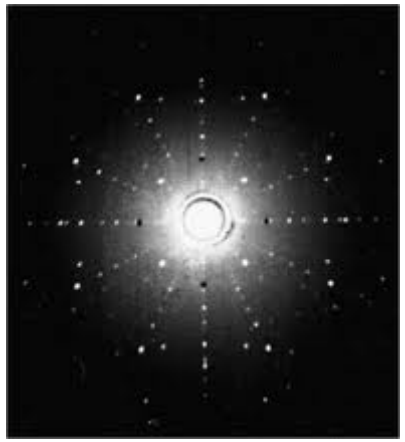
$$n\lambda = 2d_{hkl}\sin\theta$$

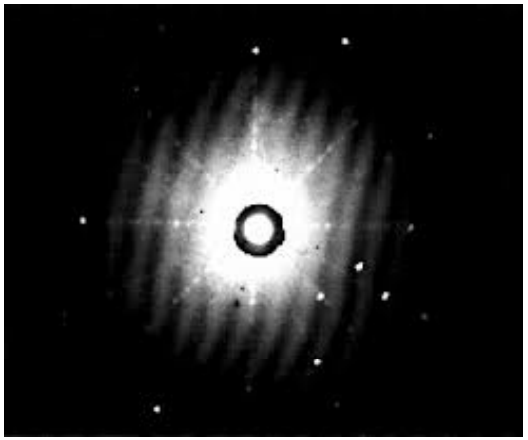
n=?

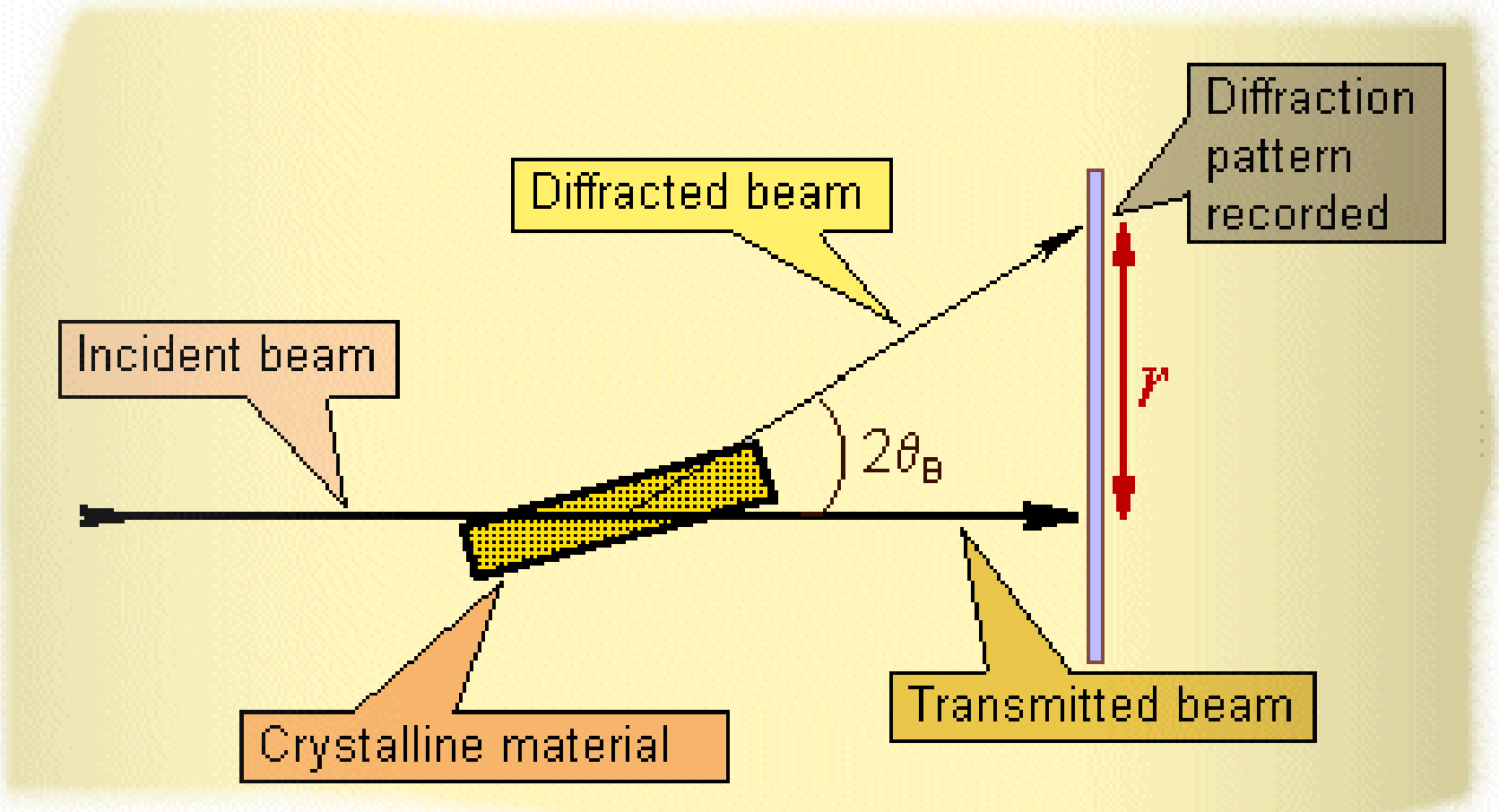










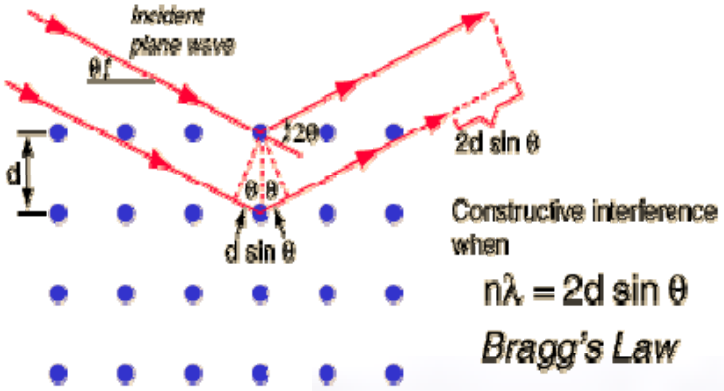

Diffraction pattern recorded
Diffracted beam
Incident beam
$2\theta_B$
Y
Crystalline material
Transmitted beam

fixed θ, variable λ

$$n\lambda = 2d_{hkl}\sin\theta$$

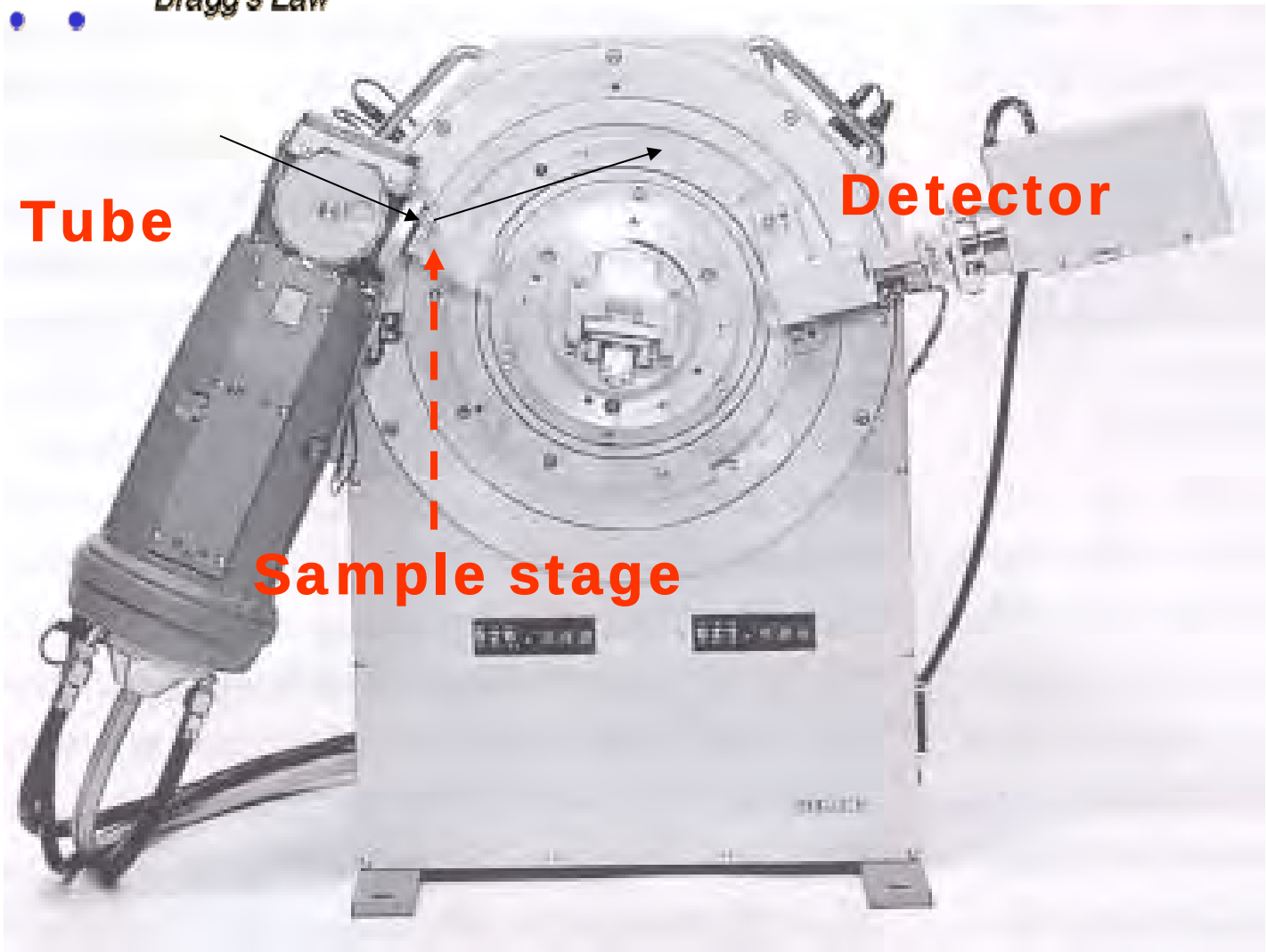
n=?

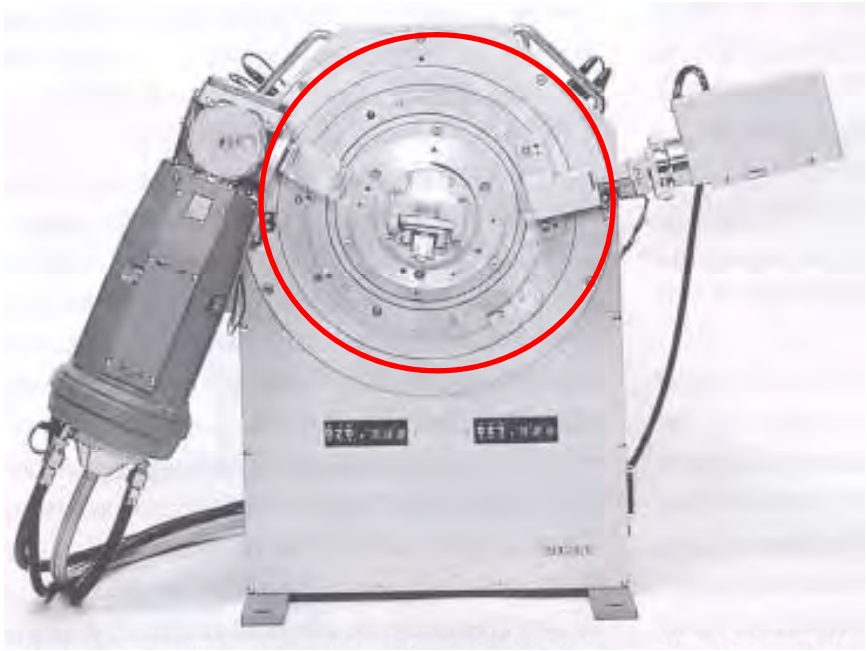
Anything else we can play around



$$n\lambda = 2d_{hkl}\sin\theta$$

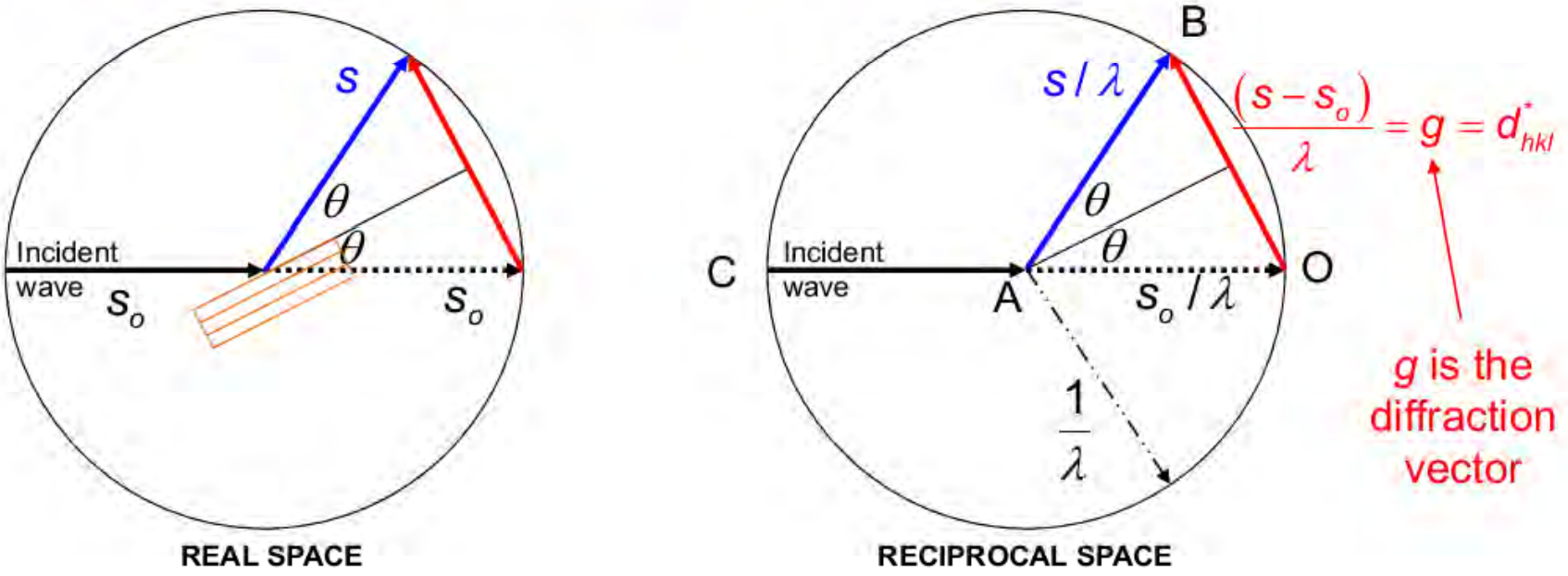
variable θ, fixed λ





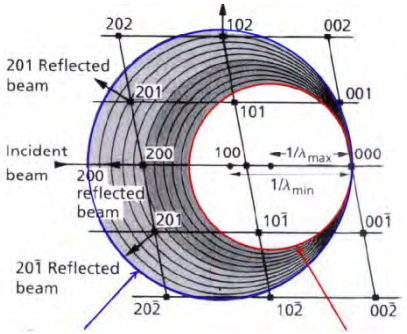
Ewald's Sphere Construction

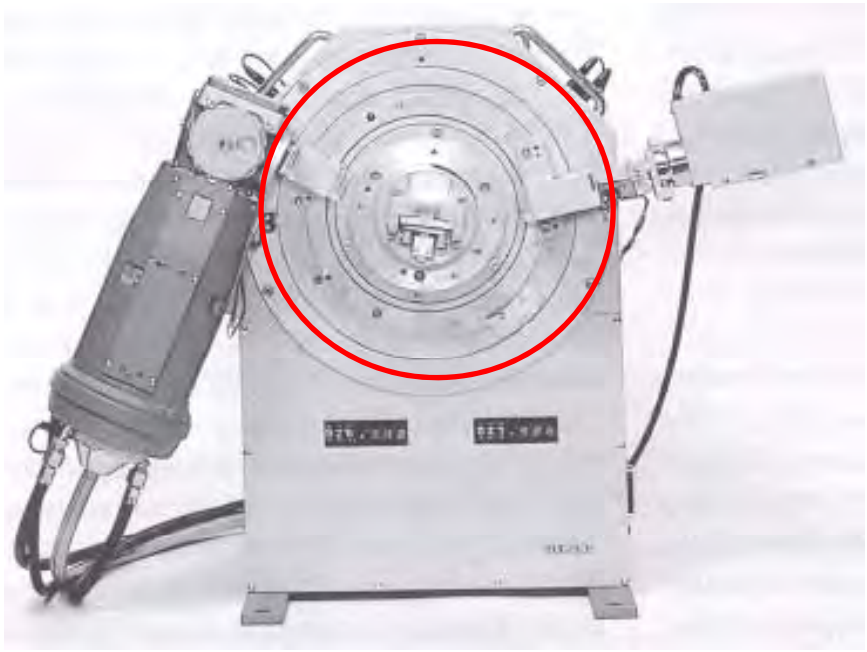
- Graphical representation of Bragg's Law in reciprocal space.

