The Reciprocal Lattice
-- continued

A set of wave vectors **K** that ensure

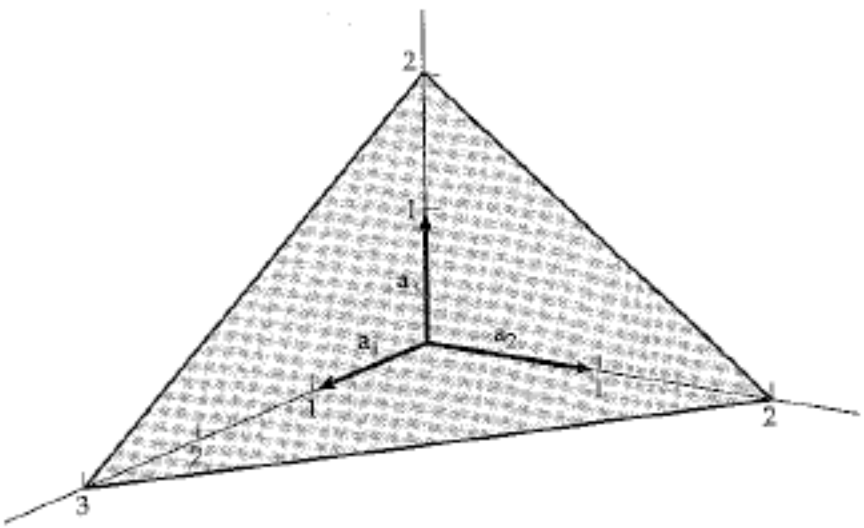
$$e^{i\boldsymbol{K}\bullet\boldsymbol{R}} = 1$$

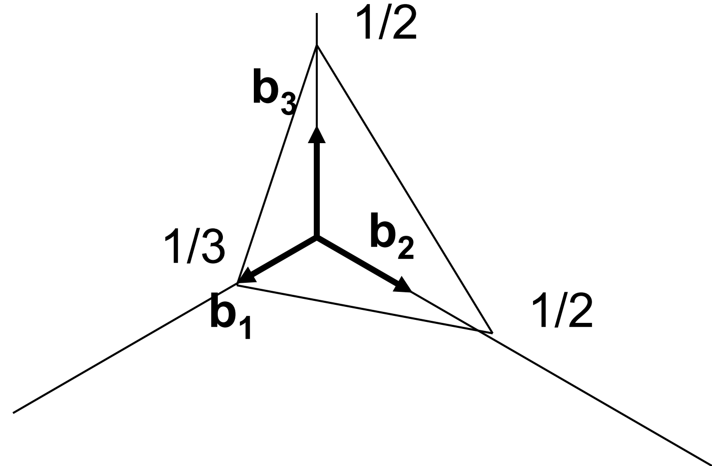
Direct lattice (Bravais lattice): $\mathbf{R} = n_1\mathbf{a_1}+n_2\mathbf{a_2}+n_3\mathbf{a_3}$

Reciprocal lattice: $\mathbf{K} = k_1\mathbf{b_1}+k_2\mathbf{b_2}+k_3\mathbf{b_3}$

Application:
Name Lattice Planes - Miller Indices

Direct lattice

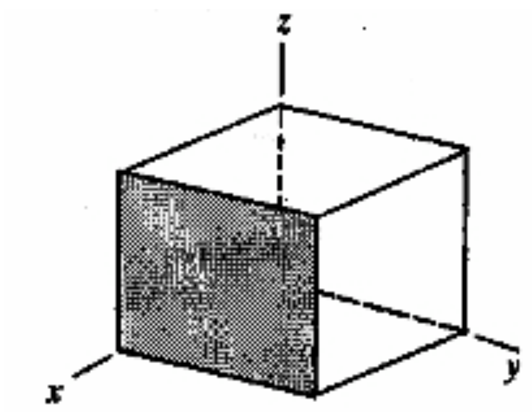


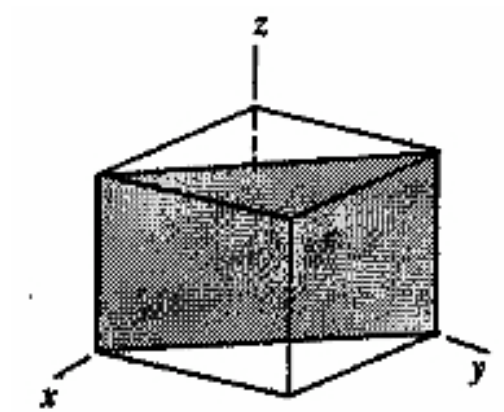


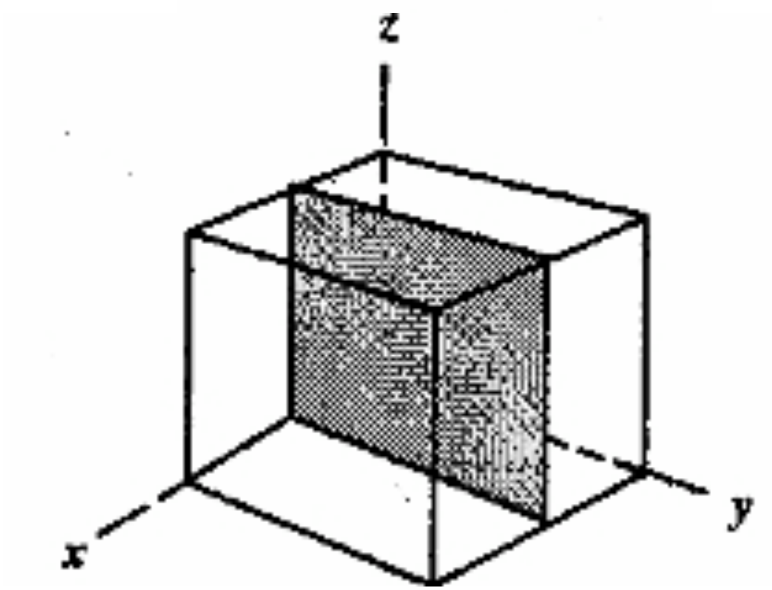
The smallest three integers having the same ratio as
1/3 : 1/2 : 1/2 = 2 : 3 : 3

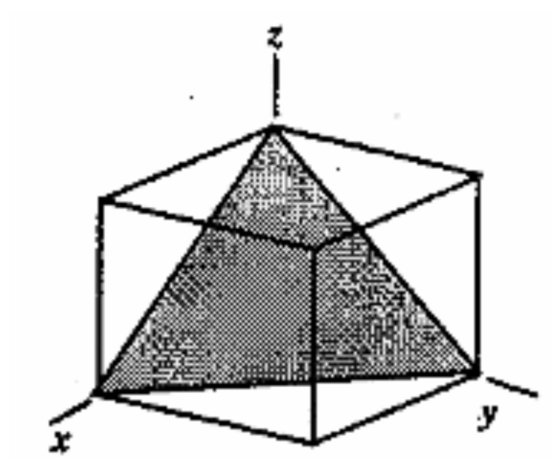
The plane is called (233) plane
- Miller Indices