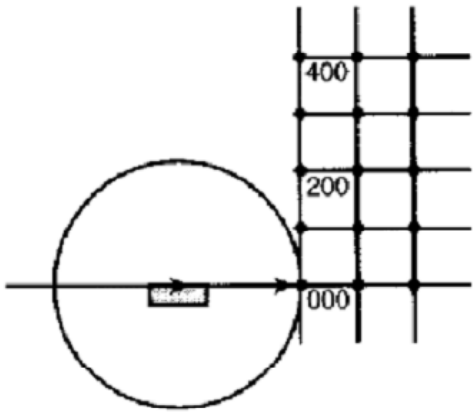


$$r_{uvw} = ua + vb + wc$$

$$r^*_{hkl} = ha^* + kb^* + lc^*$$

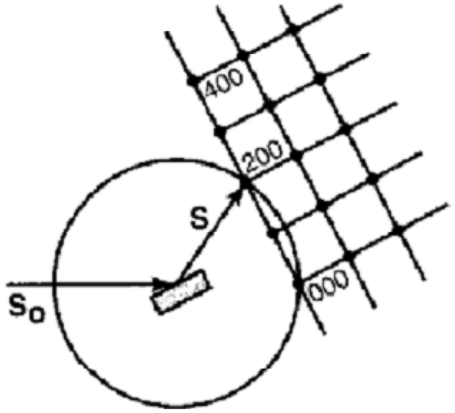






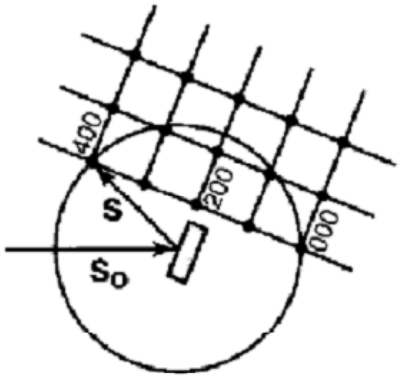
000

0°



200

θ_1°

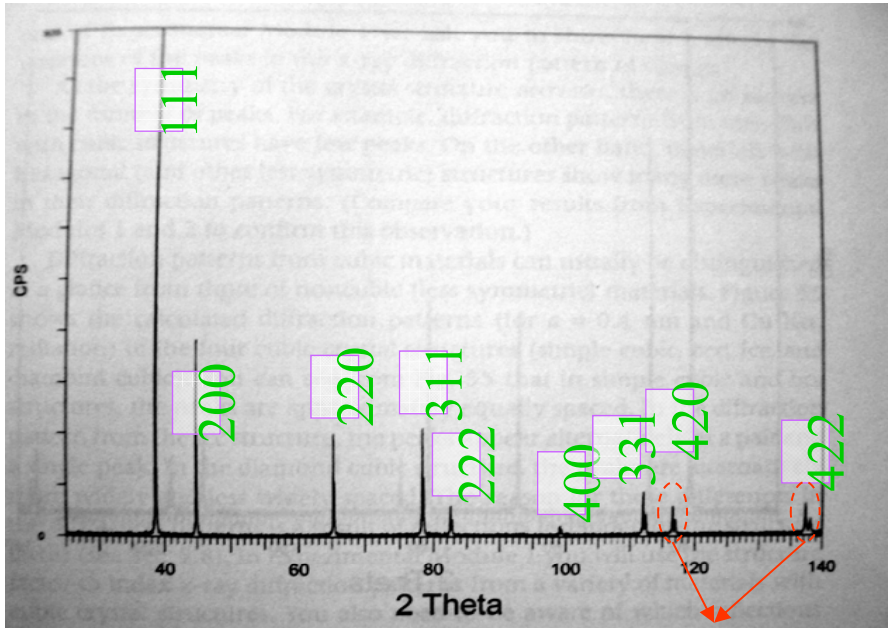


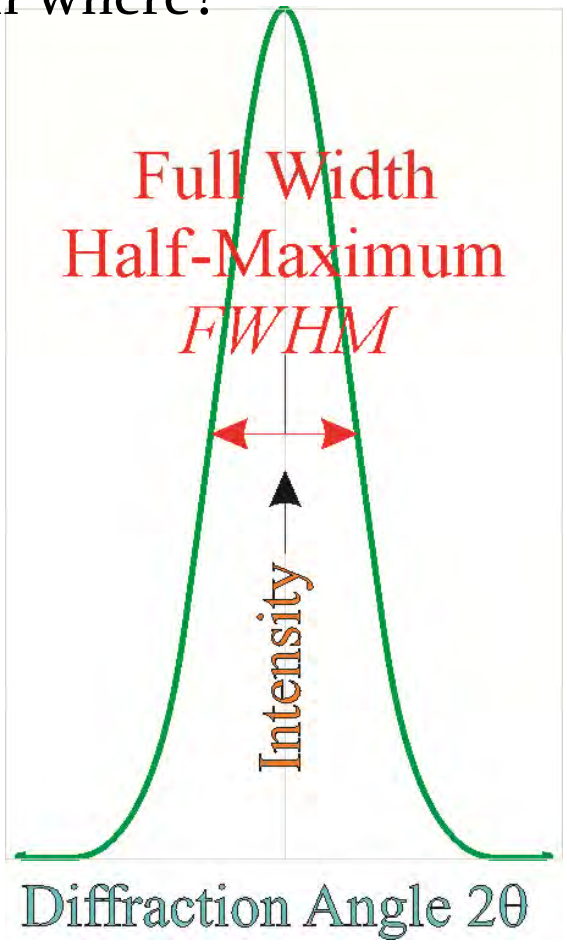
400

θ_2°

variable θ, fixed λ

What information can we get about sample? From where?





Intensity
Position
width

$$n\lambda = 2d_{hkl}\sin\theta$$

variable θ, fixed λ

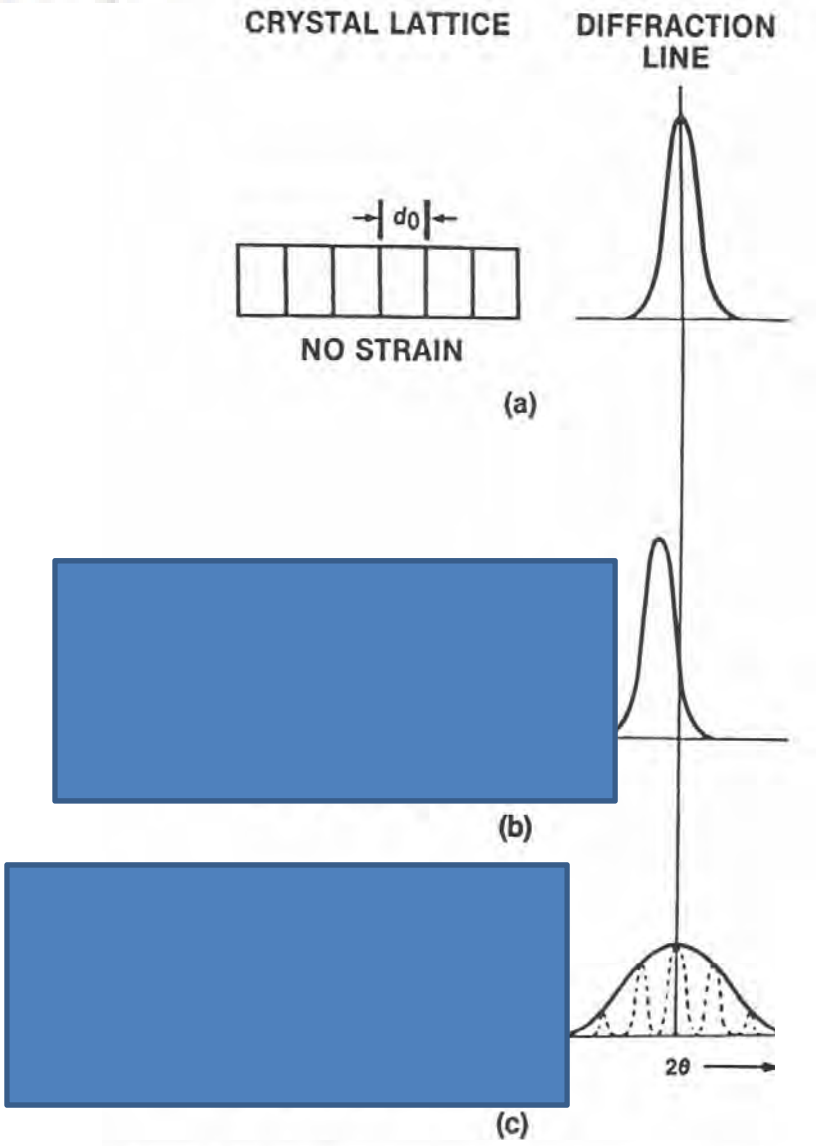


Figure 3.23. Strain expanding and contracting *d*-values.

Position

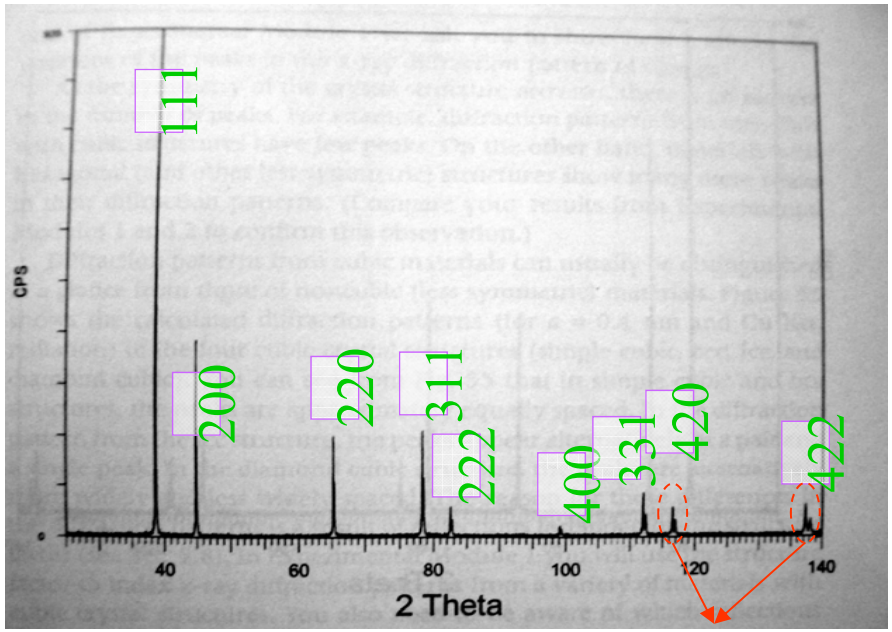
width

$$Q = \frac{4\pi \sin(\theta)}{\lambda}.$$

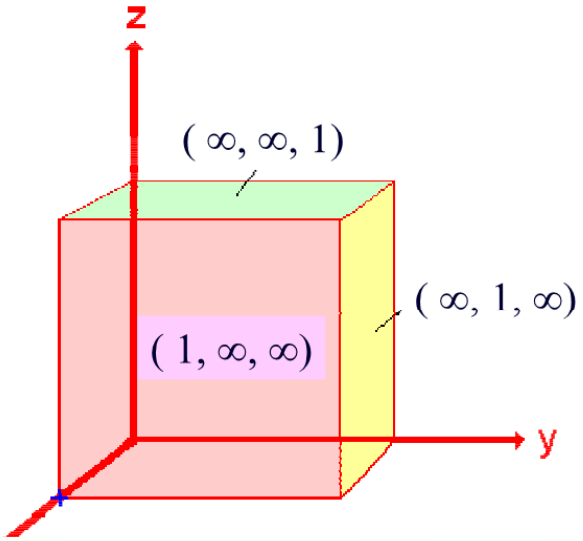
$$\mathbf{K} \cdot \mathbf{R} = 2\pi(k_1 n_1 + k_2 n_2 + k_3 n_3)$$

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Why does 111 has highest intensity?



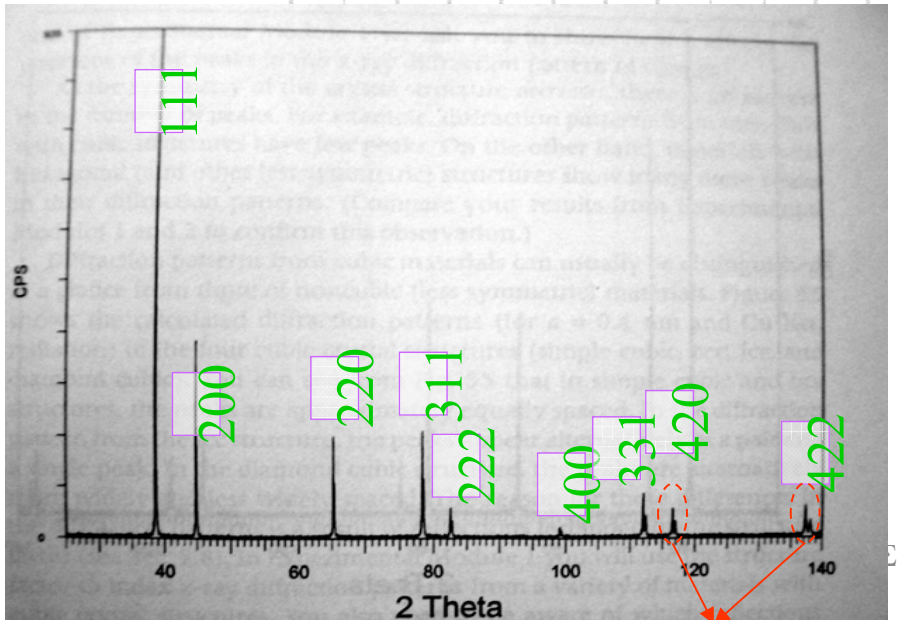
Simple cubic



Index	Members in family for **cubic lattice**
<100>	$[100],[\bar{1}00],[010],[0\bar{1}0],[001],[00\bar{1}]$
<110>	$[110],[\bar{1}10],[1\bar{1}0],[\bar{1}\bar{1}0],[101],[\bar{1}01],[10\bar{1}],[\bar{1}0\bar{1}],[011],[0\bar{1}1],[01\bar{1}],[0\bar{1}\bar{1}]$
<111>	$[111],[\bar{1}11],[1\bar{1}1],[11\bar{1}],[\bar{1}\bar{1}1],[\bar{1}1\bar{1}],[1\bar{1}\bar{1}],[\bar{1}\bar{1}\bar{1}]$

$$I_{hkl}(q) = K \times p_{hkl} \times L \times P \times A \times T \times E_{hkl} \times |F(q)|^2$$

K – scale factor, required to normalize calculated and measured intensities.
p_{hkl} – multiplicity factor. Accounts for the presence of symmetrically equivalent points in reciprocal lattice.
L – Lorentz multiplier, defined by diffraction geometry.
P – polarization factor. Account for partial polarization of electromagnetic wave.
A – absorption multiplier. Accounts for incident and diffracted beam absorption.
T_{hkl} – preferred orientation factor. Accounts for deviation from complete random grain distribution.
E_{hkl} – extinction multiplier. Accounts for deviation from kinematical diffraction model.
F_{hkl} – the structure factor. Defined by crystal structure of the material



$p_{100} = 6$
$p_{110} = 12$
$p_{111} = 8$

Index	Members in family for **cubic lattice**
<100>	$[100],[\bar{1}00],[010],[0\bar{1}0],[001],[00\bar{1}]$
<110>	$[110],[\bar{1}10],[1\bar{1}0],[\bar{1}\bar{1}0],[101],[\bar{1}01],[10\bar{1}],[\bar{1}0\bar{1}],[011],[0\bar{1}1],[01\bar{1}],[0\bar{1}\bar{1}]$
<111>	$[111],[\bar{1}11],[1\bar{1}1],[11\bar{1}],[\bar{1}\bar{1}1],[\bar{1}1\bar{1}],[1\bar{1}\bar{1}],[\bar{1}\bar{1}\bar{1}]$

$$F_{hkl} = \frac{\text{amplitude scattered by atoms in unit cell}}{\text{amplitude scattered by single electron}}$$

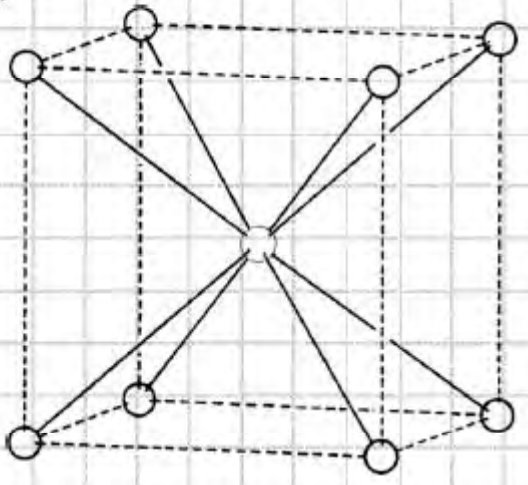
- Examples

For body-centered cell

$$F = fe^{2\pi i(h0+k0+l0)} + fe^{2\pi i(h/2+k/2+l/2)} = f\left(1+e^{\pi i(h+k+l)}\right)$$

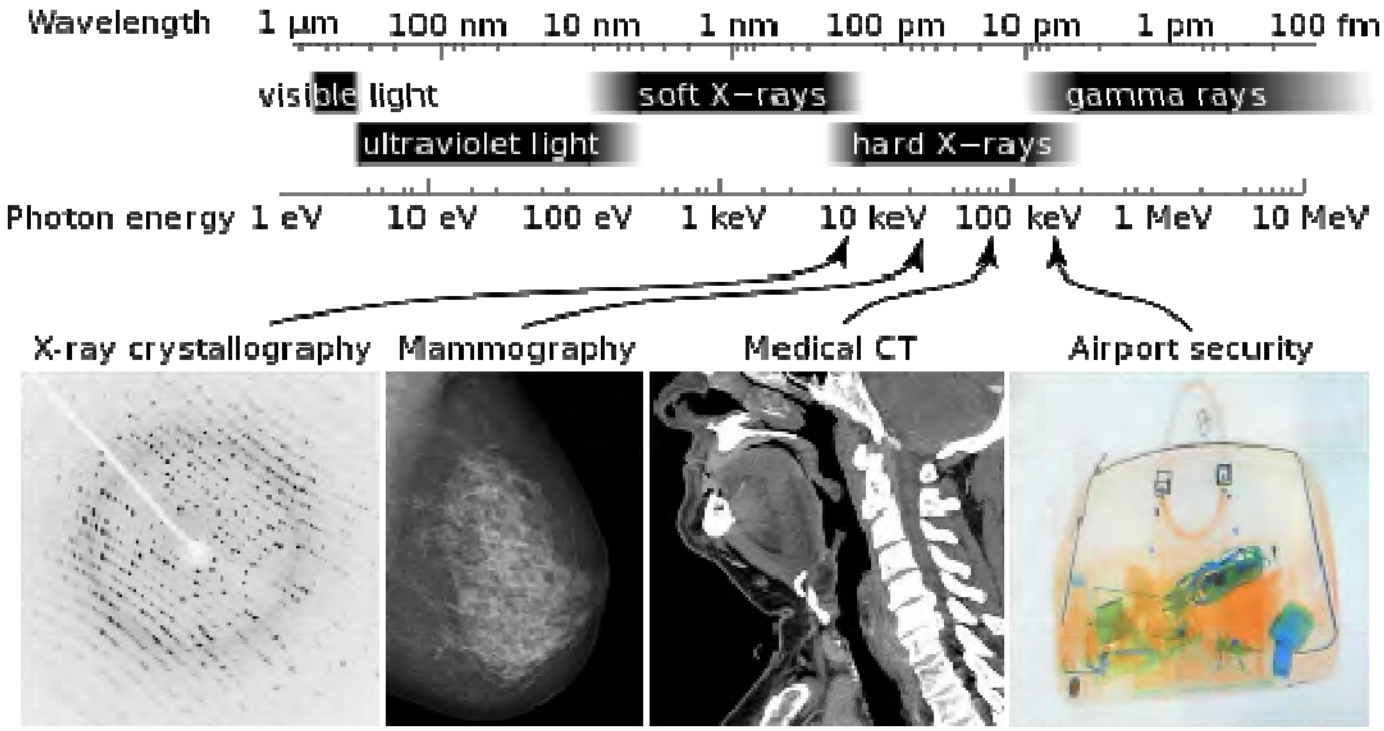
$F = 2f$ when $(h + k + l)$ is even

$F = 0$ when $(h + k + l)$ is odd

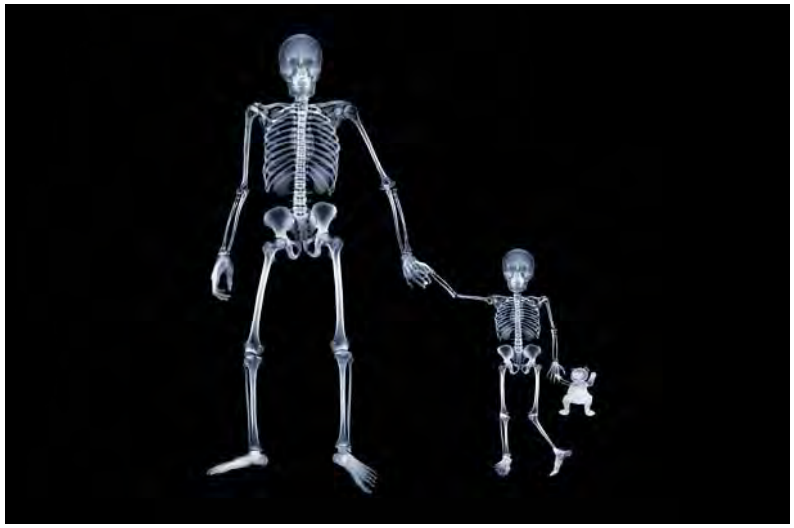


(200), (400), (220) $\cdots \Rightarrow$ $|F_{hkl}|^2 = 4f^2$

(100), (111), (300) $\cdots \Rightarrow$ $|F_{hkl}|^2 = 0$ ← "forbidden" reflections

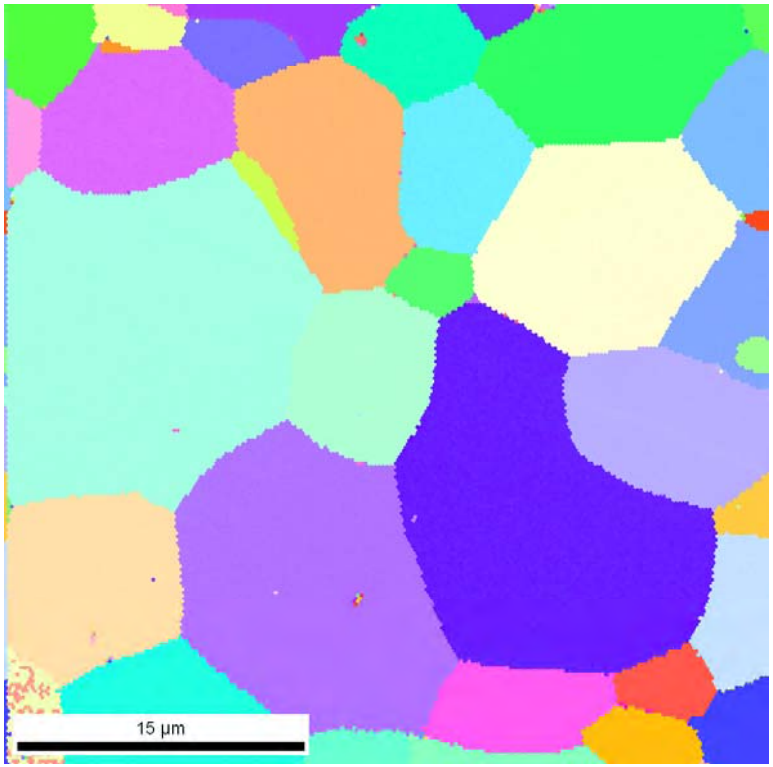

Wavelength
1 µm
100 nm
10 nm
1 nm
100 pm
10 pm
1 pm
100 fm
visible light
soft X−rays
gamma rays
ultraviolet light
hard X−rays
Photon energy
1 eV
10 eV
100 eV
1 keV
10 keV
100 keV
1 MeV
10 MeV
X-ray crystallography
Mammography
Medical CT
Airport security

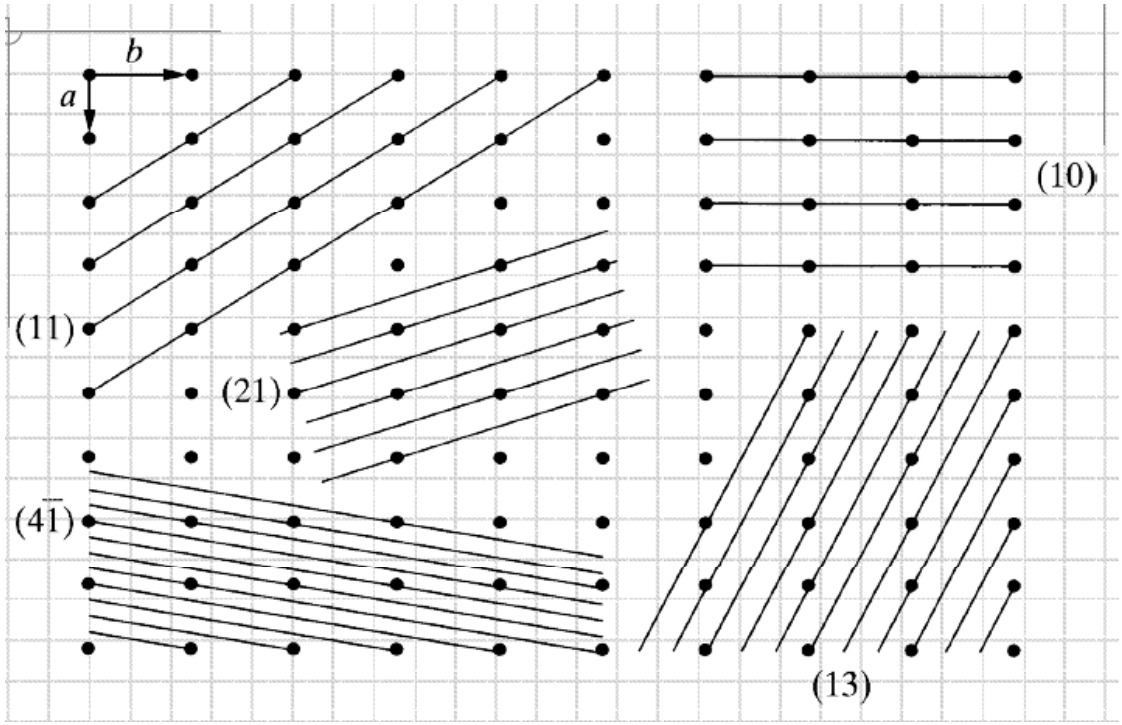
X-ray



$$I \propto Z^2$$

Good luck to your SSP study!


15 μm

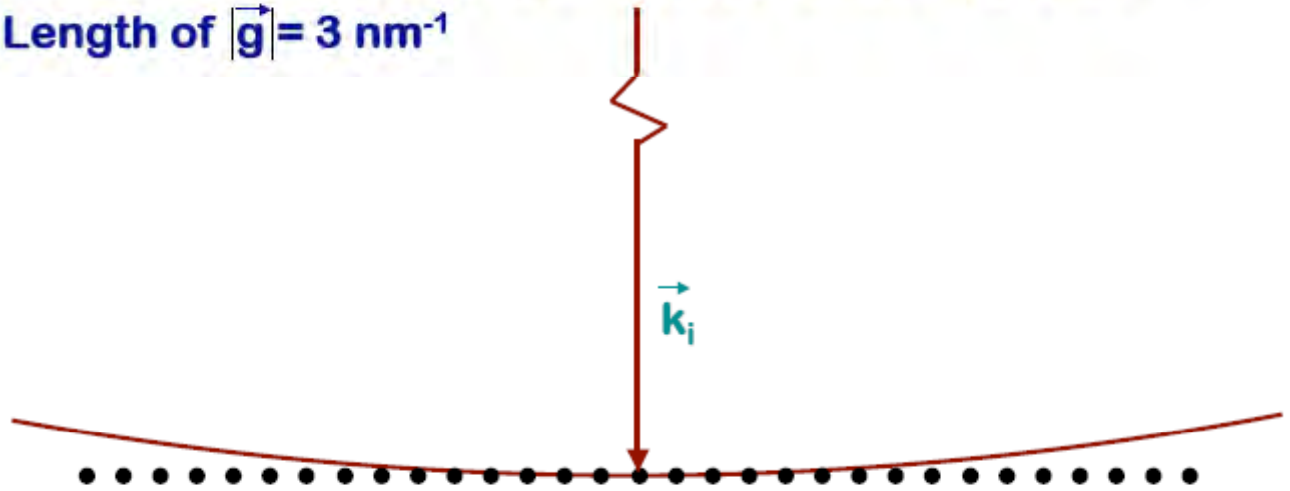

b
a
(10)
(11)
(21)
(4$\bar{1}$)
(13)

Diffraction

Diffraction occurs when the Ewald sphere intersects a reciprocal lattice vector

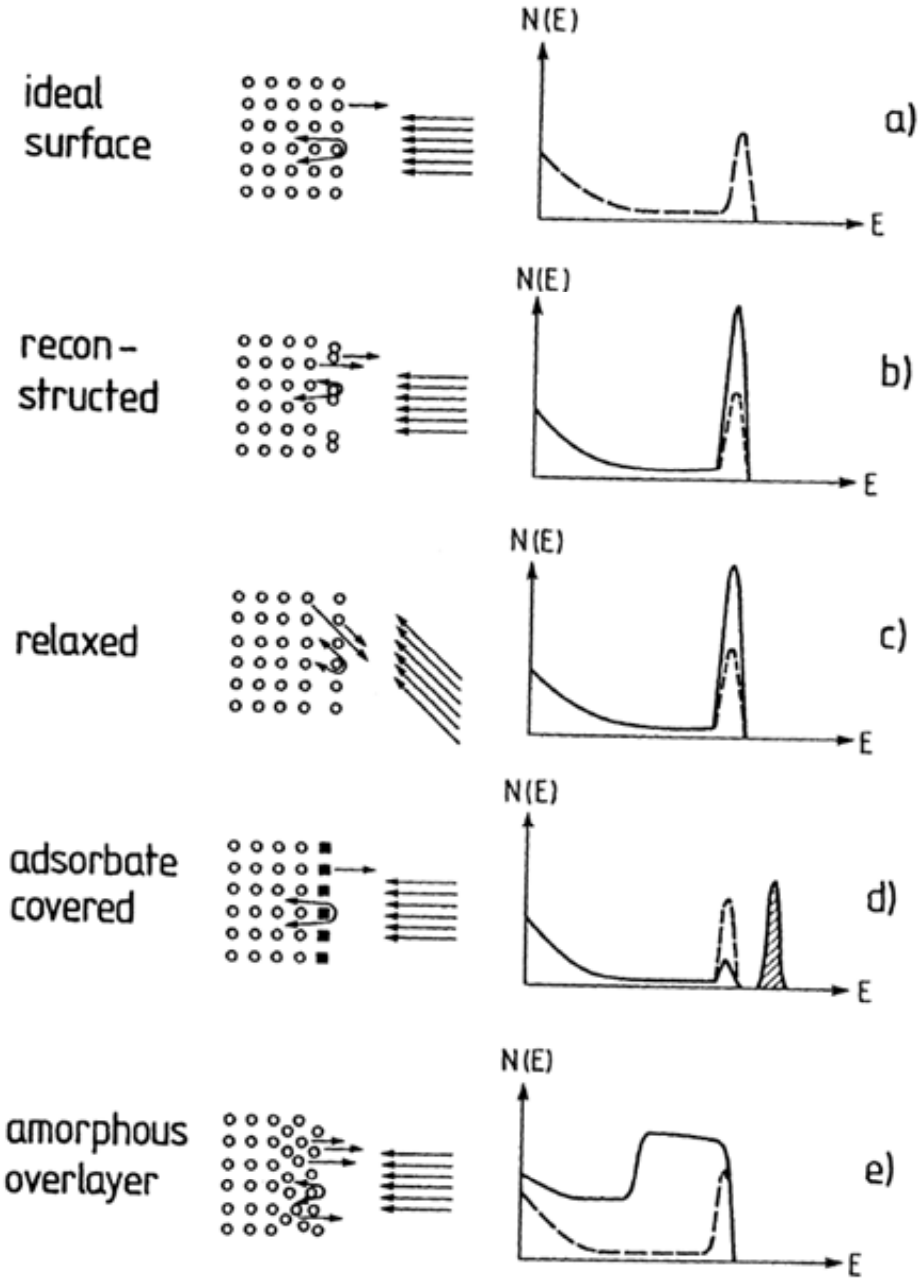
For 200 kV electrons, $1/\lambda = 1/0.00273\ \text{nm} = 366\ \text{nm}^{-1}$

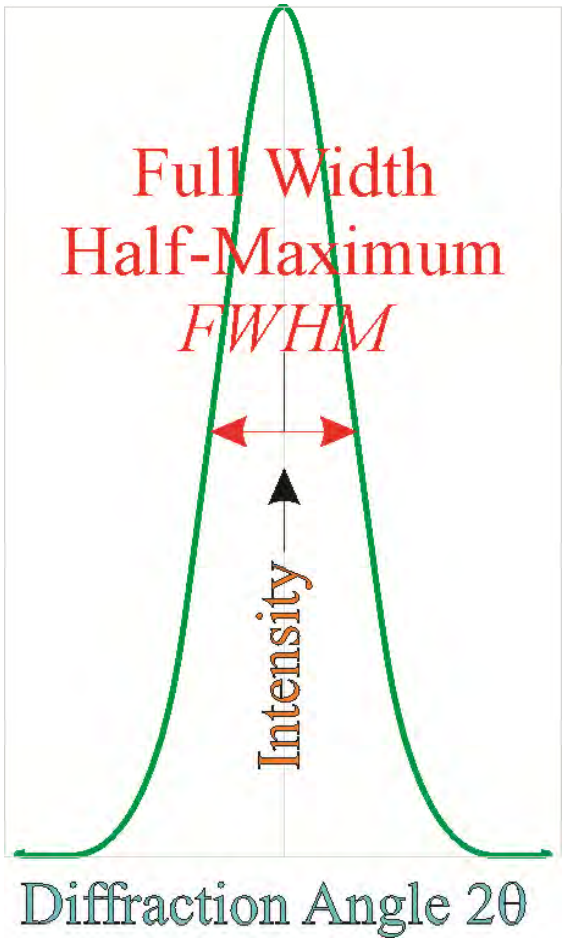
Length of $|\vec{g}| = 3\ \text{nm}^{-1}$