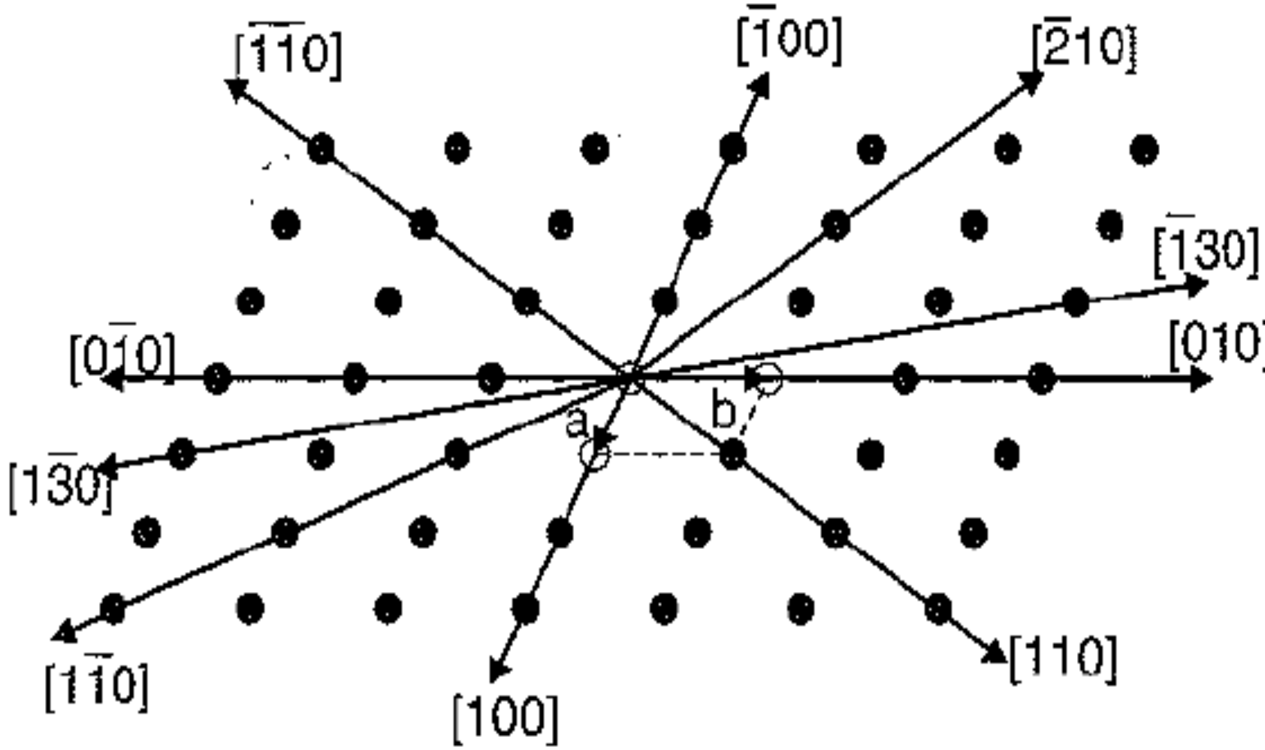
Three Miller Indices (hkl)





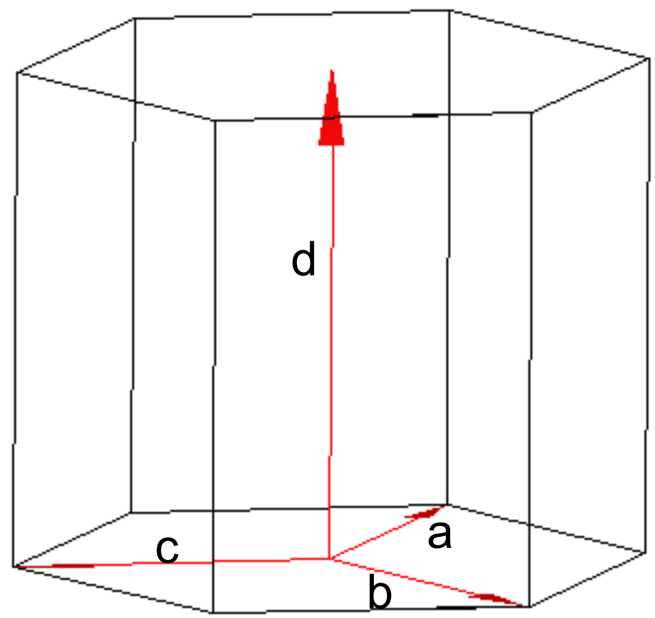






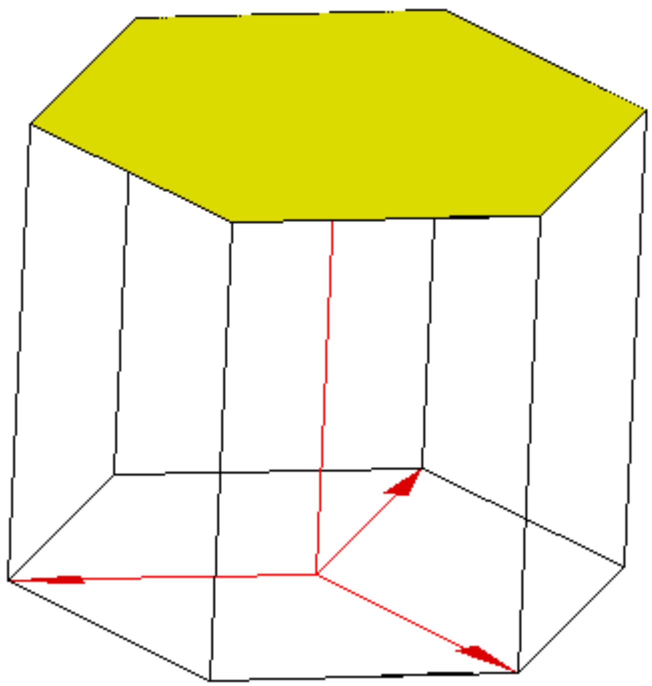
$[\bar{1}\bar{1}0]$
$[\bar{1}00]$
$[\bar{2}10]$
$[\bar{1}30]$
$[0\bar{1}0]$
$[010]$
a
b
$[1\bar{3}0]$
$[1\bar{1}0]$
$[100]$
$[110]$

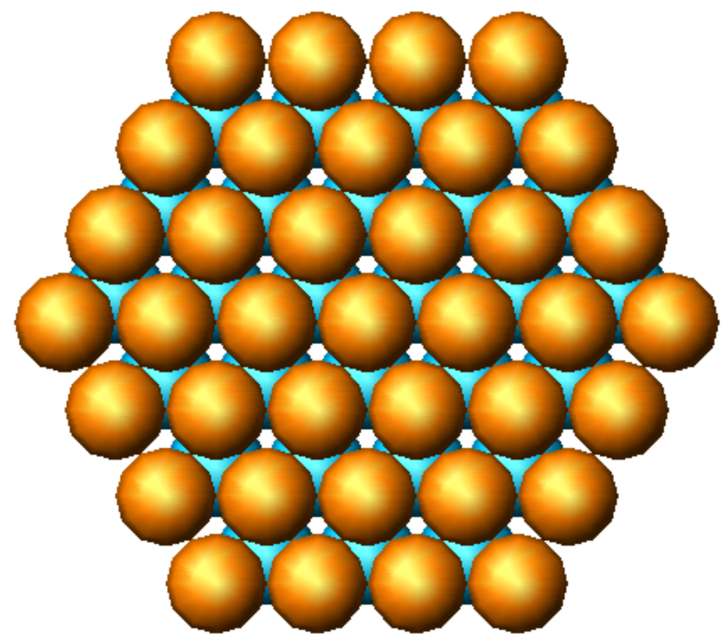
Four Miller-Bravais Indices (hkil)



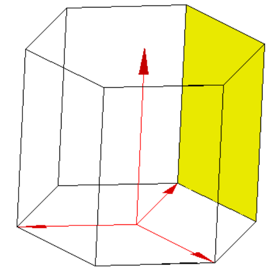
$$h + k + i = 0$$

(0001)

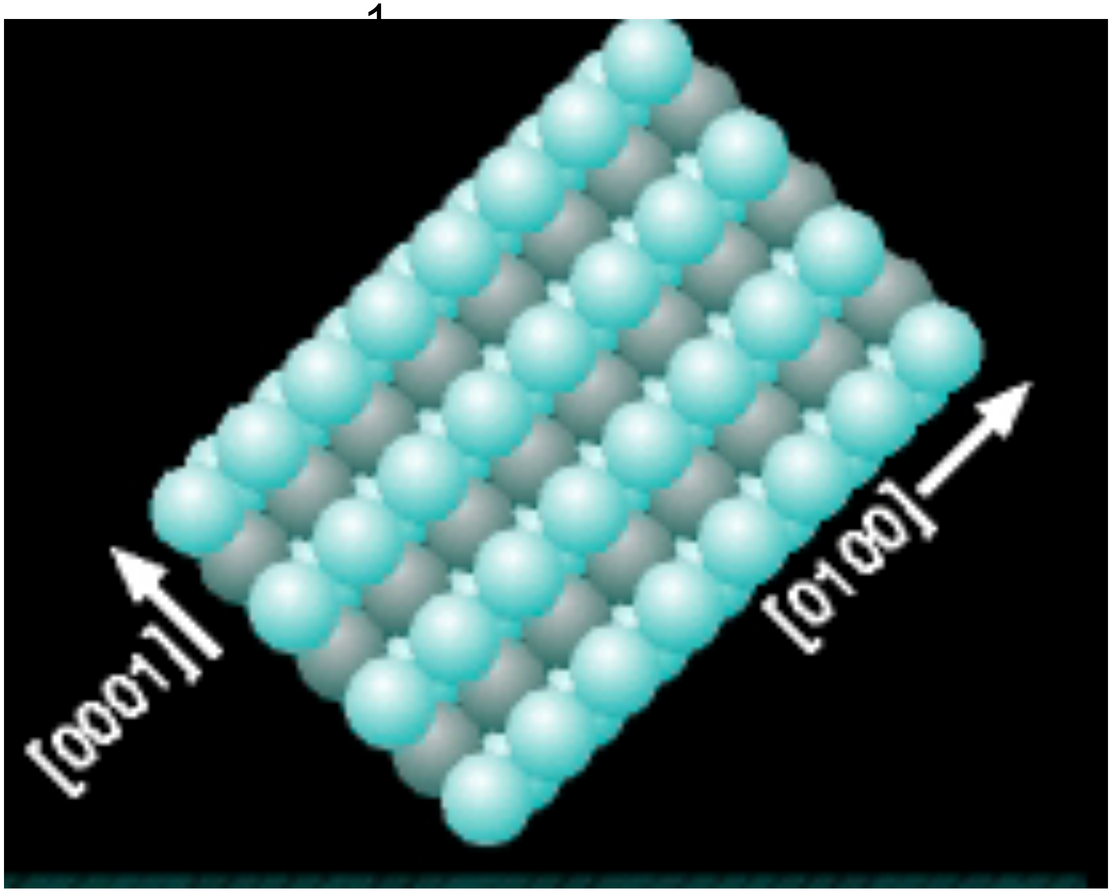




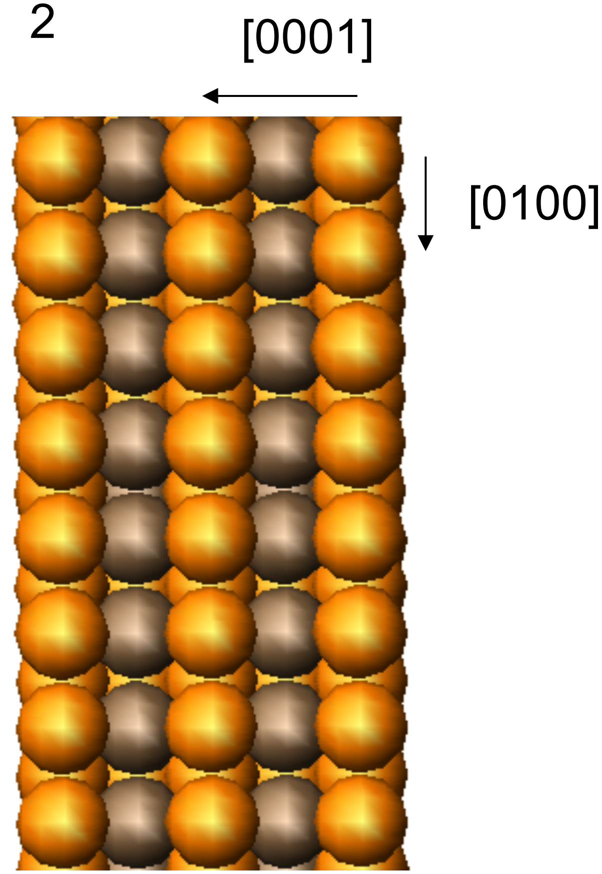
$(10\bar{1}0)$



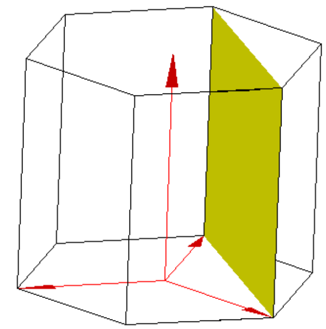
1



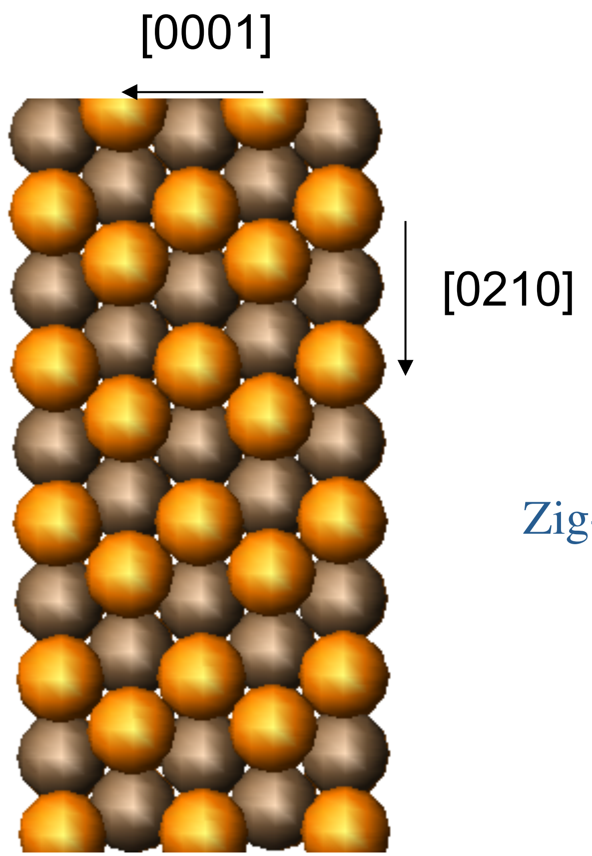
2