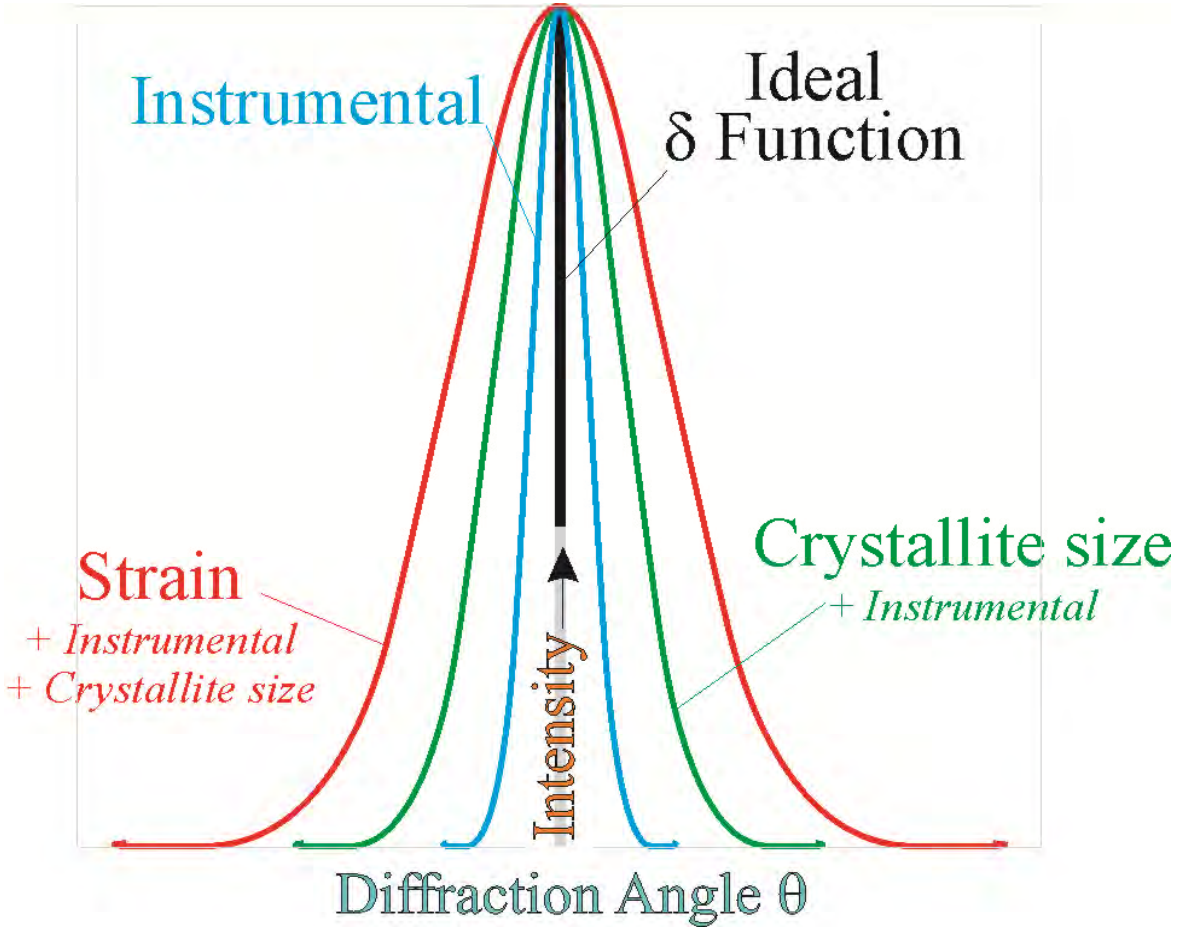


The applications

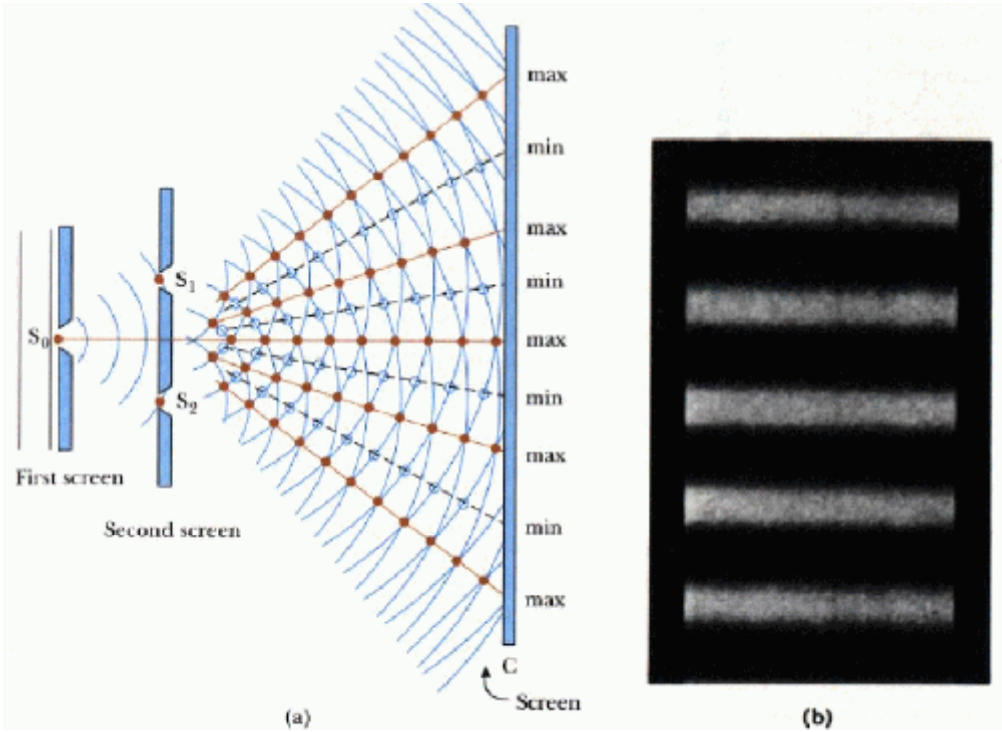
a) First layer atoms scatter;
b) First and second layer atoms scatter;
c) At certain angle first and second layer atoms scatter, while along normal only first layer atoms scatter;
d) Adsorbate overlayers' first layer atoms scatter, the first layer atoms of substrate scattering reduced.
e) Amorphous overlayer atoms scatter, there is no peak but a bump and the size of the bump depends on thickness of the overlayer.

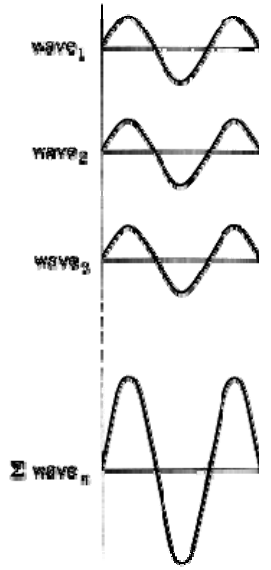


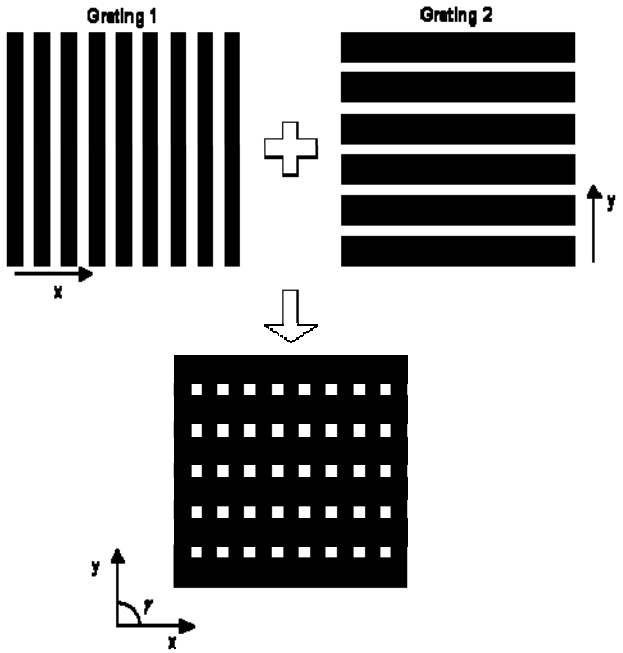




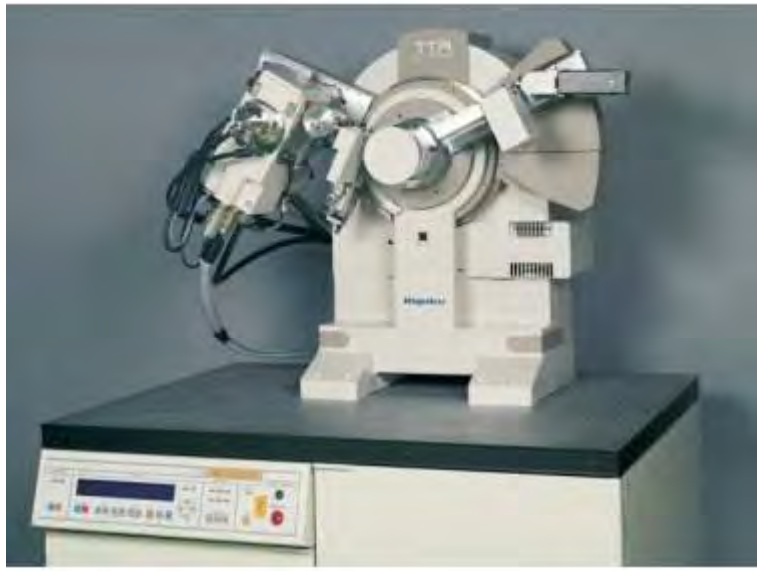
$$B(FWHM) = B_i + B_c + B_s + B_{SF} + \ldots$$

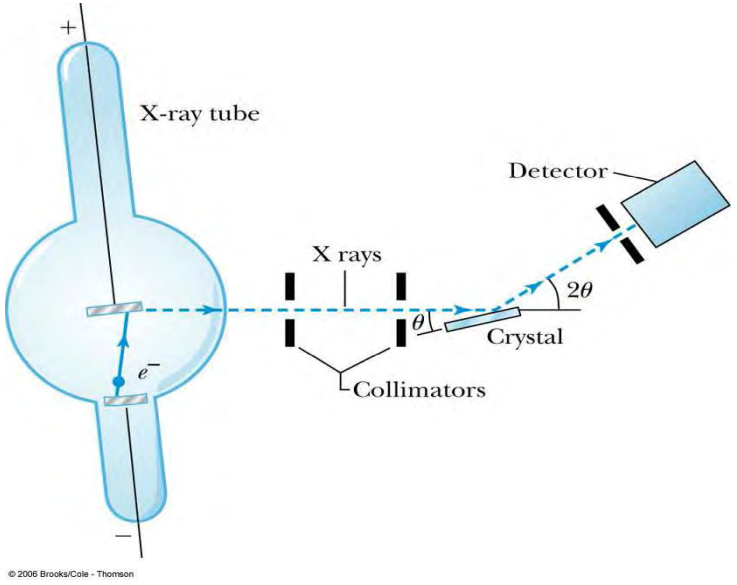






http://www.youtube.com/watch?v=ACjr66v4gyo





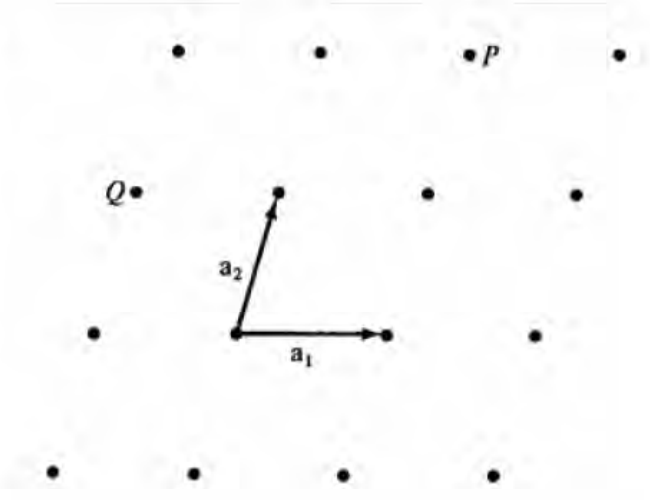
Periodic Lattice in a solid.

Bravais Lattice:

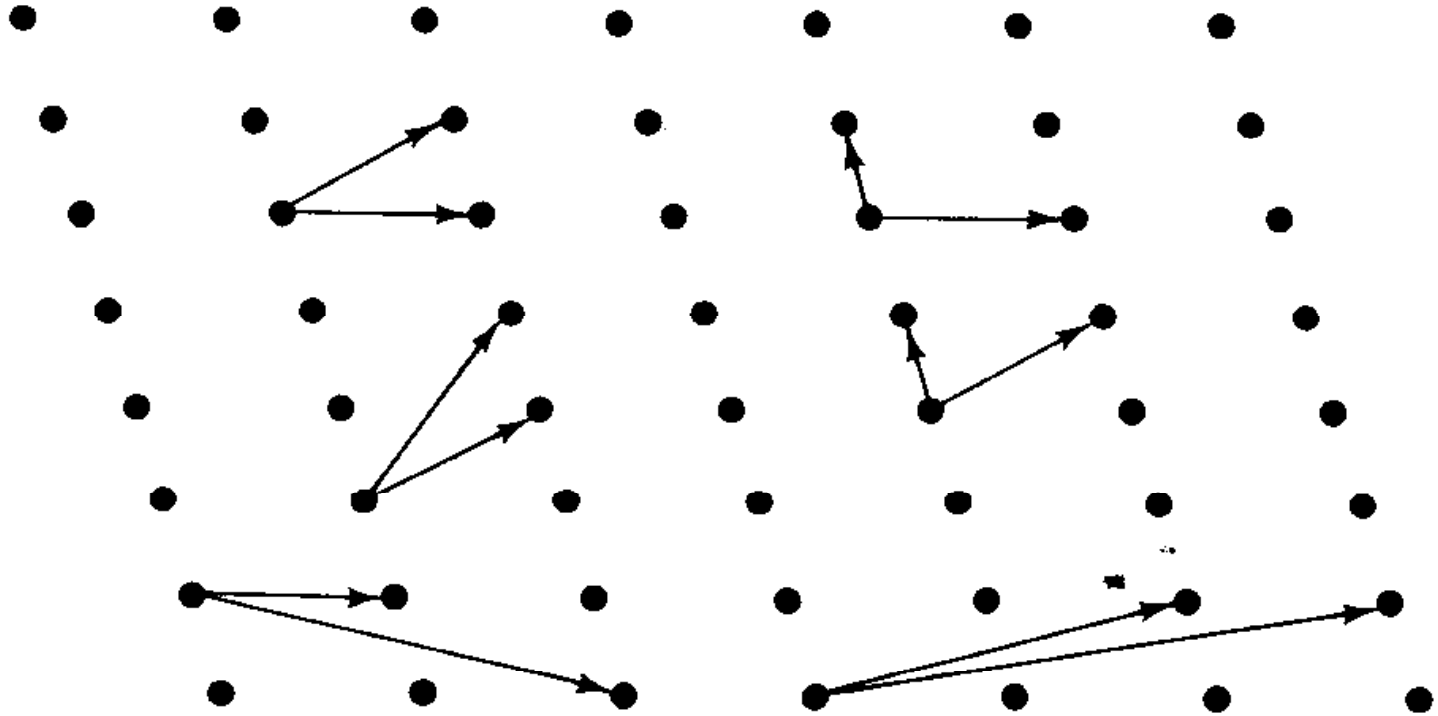
(a) A Bravais lattice is an infinite array of discrete points with an arrangement and orientation that appears exactly the same, for whichever of the points the array is viewed.

(b) A (3D) Briavais lattice consists of all points with position vectors $\vec{R}$ of the form: $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$, where $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ are any three vectors not all in the same plane, and n_1, n_2, n_3 are all integeral values.

Thus the point $\sum n_i\vec{a}_i$ is reached by moving n_i steps of $\vec{a}_i$ length in the direction of $\vec{a}_i$ for $i = 1, 2, 3...$



For any given Bravais lattice, the set of primitive vectors is not unique. There are many nonequivalent choices.



Primitive lattice cell :

The vectors $\vec{a}_i$ appearing in definition of a Bravais lattice are called primitive vectors and are said to generate or span lattice.

Primitive cell is a minimum-volume cell:

A volume of space that, when translated through all the vectors in a Bravais lattice, just fills all of space without either overlapping itself or leaving voids is called a primitive cell or primitive unit cell. There is no unique way of choosing a primitive cell for a given Bravias lattice.

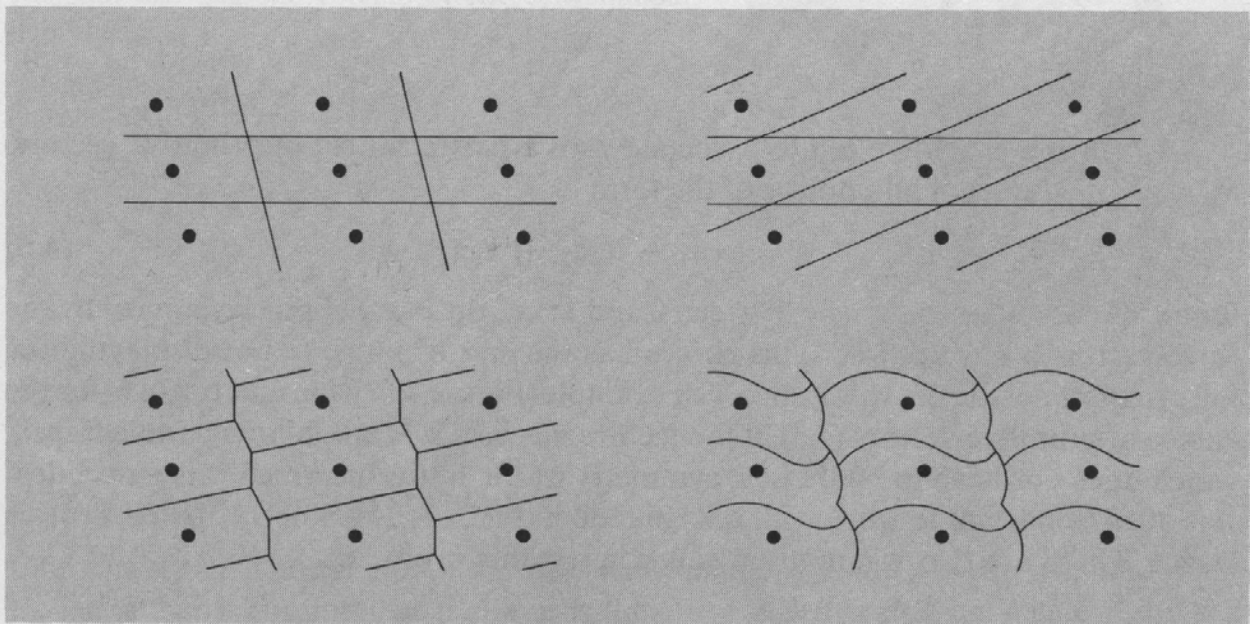
The volume of a primitive cell is independent of the choice of cell:

$V_c = |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|$,

A primitive cell must contain precisely one lattice point.

Primitive unit cell:

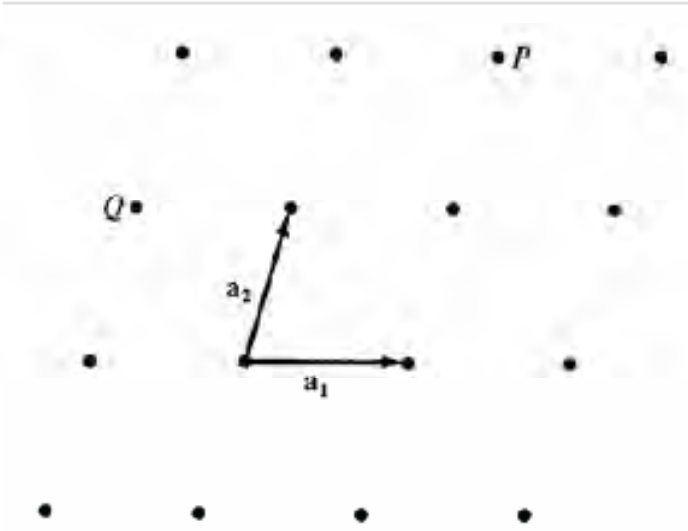
Given any two primitive cells of arbitrary shape, it is possible to cut the first up into pieces, which, when translated through appropriate lattice vectors, can be reassembled to give the second.



Bravais Lattice:

(a) A Bravais lattice is an infinite array of discrete points with an arrangement and orientation that appears exactly the same, for whichever of the points the array is viewed.