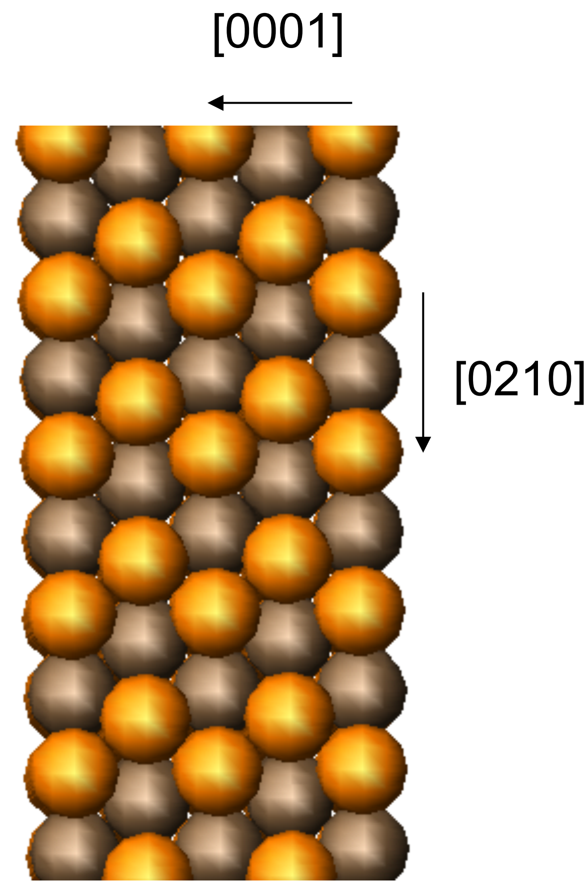
$(11\bar{2}0)$



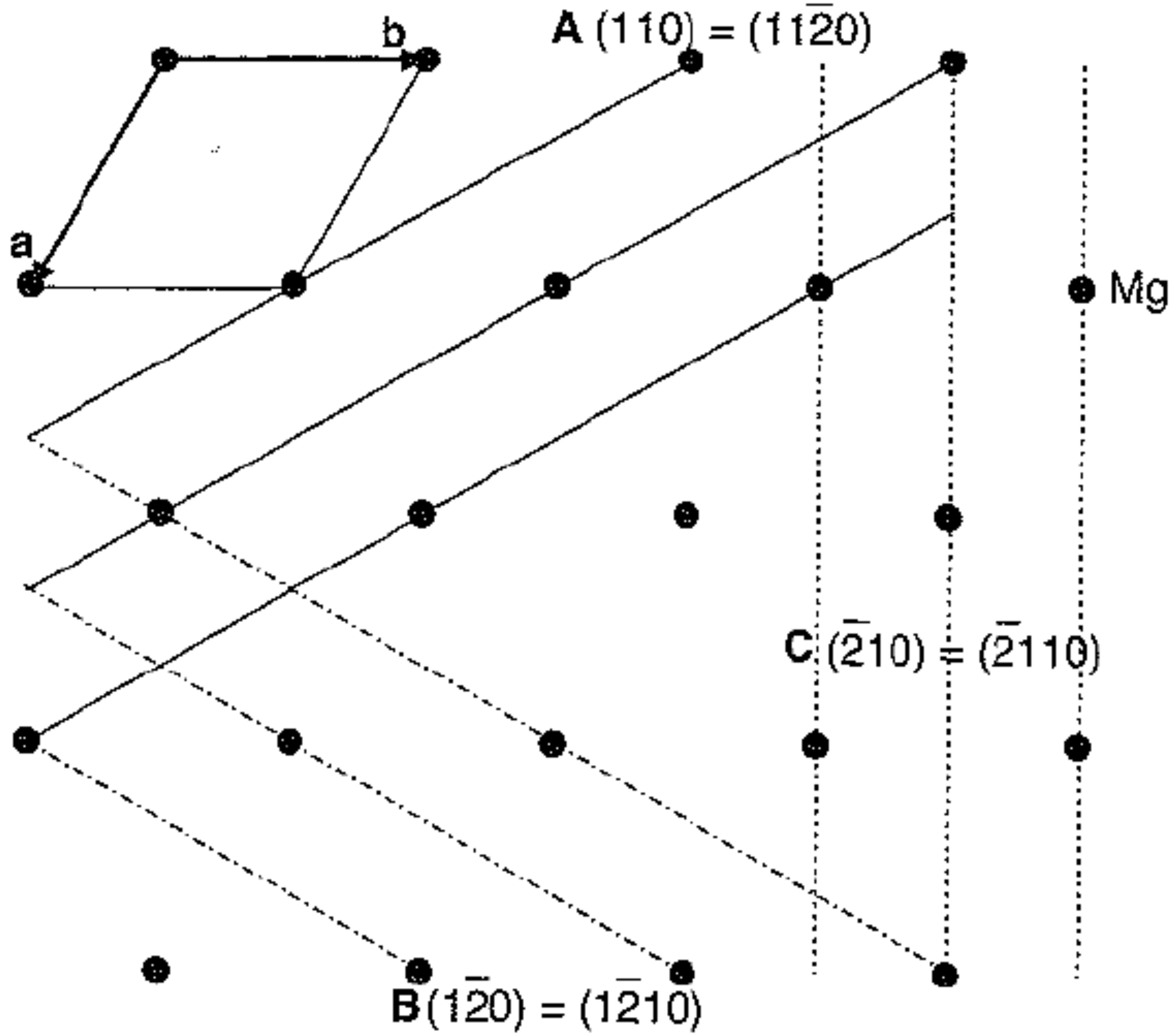
1



2



Zig-Zag Rows



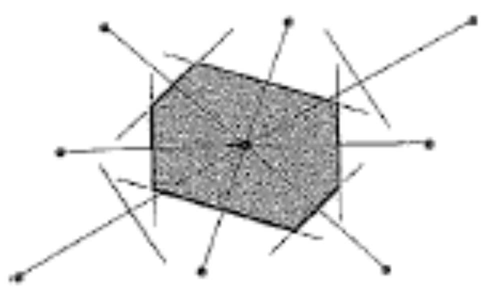
b
a
A (110) = (11$\bar{2}$0)
Mg
C ($\bar{2}$10) = ($\bar{2}$110)
B (1$\bar{2}$0) = (1$\bar{2}$10)