(b) A (3D) Briavais lattice consists of all points with position vectors $\vec{R}$ of the form: $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$, where $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ are any three vectors not all in the same plane, and n_1, n_2, n_3 are all integeral values. Thus the point $\sum n_i\vec{a}_i$ is reached by moving n_i steps of $\vec{a}_i$ length in the direction of $\vec{a}_i$ for $i = 1, 2, 3...$



Definition of reciprocal lattice:

Consider a set of point $\vec{R}$ constituting a Bravais lattice, and a plane wave, $e^{i\vec{k}\cdot\vec{r}}$. For general $\vec{k}$, such a plane wave will not have the periodicity of the Bravais lattice, but for certain special choices of wave vectors it will. The set of all wave vectors $\vec{k}$ that yield plane waves with the periodicity of a given Bravais lattice is known as it reciprocal lattice.

$\vec{k}$ belongs to the reciprocal lattice of a Bravais lattice of points $\vec{R}$, provided that $e^{i\vec{k}\cdot(\vec{R}+\vec{r})} = e^{i\vec{k}\cdot\vec{r}}$ holds for any $\vec{r}$, and for all $\vec{R}$ in the Bravais lattice. The reciprocal lattice is a set of wave vectors $\vec{k}$ satisfying $e^{i\vec{k}\cdot\vec{R}} = 1$.

Reciprocal lattice is a Bravais lattice:

Let $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$ be a set of primitive vectors for the direct lattice.

Then the reciprocal lattice

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

Note $\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$, if $i \neq j$, $\delta_{ij} = 0$; if $i = j$, $\delta_{ij} = 1$.

For any vector $\vec{k}$ in reciprocal space, $\vec{k} = k_1\vec{b}_1 + k_2\vec{b}_2 + k_3\vec{b}_3$.

For any vector $\vec{R}$ in reciprocal space, $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$.

$\vec{k} \cdot \vec{R} = 2\pi(k_1n_1 + k_2n_2 + k_3n_3)$.

Since $\vec{k} \cdot \vec{R}$ must be times an integer for any choices of integers n_i.

This requires the coefficients k_i to be integers.

The reciprocal of the reciprocal space is the real space. Examples of reciprocal lattice units.

Reciprocal lattice units in simple cubic case:

Let $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = a\hat{y}$, and $\vec{a}_3 = a\hat{z}$

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi}{a}\hat{x}, \vec{b}_2 = \frac{2\pi}{a}\hat{y}, \vec{b}_3 = \frac{2\pi}{a}\hat{z}.$$

Prove that the reciprocal lattice primitive vectors satisfy

$$\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \frac{(2\pi)^3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}.$$

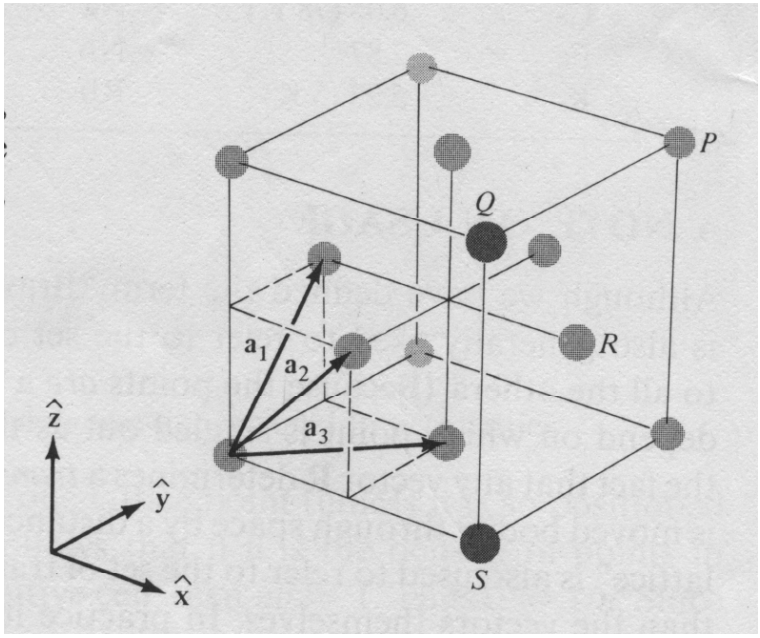
Note vector identity: $(\vec{c} \times \vec{a}) \times (\vec{a} \times \vec{b}) = (\vec{c} \cdot \vec{a} \times \vec{b})\vec{a}$

Reciprocal lattice units in fcc case:

Primitive vectors

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

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{y}+\hat{z}-\hat{x}), \vec{b}_2 = \frac{2\pi}{a}(\hat{z}+\hat{x}-\hat{y}), \vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z}).$$

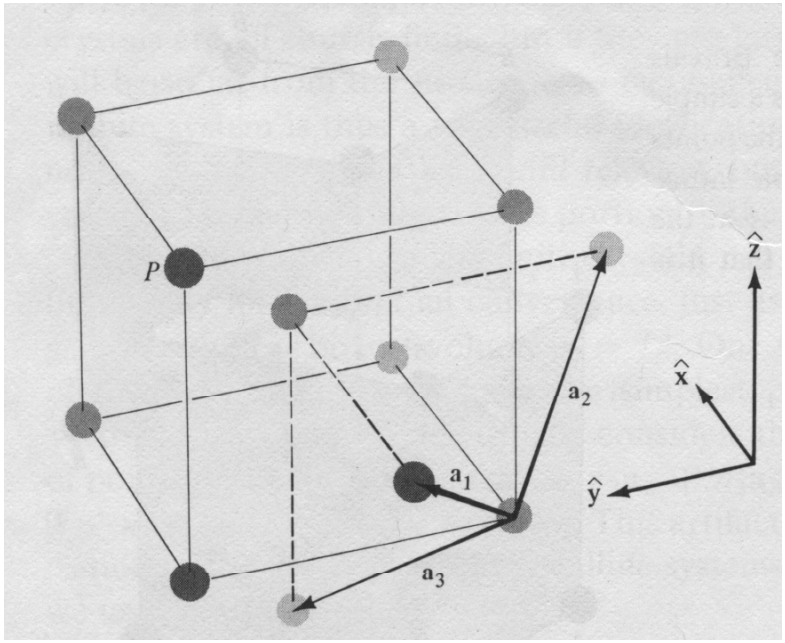


Reciprocal lattice units in bcc case:

Primitive vectors

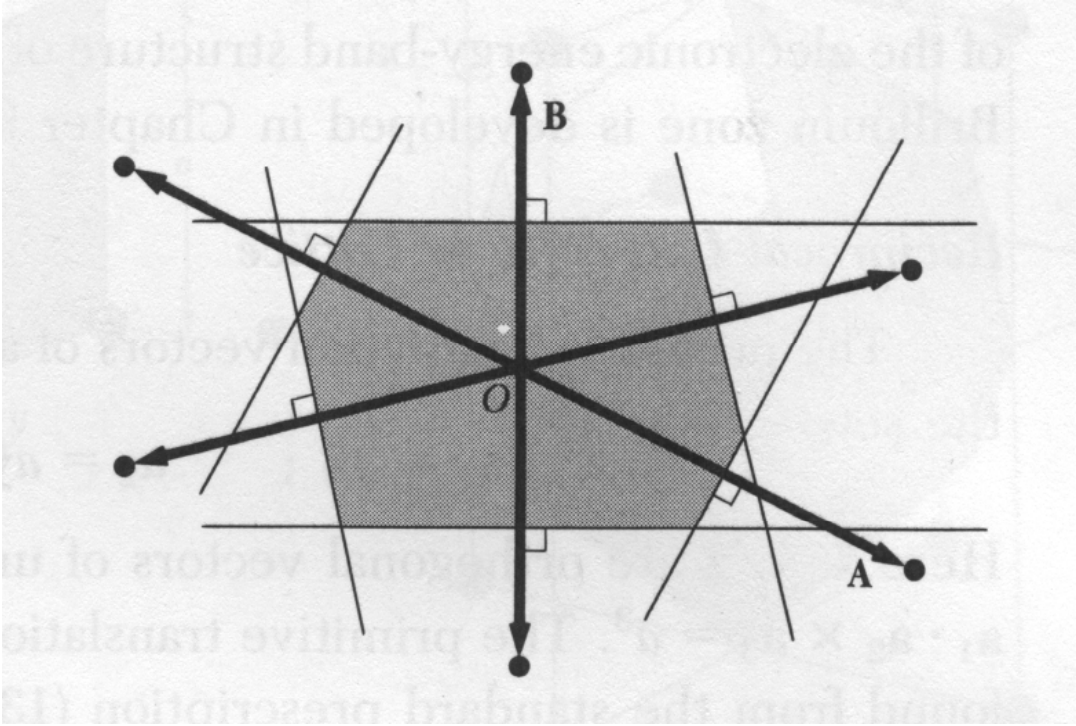
$$\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z}-\hat{x}), \vec{a}_2 = \frac{a}{2}(\hat{z}+\hat{x}-\hat{y}), \vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z}).$$

$$\vec{b}_1 = \frac{2\pi}{a}(\hat{y}+\hat{z}), \vec{b}_2 = \frac{2\pi}{a}(\hat{z}+\hat{x}), \vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}).$$

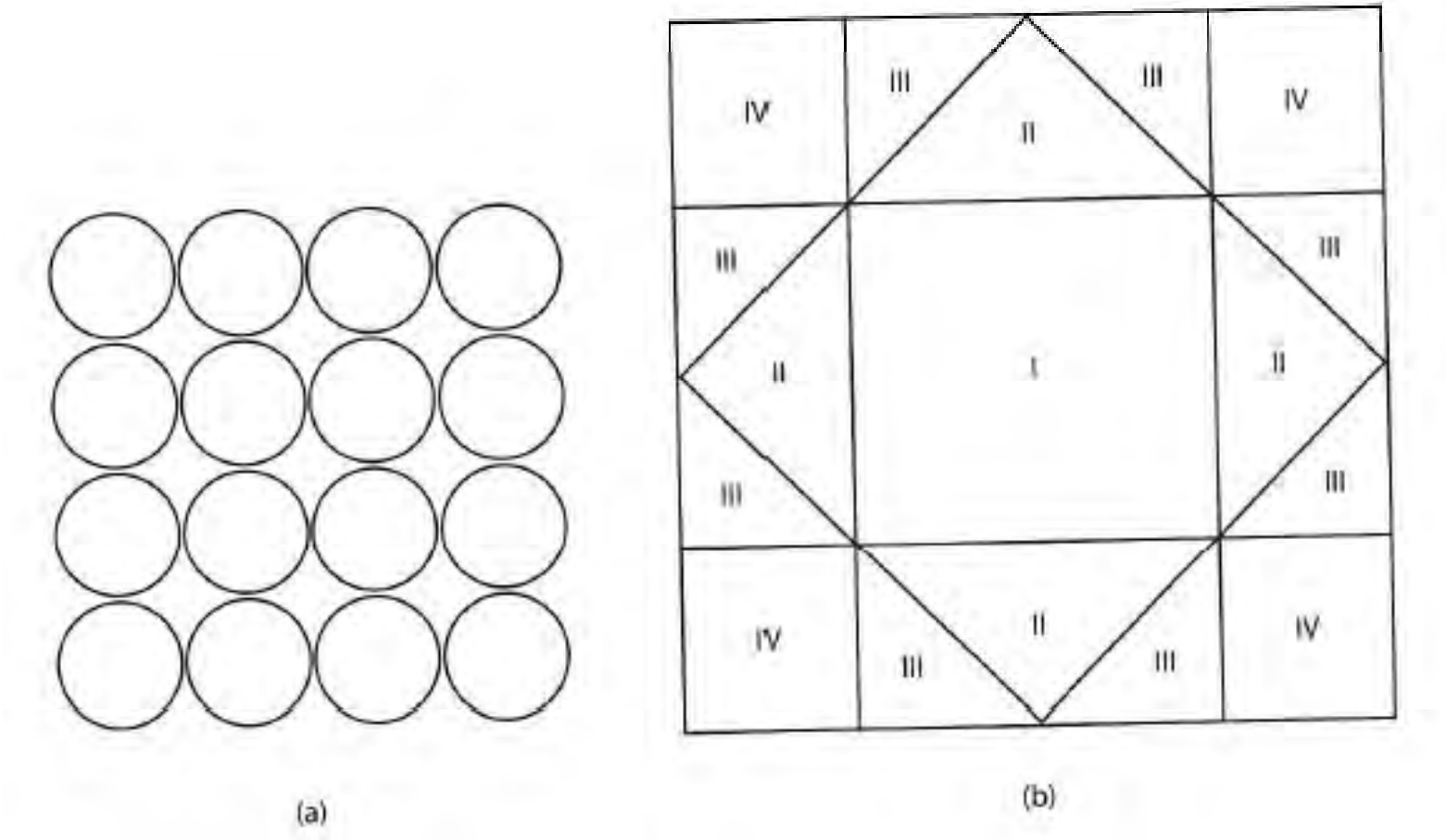


First Brillouin zone

The Wigner-Seitz primitive cell of the reciprocal lattice is known as the first Brillouin zone. (Wigner-Seitz is real space concept while Brillouin zone is a reciprocal space idea).



Two dimensional real and reciprocal space



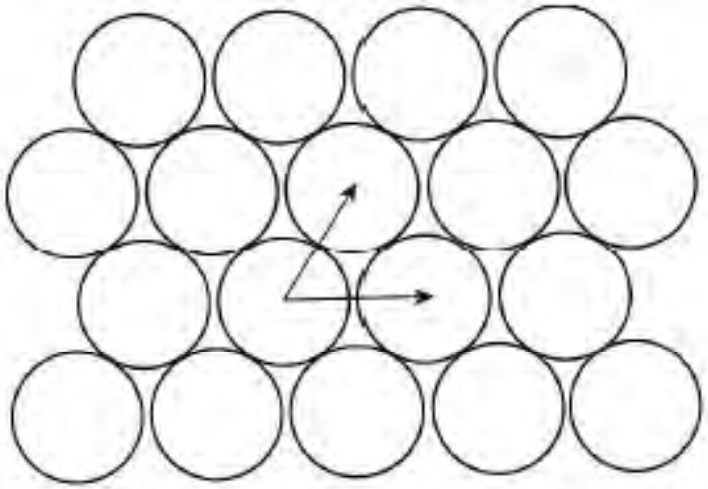
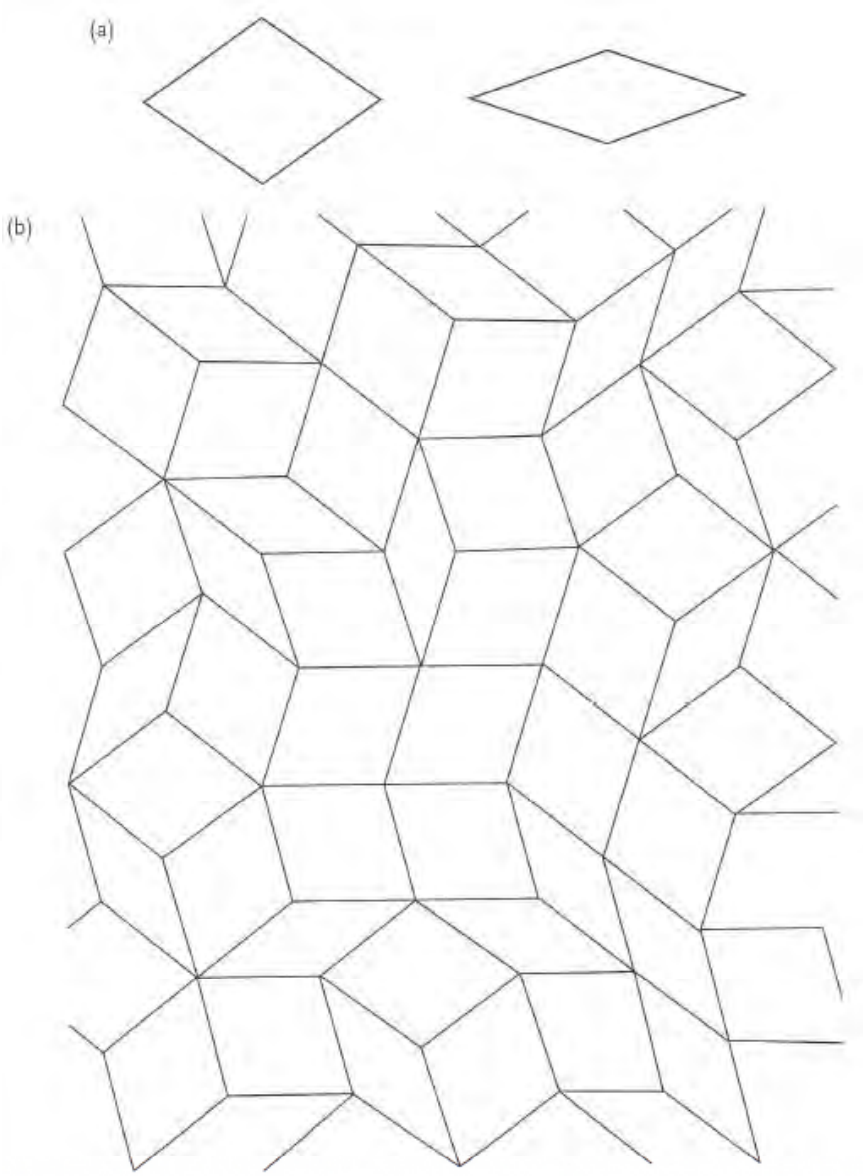


FIGURE 2.4. Two-dimensional plane triangular lattice.



Solve a problem

The primitive translation vectors of the hexagonal space lattice may be taken as

$\vec{a}_1 = (3^{1/2}a/2)\hat{x} + (a/2)\hat{y}$;

$\vec{a}_2 = -(3^{1/2}a/2)\hat{x} + (a/2)\hat{y}$;

$\vec{a}_3 = c\hat{z}$.

(a) Show that the volume of the primitive cell is $(3^{1/2}a/2)a^2c$.