Application:
Construction of Brillouin Zones

In Bravais lattices

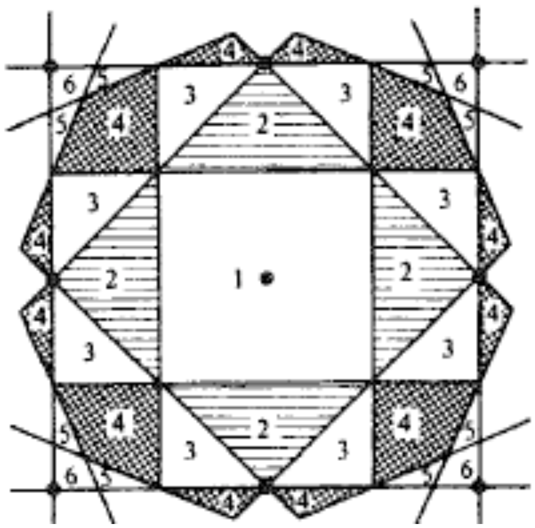
(direct lattices)

Winger-Seitz cell



In reciprocal lattices

Winger-Seitz cell
= first Brillouin Zone



Determination of Crystal Structures

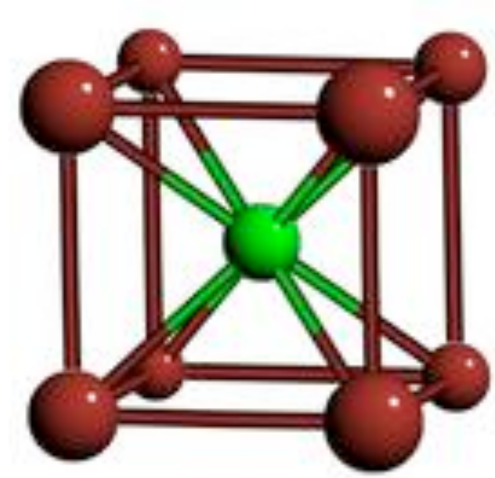
	2D	3D
Crystal structures	5	7

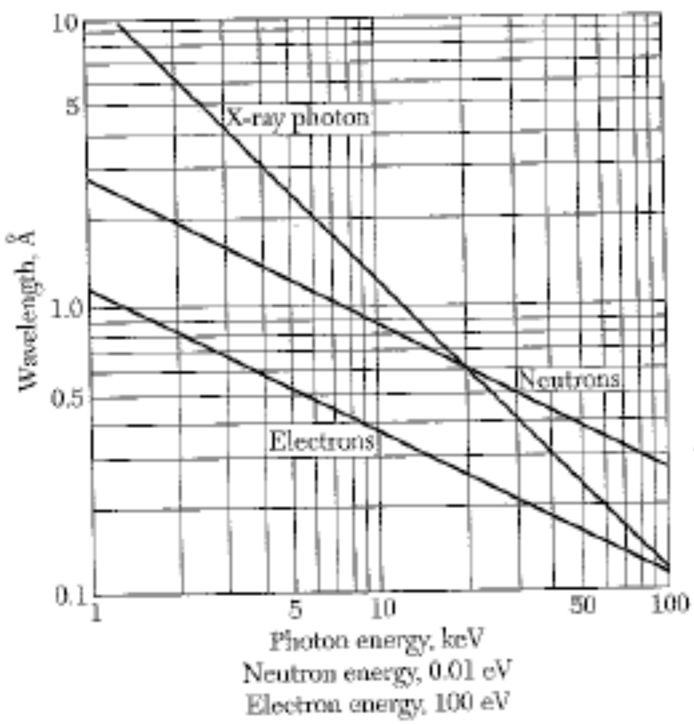
Distance between atoms
in the order of

Å ~ 10^{-8} cm ~ 10^{-10} m

requires

Wave length $\lambda \sim$ Å

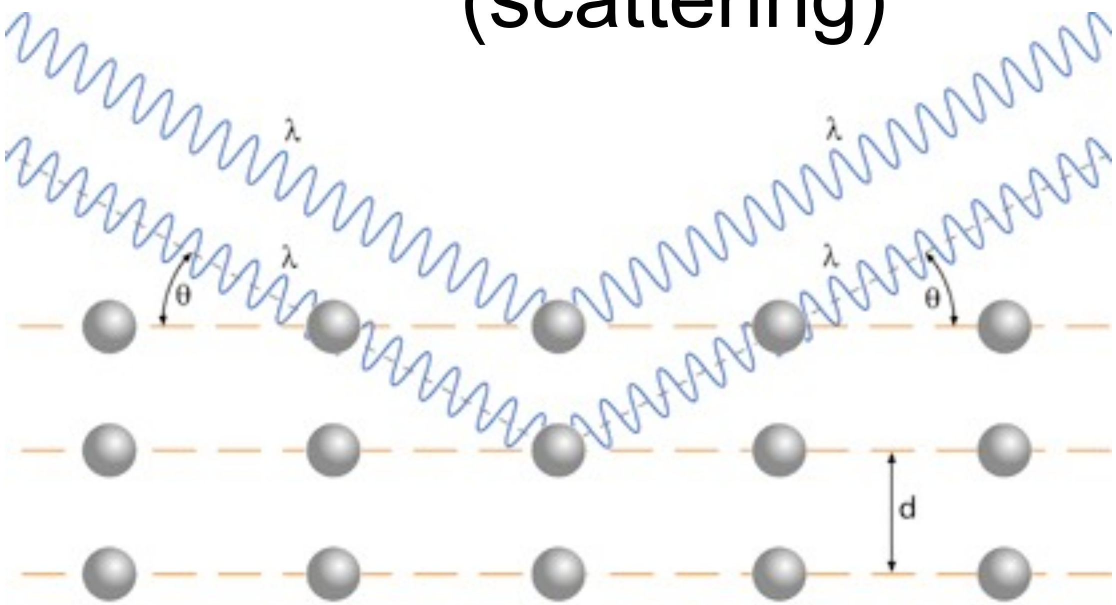




Determination of Crystal Structures:

X-ray diffraction

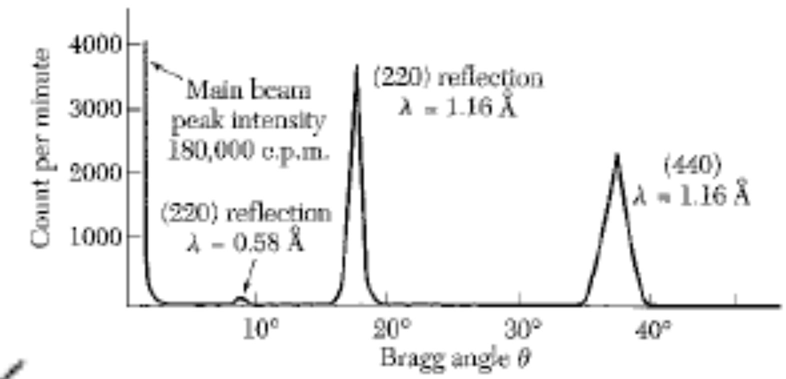
(scattering)



Bragg Law:

$$2d\sin\theta = n\lambda$$

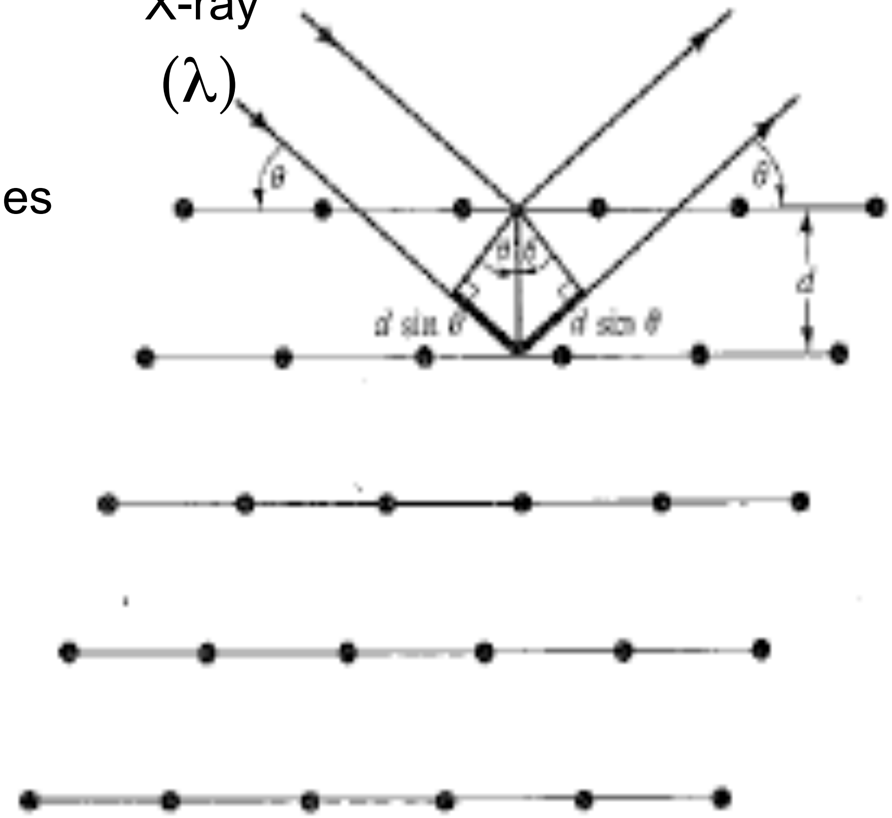
(n = integer)



X-ray

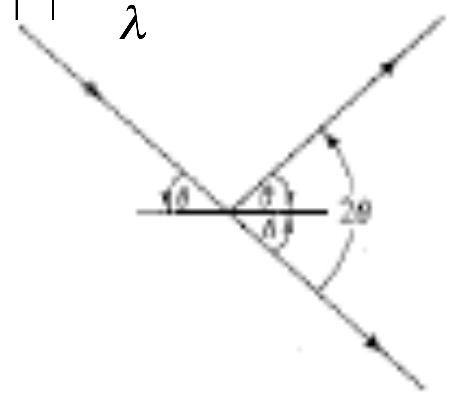
(λ)

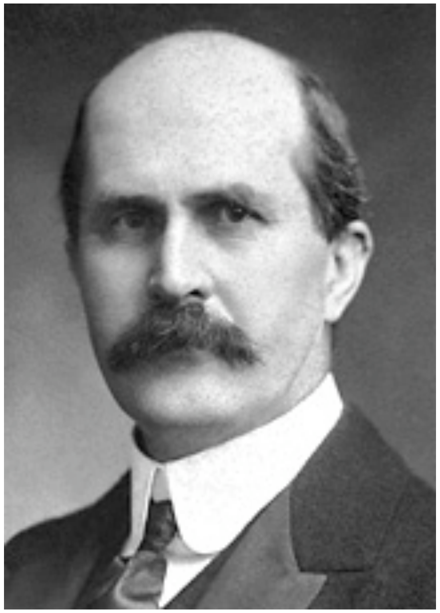
Lattice planes



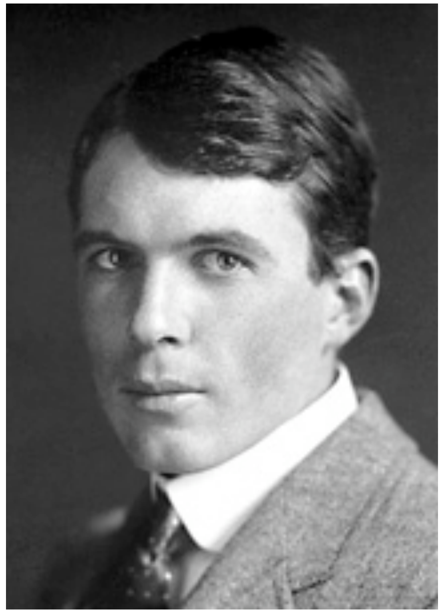
Wave vector

$$|\mathbf{k}| = \frac{2\pi}{\lambda}$$





Sir W. Henry Bragg



W. Lawrence Bragg

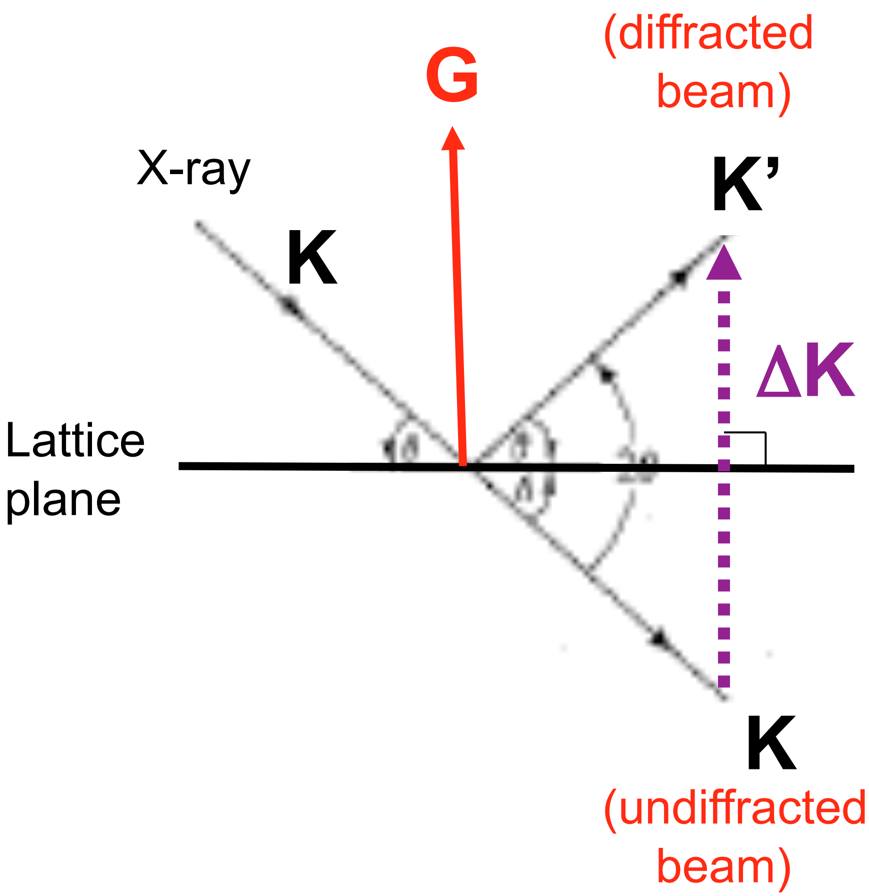
1915:
The Nobel Prize in Physics was awarded jointly to Sir William Henry Bragg and William Lawrence Bragg