(b) Show that the primitive translations of the reciprocal lattice are

$\vec{b}_1 = (2\pi/3^{1/2}a)\hat{x} + (2\pi/a)\hat{y}$;

$\vec{b}_2 = -(2\pi/3^{1/2}a)\hat{x} + (2\pi/a)\hat{y}$;

$\vec{b}_3 = (2\pi/c)\hat{z}$,

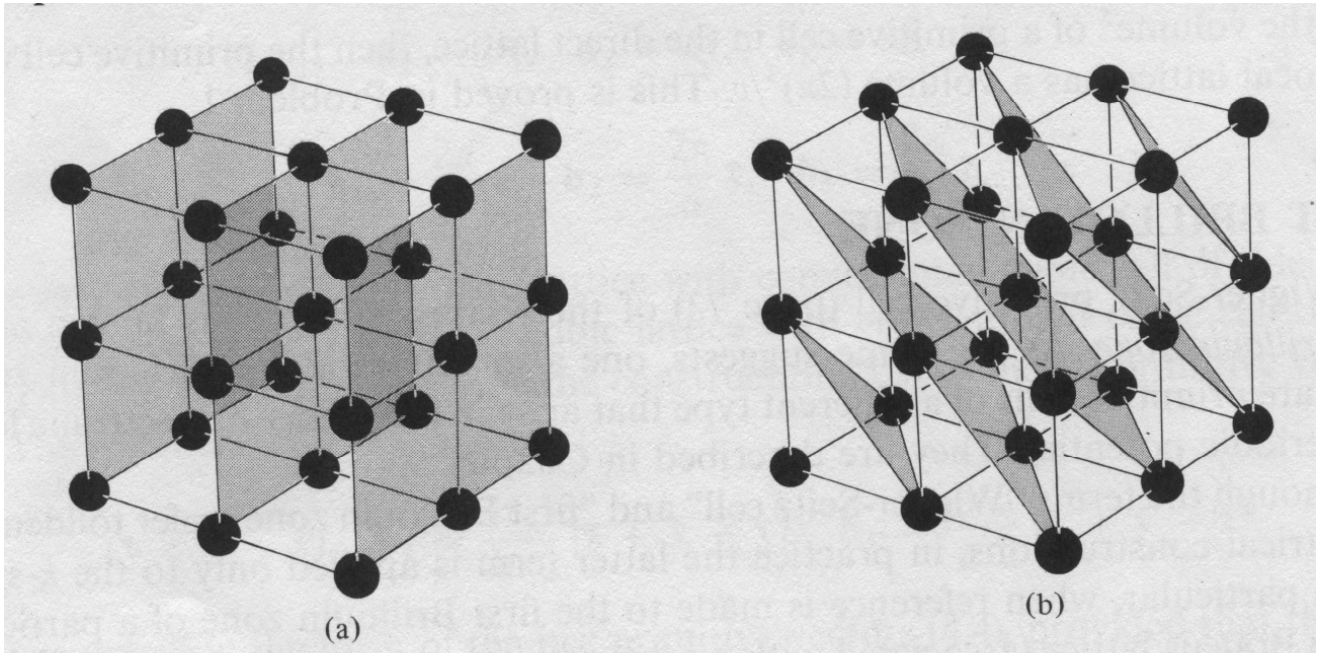
so that the lattice is its own reciprocal, but with a rotation of axes.

(c) describe and sketch the first Brillouin zone of the hexagonal space lattice.

Lattice planes

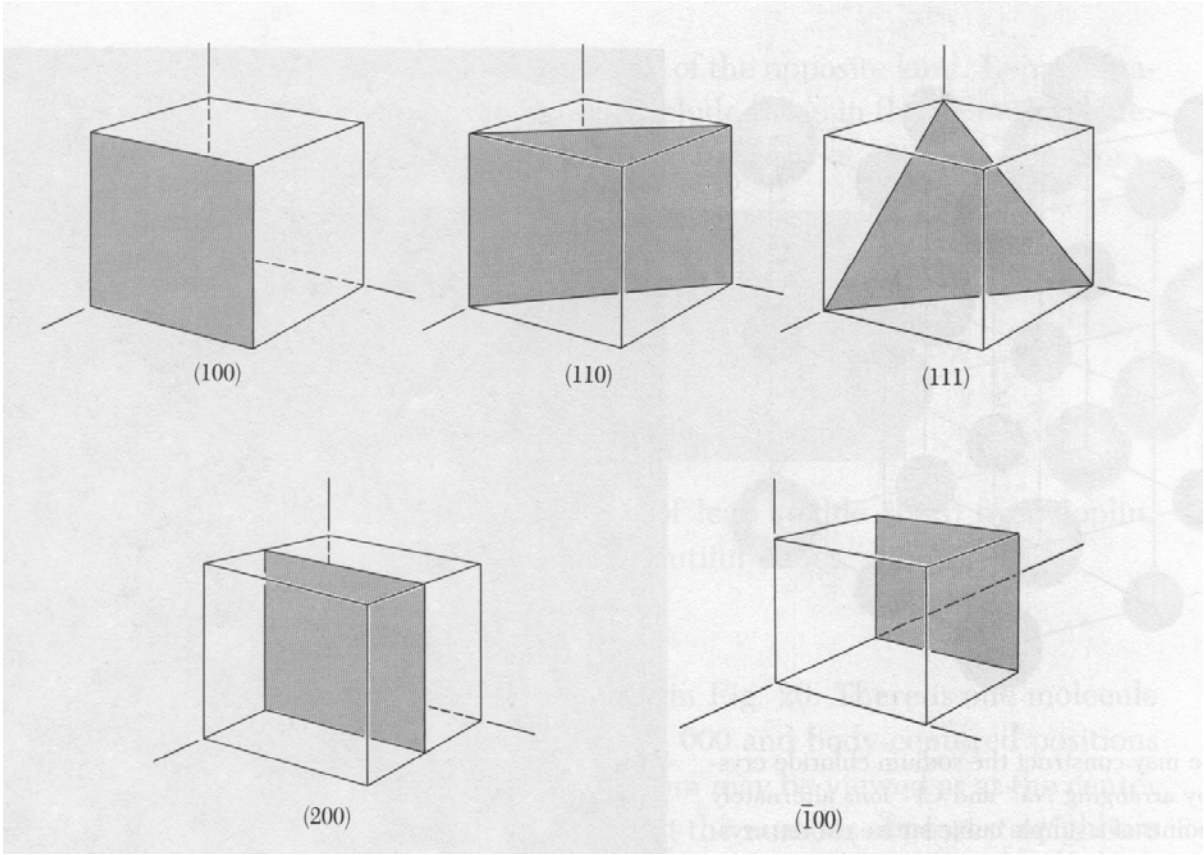
A lattice plane is defined to be any plane containing at least three noncollinear Bravais lattice points. A family of lattice planes is a set of parallel, equally spaced lattice planes, with together contain all the points of the 3D Bravais lattice.

For any family of lattice planes separated by a distance d, there are reciprocal lattice vectors perpendicular to the planes, the shortest of which have a length of $2\pi/d$. Conversely, for any reciprocal lattice vector K, there is a family of lattice planes normal to K and separated by a distance d, where $2\pi/d$ is the length of the shortest reciprocal lattice vector parallel to K.



(100) (111)

Index of the plane
1. Find the intercepts on the axes in terms of lattice constants.
2. Take the reciprocals of these numbers and then reduce to three integers having the same ratio, usually the smallest three integers. (*hkl*)-plane



Miller indices:

The Miller indices of a lattice plane are the coordinates of the shortest reciprocal lattice vectors normal to that plane, with respect to a specified set of primitive reciprocal lattice vectors.

A plane with Miller indices h, k, l, is normal to the reciprocal lattice vector: $h\vec{b}_1 + h\vec{b}_2 + h\vec{b}_3$.

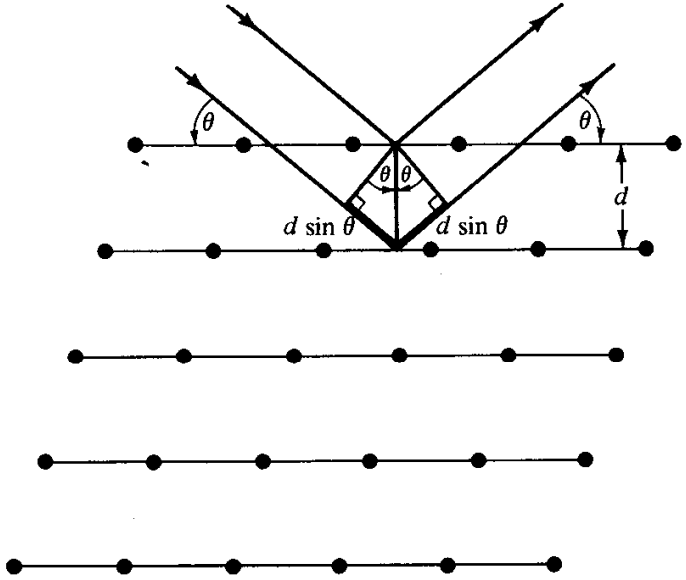
the Miller indices are integers, can have no common factors, and depend on the particular choice of primitive vectors.

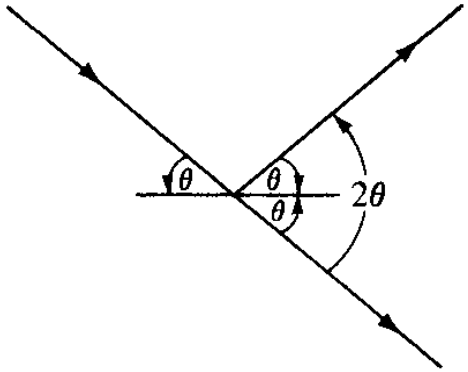
Conventions for specifying directions:

Lattice planes are usually specified by giving their Miller indices in parentheses (h,k,l). When specifying directions in the direct lattice, we use the notation $[n_1,n_2,n_3]$ from the origin. Since the (100), (010), and (001) planes are all equivalent in a cubic crystal. One denotes these planes as $\{100\}$ planes. Similarly, the [100], [010], [001], $[\bar{1}00]$, $[0\bar{1}0]$, and $[00\bar{1}]$ in a cubic crystal are equivalent, and referred to collectively as the $\langle 100\rangle$ direction.

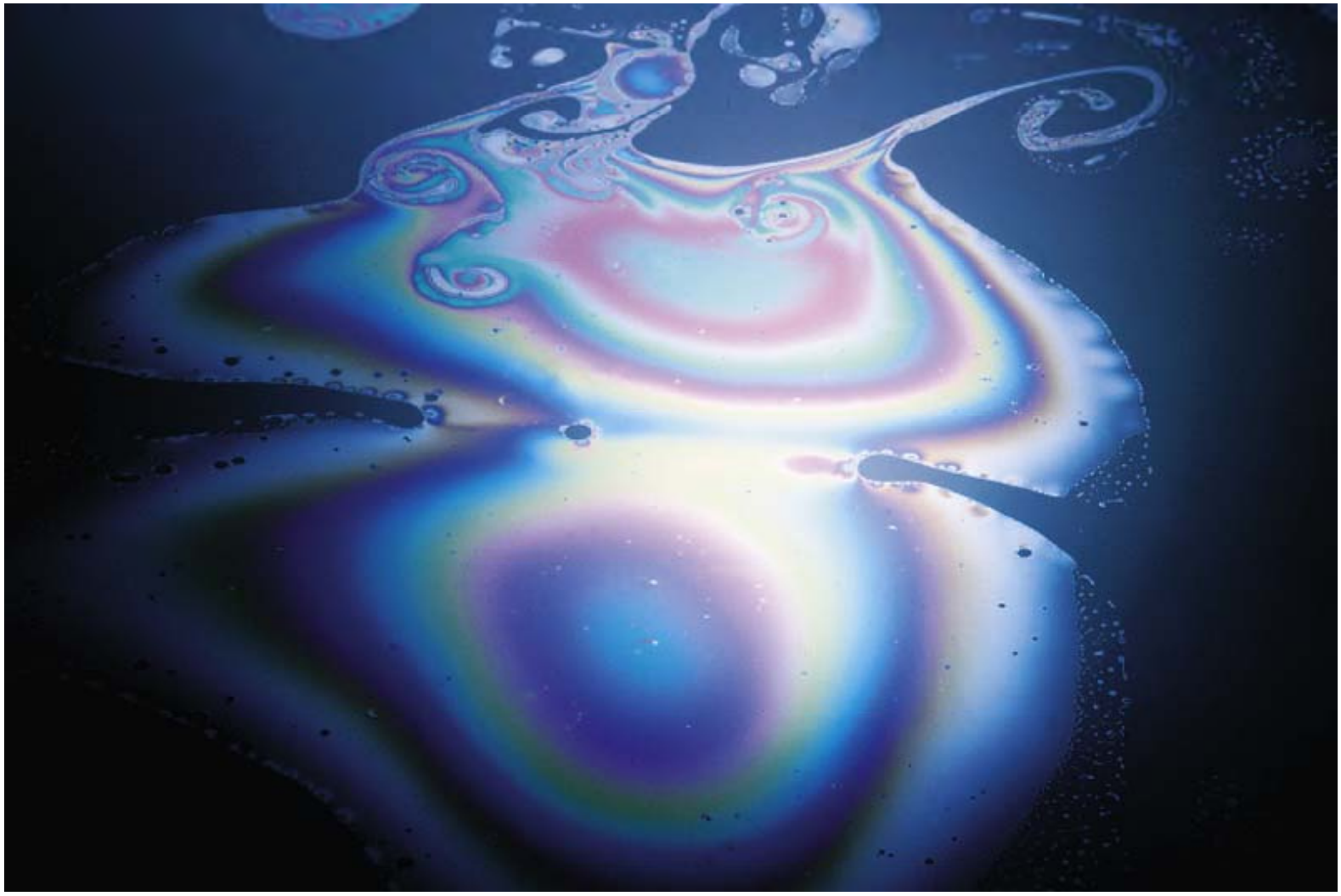
Bragg Law: $2d\sin\theta = n\lambda,\ \lambda \approx 10^{-8}$ cm.

The crystal is made out of parallel planes of ions, spaced d apart. (1) the x-rays are specularly reflected by the ions in any one plane. (2) the reflected rays from successive planes should interfere constructively.





Thin films: gasoline on water



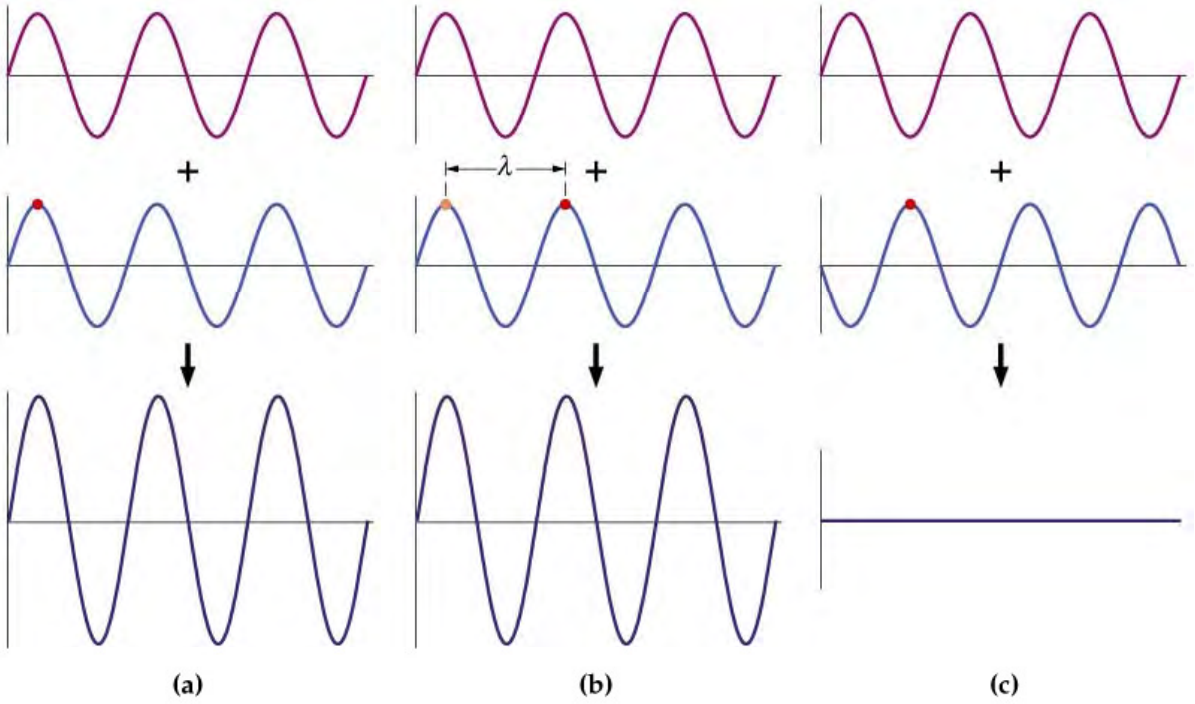
Constructive and destructive interference

Cases (a) & (b): constructive interference

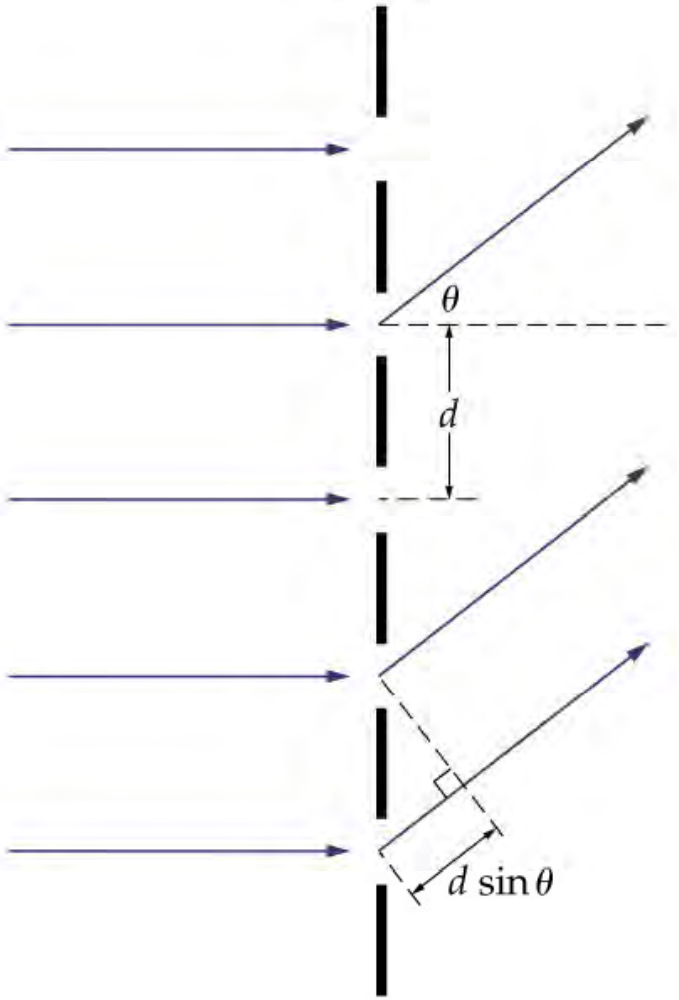
$d \sin\theta = m\lambda \qquad m = 0, \pm 1, \pm 2..$