"for their services in the analysis of crystal structure by means of X-rays"

Bragg Law:

$$2d \sin\theta = n\lambda$$

(n = integer)



Diffraction conditions:

The set of reciprocal lattice vectors **G** determines the possible x-ray reflection

$$\Delta \mathbf{K} = \mathbf{K}' - \mathbf{K} = \mathbf{G}$$

$$\mathbf{K} + \mathbf{G} = \mathbf{K}'$$

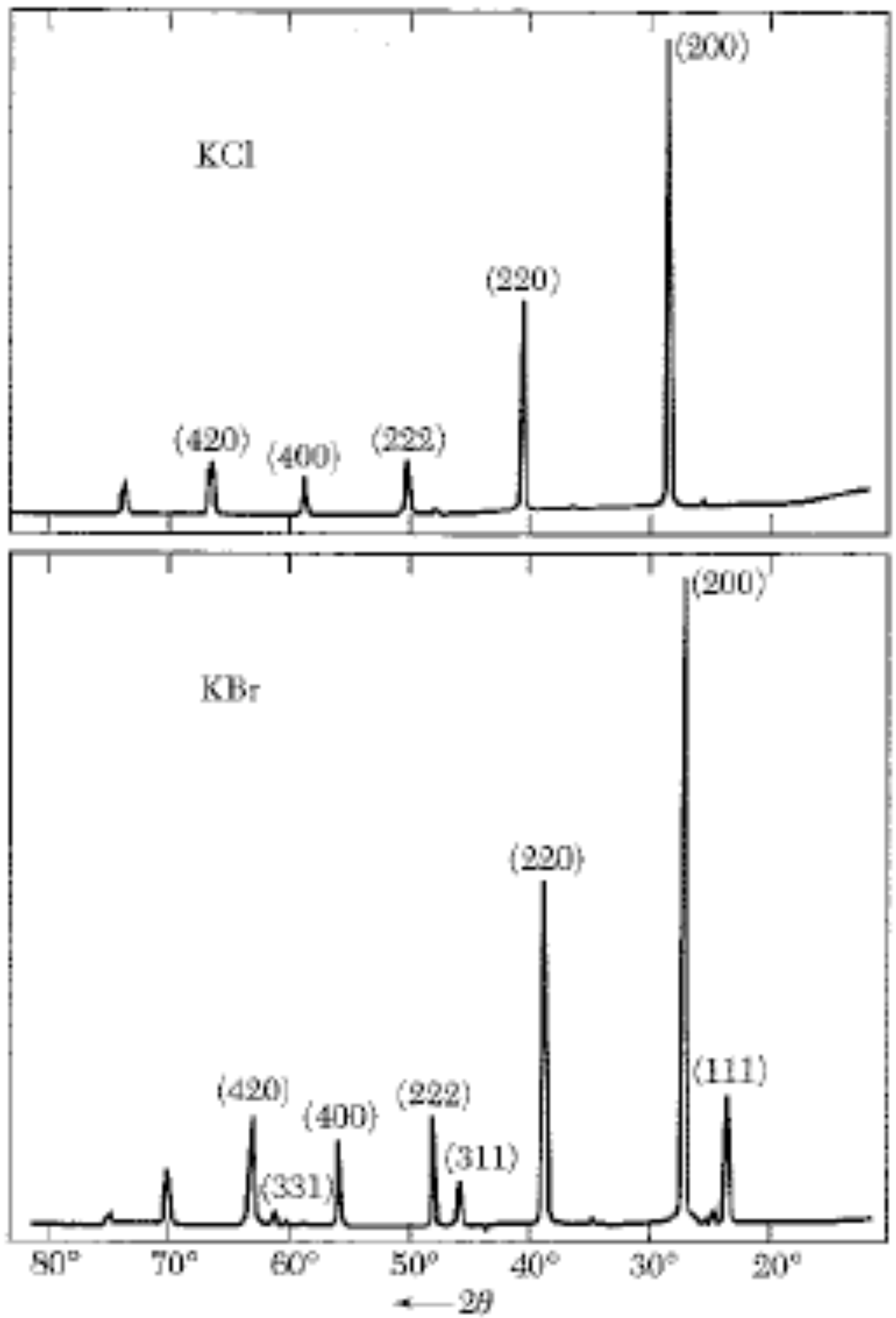
Elastic scattering: K = K'