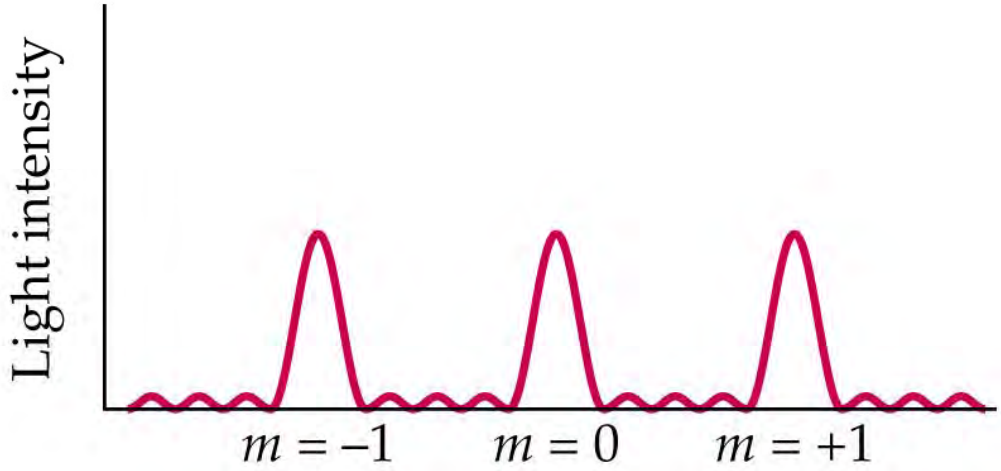
Case (c): destructive interference

$d \sin\theta = (m + 1/2)\lambda \quad m = 0, \pm 1, \pm 2, ..$



Diffraction gratings





Diffraction maxima

$d\sin\theta = m\lambda$ $(m=0,\pm1,\pm2..)$

m=order of diffraction

First minimum

$\sin\theta = \frac{\lambda}{Nd}$ (N:total number of slits covered by wave)

There are N-2 secondary maxima between two primary maxima

Von Laue formulation of x-ray diffraction

If one regards the crystal as composed of idential atoms at sites $\vec{R}$ of a Bravais lattice, each of which can reradiate incident beam in all directions. Sharp peaks will be observed only in directions and at wavelengths for which the rays scattered from all lattice points interfere constructively.

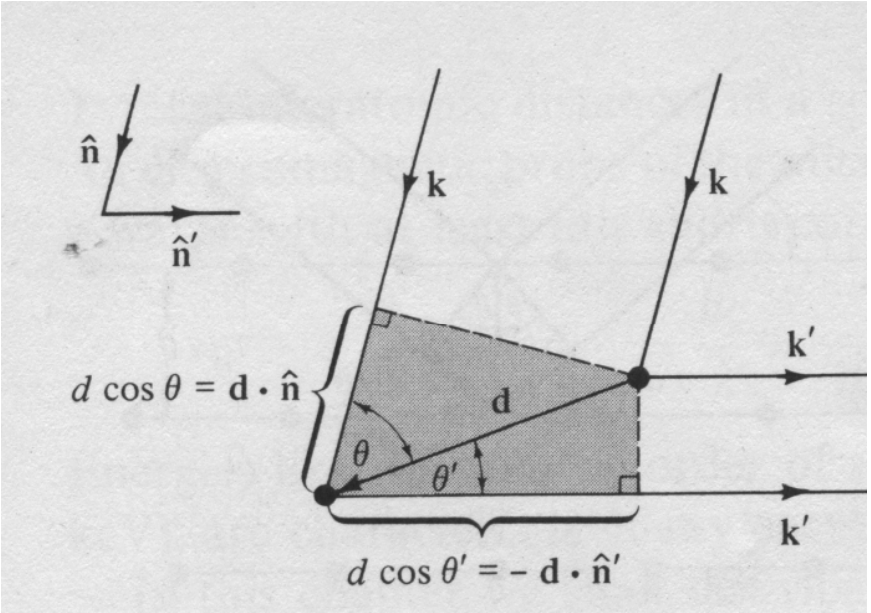
Incident beam wavevector $\vec{k} = 2\pi\hat{n} / \lambda$

Scattered beam wavevector $\vec{k}' = 2\pi\hat{n}' / \lambda$

Constructive interference:

$d\cos\theta + d\cos\theta' = \vec{d}\cdot(\hat{n} - \hat{n}') = \mathrm{m}\lambda \quad (\mathrm{m}=0, \pm 1, \pm 2..)$

This can also be written as $\vec{d}\cdot(\vec{k} - \vec{k}') = 2\pi\mathrm{m}$



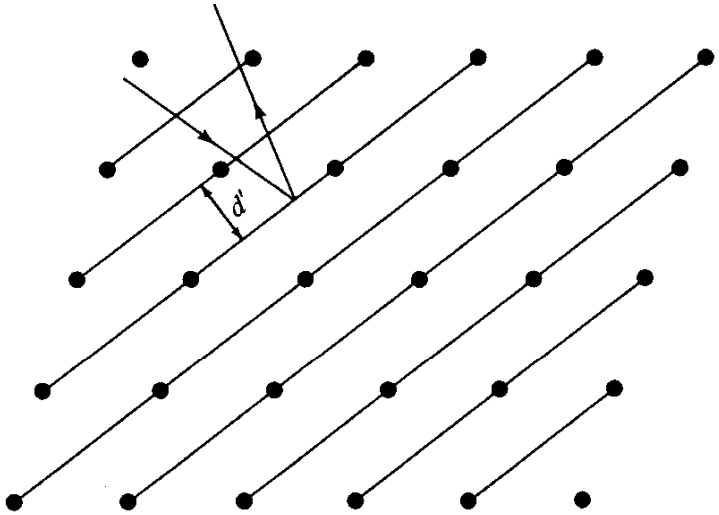
Since the lattice sites are displaced from one another by the Bravais lattice vector $\vec{R}$, the condition that all scattered rays interfere constructively means that $\vec{d} = \vec{R}$

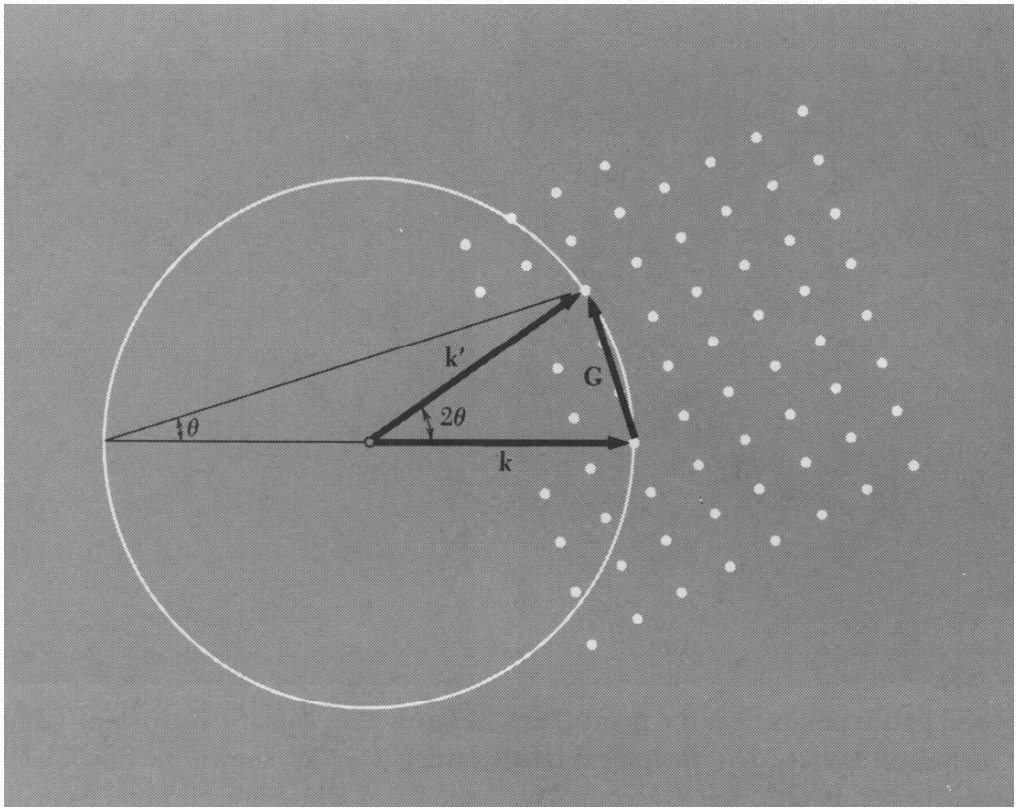
or $$\vec{R} \cdot (\vec{k} - \vec{k}') = 2\pi \mathrm{m}$$

or $e^{i\vec{R}\cdot(\vec{k}-\vec{k}')} = 1,$ for all Bravais lattice vector $\vec{R}$.

Constructive interference will occur if the change in wavevector, $\vec{K} = \vec{k} - \vec{k}',$ is a vector of the reciprocal lattice.

Constructive and destructive interference





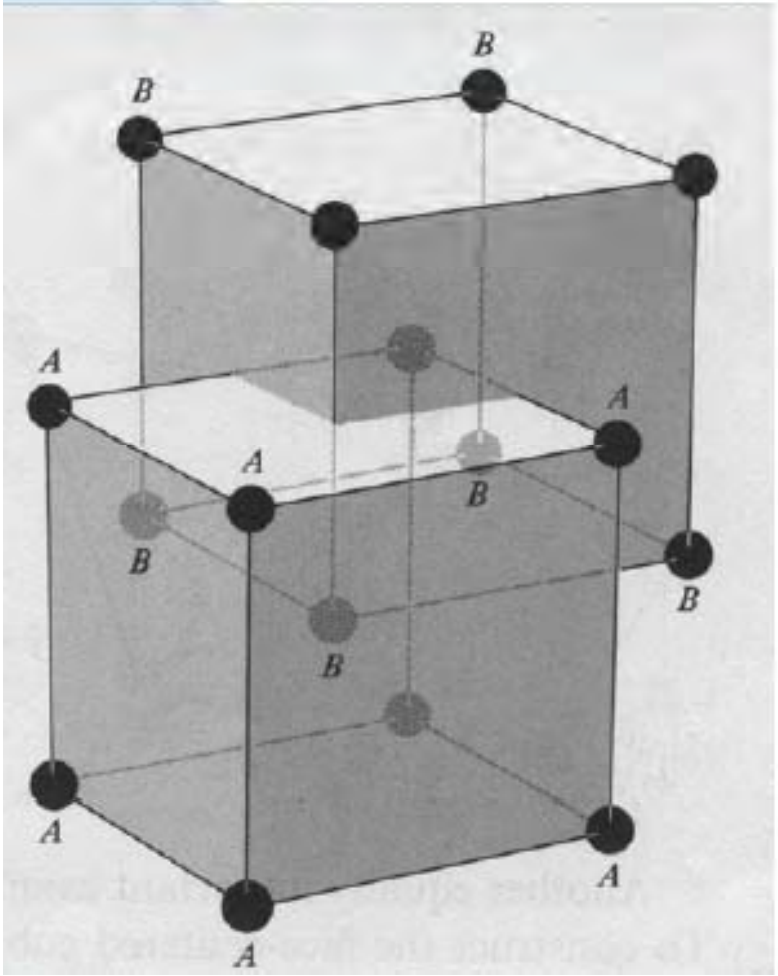
The geometrical structure factor

If the crystal structure has n-atoms per unit cell, monatomic, then the contents of each primitive cell can be further analyzed into a set of identical scatters at $d_1, \ldots, d_n$. The phase differences between the rays scattered at $\vec{d}_i$ and $\vec{d}_j$ will be $\vec{K} \cdot (\vec{d}_i - \vec{d}_j)$. The phases of the rays at $\vec{d}_i$ are in ratio $e^{i\vec{K}\cdot\vec{d}_i}$. The net ray scattered by the entire primitive cell is the sum of the individual rays, and will therefore have an amplitude containing the factor, called the geometrical structure factor

$$S_K = \sum_{i=1}^{n} e^{i\vec{K}\cdot\vec{d}_i}$$

Bragg peak intensity is proportional to $|S_K|^2$

BCC considered as simple cubic with a basis



Primitive vectors $a\hat{x}$, $a\hat{y}$, and $a\hat{z}$,

with a two-point basis of $d = 0$

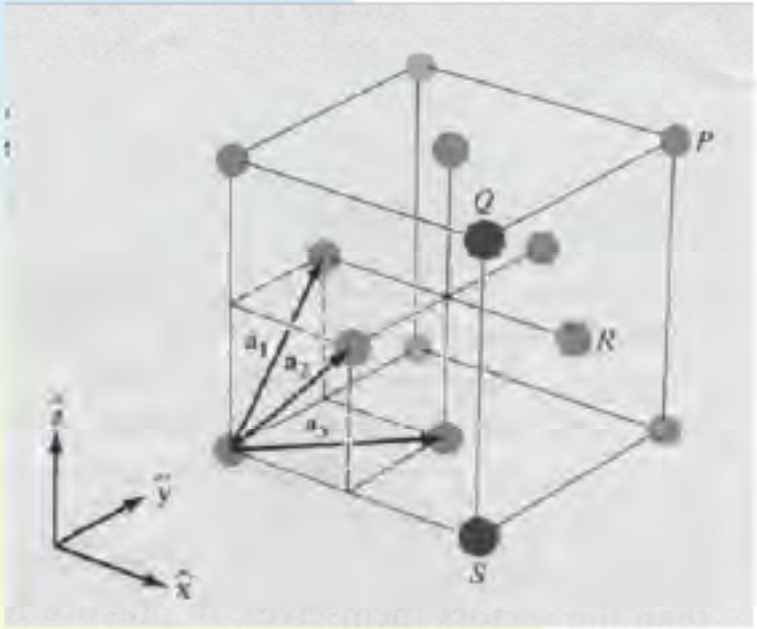
and $d_2 = \frac{a}{2}(\hat{x} + \hat{y} + \hat{z})$

$$S_K = 1 + \exp[i\vec{K} \bullet \frac{a}{2}(\hat{x} + \hat{y} + \hat{z})]$$

$$\vec{K} = \frac{2\pi}{2}(n_1\hat{x} + n_2\hat{y} + n_3\hat{z})$$

$$S_K = 1 + (-1)^{(n1+n2+n3)} = \begin{cases} 2, n_1 + n_2 + n_3 \text{ even} \\ 0, n_1 + n_2 + n_3 \text{ odd} \end{cases}$$

FCC considered as simple cubic with a basis



Primitive vectors $a\hat{x}$, $a\hat{y}$, and $a\hat{z}$, with four atoms per unit cell at

$$(000),(0\frac{1}{2}\frac{1}{2}),(\frac{1}{2}0\frac{1}{2}),(\frac{1}{2}\frac{1}{2}0)$$

$$S_K = 1 + \sum_{i=1}^{4} \exp[i\vec{K}\bullet\vec{d}_i]$$

$$\vec{K} = \frac{2\pi}{a}(n_1\hat{x} + n_2\hat{y} + n_3\hat{z})$$

$$S_K = 1 + (-1)^{(n1+n2)} + (-1)^{(n2+n3)} + (-1)^{(n3+n1)}$$

$$= \begin{Bmatrix} 4, n_1, n_2, n_3 \text{ are even or odd} \\ 0, n_1, n_2, n_3 \text{ mixed even/odd} \end{Bmatrix}$$

Atomic form factor for x-rays

$$S_K = \sum_{j=1}^{n} f_j(\vec{K}) e^{i\vec{K}\cdot\vec{d}_j}$$

where $f_j(\vec{K})$ is the atomic form factor, and is determined by the internal structure of the ion that occupies position $\vec{d}_j$ in the basis. The atomic form factor at $\vec{K}$ is taken to be proportional to the Fourier transform of the electron charge distribution of the corresponding ion:

$$f_j(\vec{K}) = \int dV n_j(\vec{r}) \exp(-i\vec{K}\bullet\vec{r})$$

Here $n_j(\vec{r})$ is electron density concentration.

X-ray diffraction by a small crystal

Structure factor F of the system is then

$$F = \sum_{j=1}^{n} f e^{i\bar{K}\cdot\bar{R}_j} = f \sum_{j=0}^{N_{1,2,3}-1} e^{i\bar{K}\cdot(n_1\bar{a}_1+n_2\bar{a}_2+n_3\bar{a}_3)}$$

$$= f \frac{e^{i\bar{K}\cdot N_1\bar{a}_1}-1}{e^{i\bar{K}\cdot\bar{a}_1}-1} \frac{e^{i\bar{K}\cdot N_2\bar{a}_2}-1}{e^{i\bar{K}\cdot\bar{a}_2}-1} \frac{e^{i\bar{K}\cdot N_3\bar{a}_3}-1}{e^{i\bar{K}\cdot\bar{a}_3}-1}$$

where f_n is the structural factor of the unit cell.

The total scattered intensity then

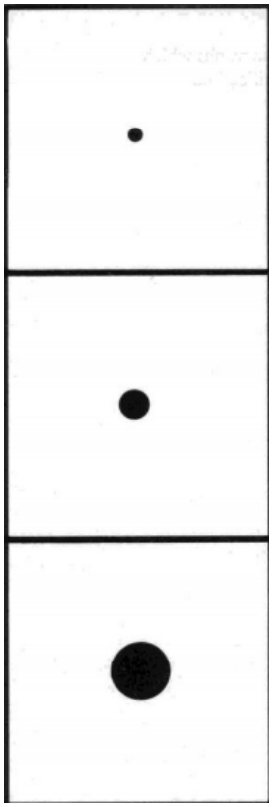
$$I = F \bullet F^*$$

We suppose that in a linear crystal there are identical point scattering centers at every lattice point $\bar{\rho}_m = m\bar{a}$, where m is an integer. Show that the scattering intensity is proportional to $|F|^2$

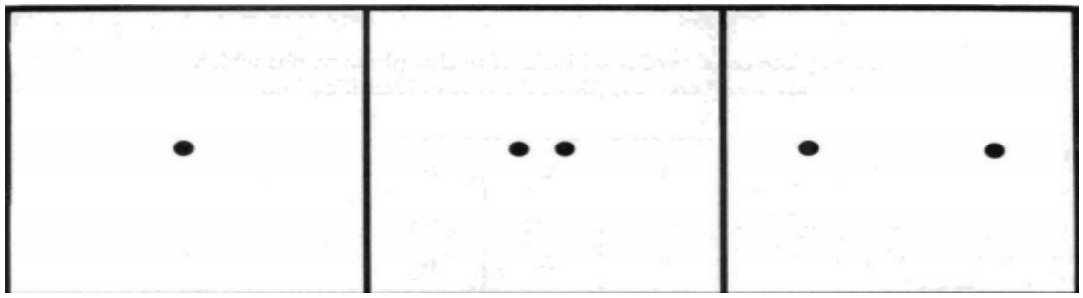
a) $I = F \cdot F^* = \dfrac{\sin^2 M(a \cdot \Delta k)/2}{\sin^2 (a \cdot \Delta k)/2}$

b) We know that a diffraction maximum appears when $a \cdot \Delta k = 2\pi h$, where h is an integer. We change Δk slightly and define ε in $a \cdot \Delta k = 2\pi h + \varepsilon$ such that ε gives the position of the first zero in $\sin^2 M(a \cdot \Delta k)/2$. Show that $\varepsilon = 2\pi / M$, so that the width of the diffraction maximum is proportional to $1/M$ and can be extremely narrow for macroscopic values of M.

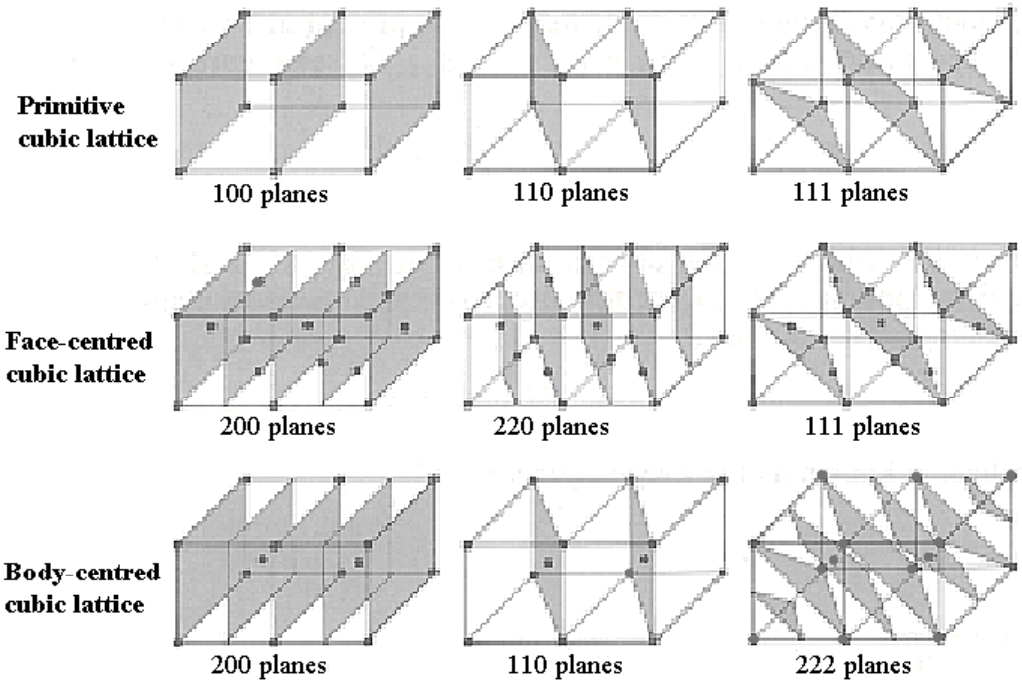
Real space (1)



Real space (2)



Lattice planes in crystals: Miller indexes

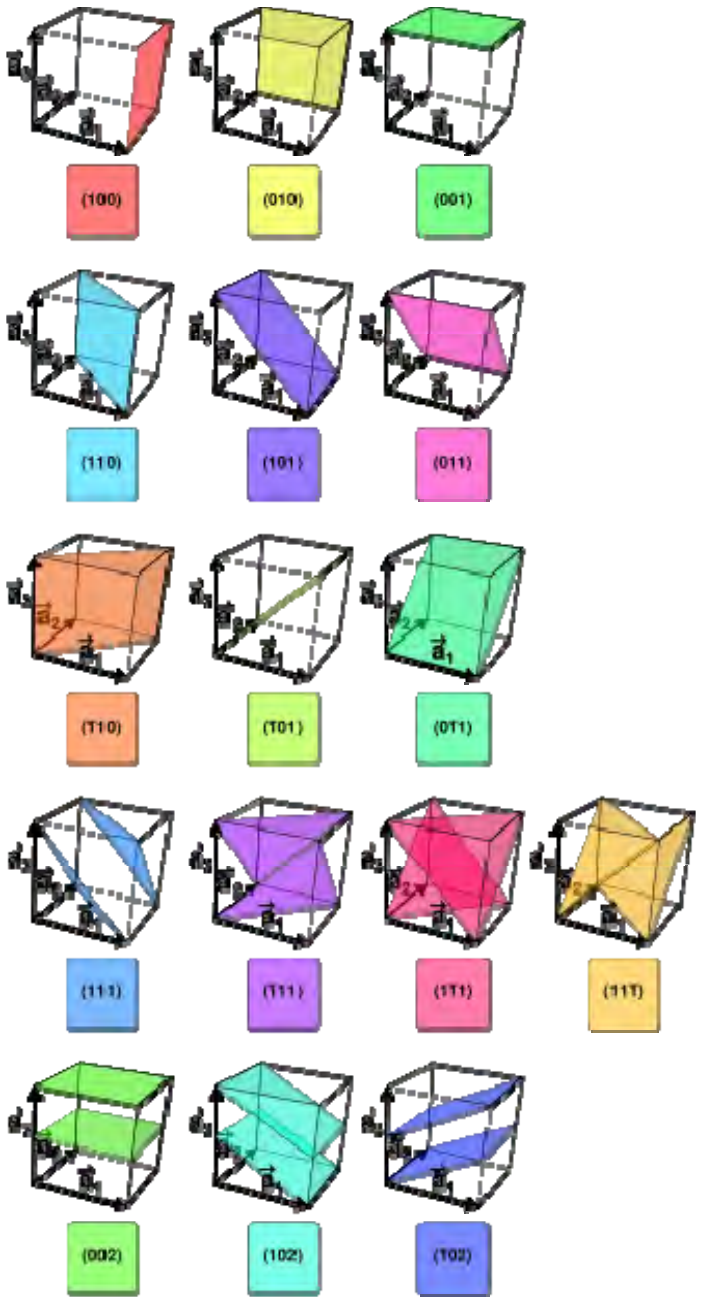


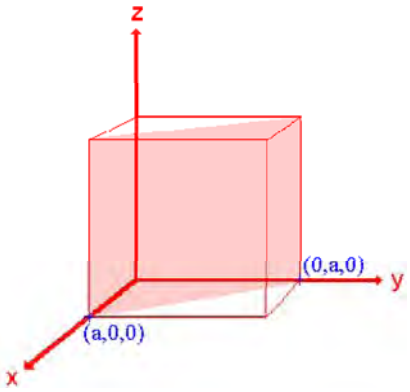
Miller indices for three types of cubic lattices.

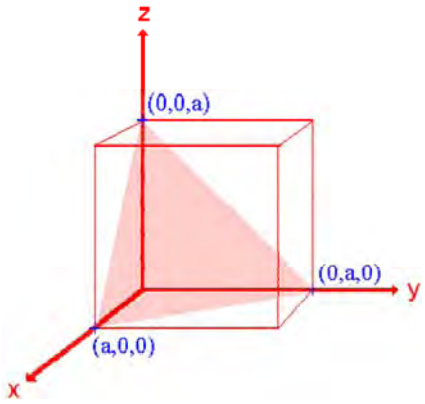
Σιλιχον ανδ Γερμανιυμ βρεακ ον {1,1,1} πλανεσ

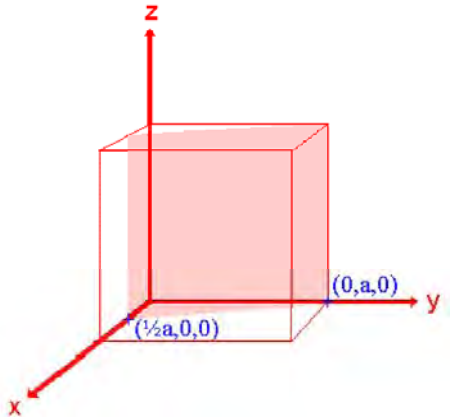
νεωερ χονφυσε τηε σπαχινγ βετωεεν λαττιχε πλανεσ

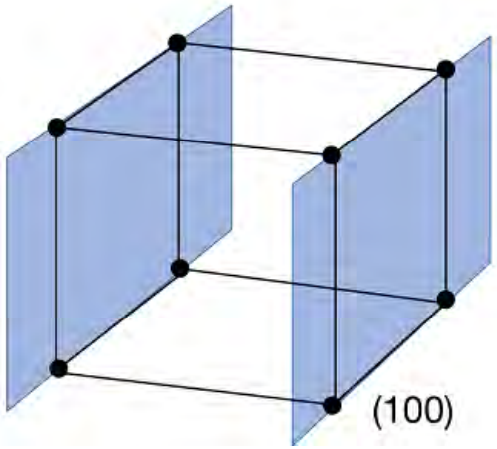
ωιτη τηε σπαχινγ βετωεεν χρωσταλ πλανεσ

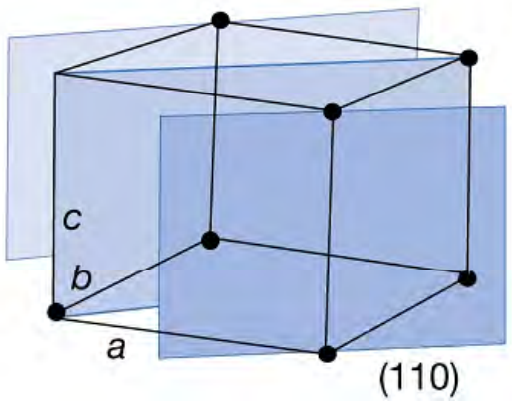

(100)
(010)
(001)
(110)
(101)
(011)
(T10)
(T01)
(0T1)
(111)
(T11)
(1T1)
(11T)
(002)
(102)
(T02)

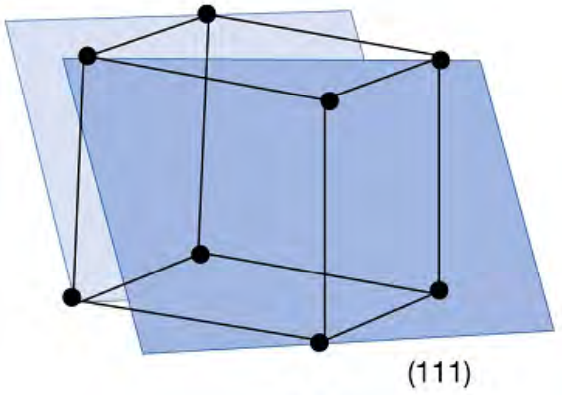








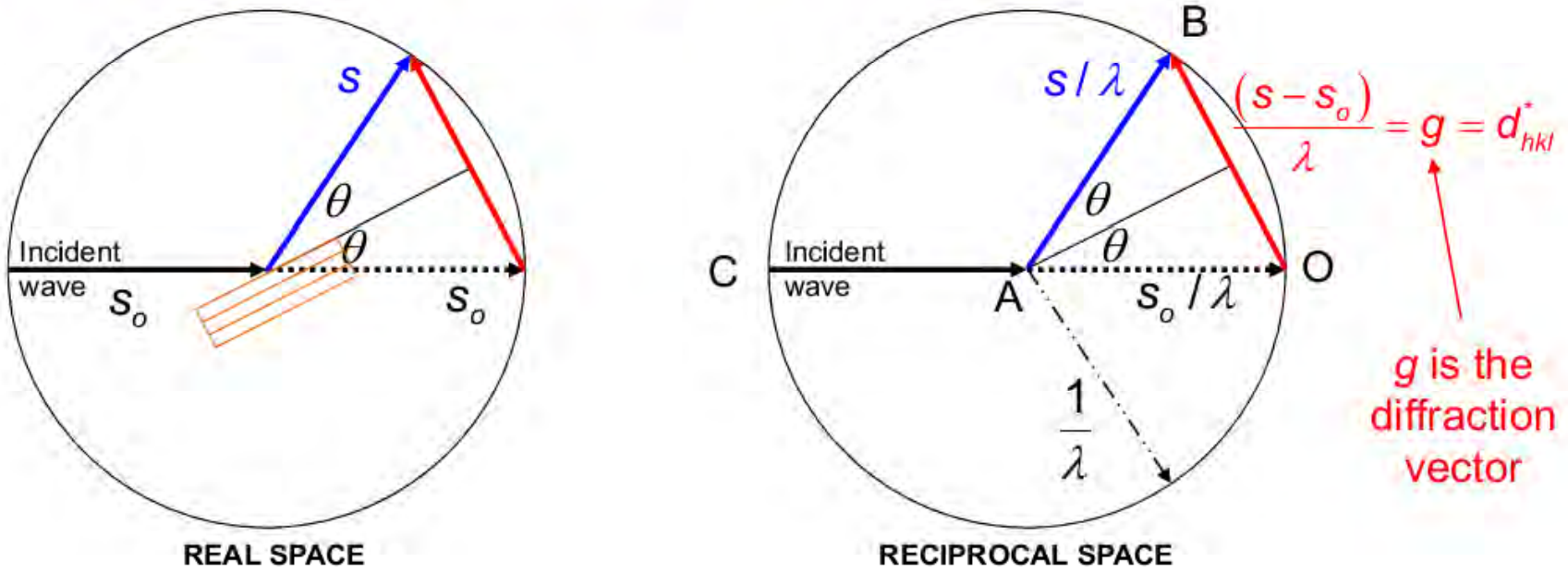




$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

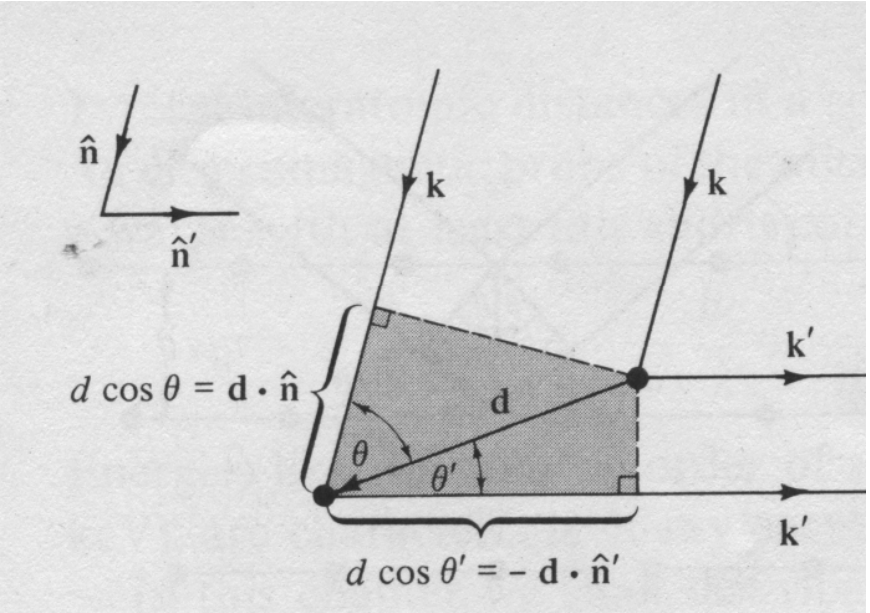
Ewald's Sphere Construction

- Graphical representation of Bragg's Law in reciprocal space.



$$r_{uvw} = ua + vb + wc$$

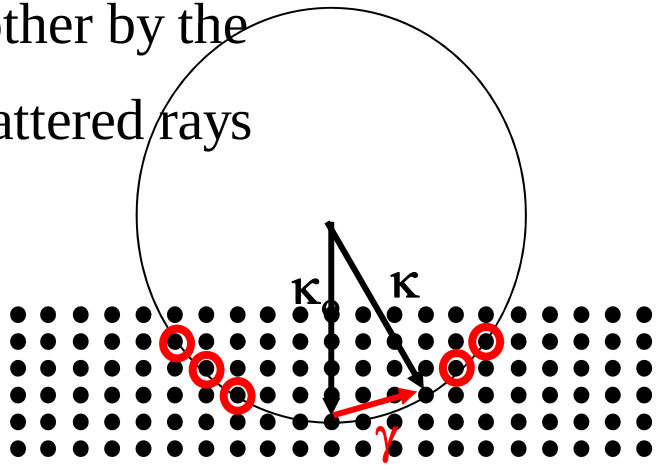
$$r^*_{hkl} = ha^* + kb^* + lc^*$$



Since the lattice sites are displaced from one another by the Bravais lattice vector $\vec{R}$, the condition that all scattered rays interfere constructively means that $\vec{d} = \vec{R}$

or $$\vec{R} \cdot (\vec{k} - \vec{k}') = 2\pi \boxed{\text{m}}$$

or $e^{i\vec{R}\cdot(\vec{k}-\vec{k}')} = 1,$ for all Bravais lattice vector $\vec{R}$.



Constructive interference will occur if the change in wavevector, $\vec{K} = \vec{k} - \vec{k}',$ is a vector of the reciprocal lattice.