$$(\mathbf{K}+\mathbf{G})^2 = K^2$$

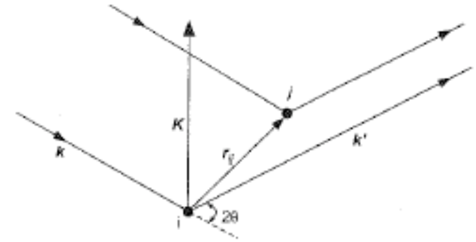
$$2\mathbf{K} \cdot \mathbf{G} = G^2$$

$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$$

If cubic $d^{-1} \propto \sqrt{h^2 + k^2 + l^2}$



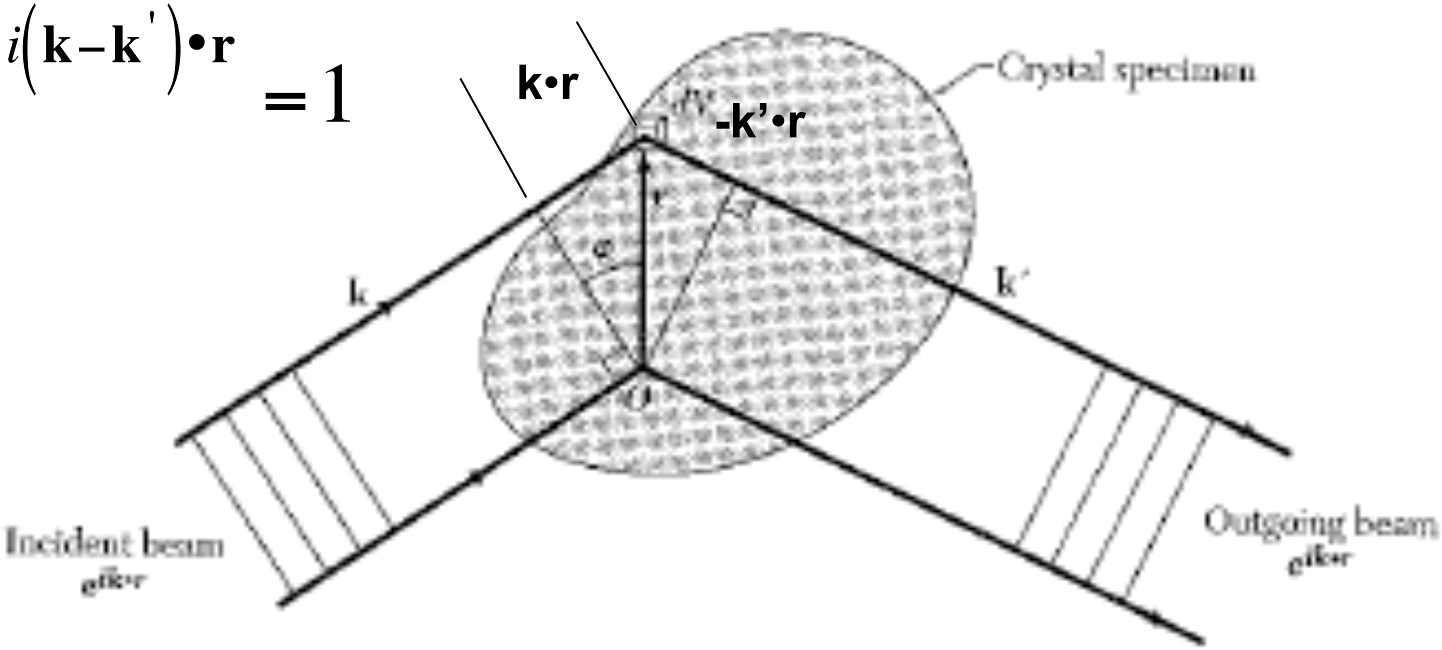
(200)
KCl
(220)
(420)
(400)
(222)
(200)
KBr
(220)
(111)
(420)
(400)
(222)
(311)
(331)
80°
70°
60°
50°
40°
30°
20°
← 2θ



Von Laue Approach

Condition: $(\mathbf{K}-\mathbf{K'})\bullet\mathbf{r} = 2\pi n$ (n = integer)

$$e^{i(\mathbf{k}-\mathbf{k}')\bullet\mathbf{r}} = 1$$

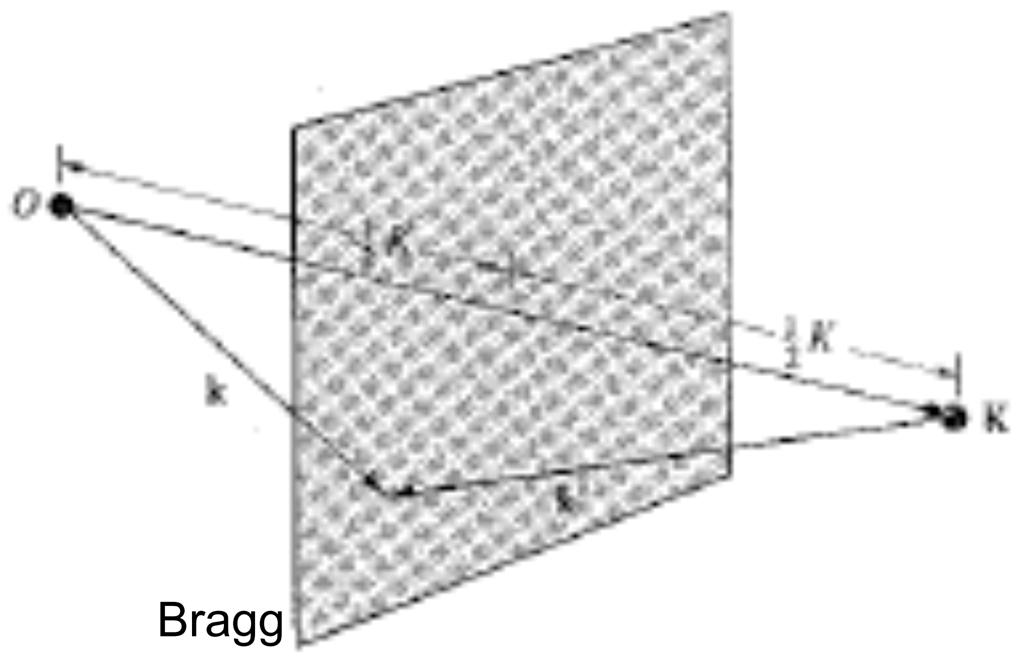


Constructive interference will occur if ΔK = K'-K is a vector of the reciprocal lattice.

In the case of elastic scattering: K = K'

$$k = |\mathbf{k} - \Delta\,\mathbf{K}|$$

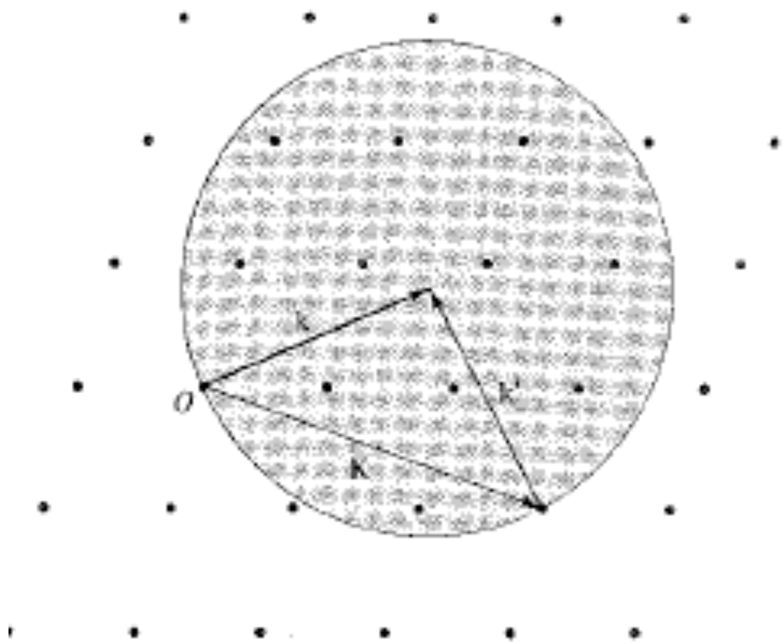
$$2\mathbf{k} \bullet \Delta\mathbf{K} = K$$

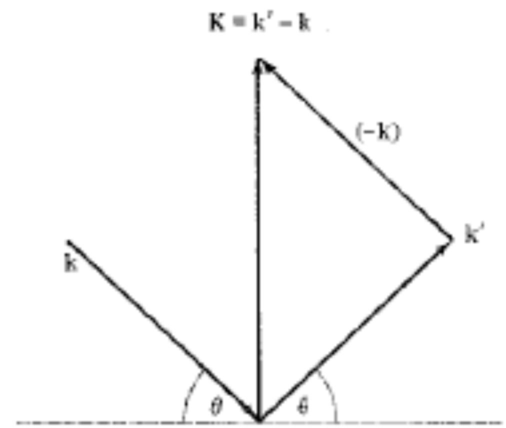


Bragg plane

ΔK is the reciprocal lattice vector: $K=n(2\pi/d)=2k\sin\Theta$

The Ewald Construction

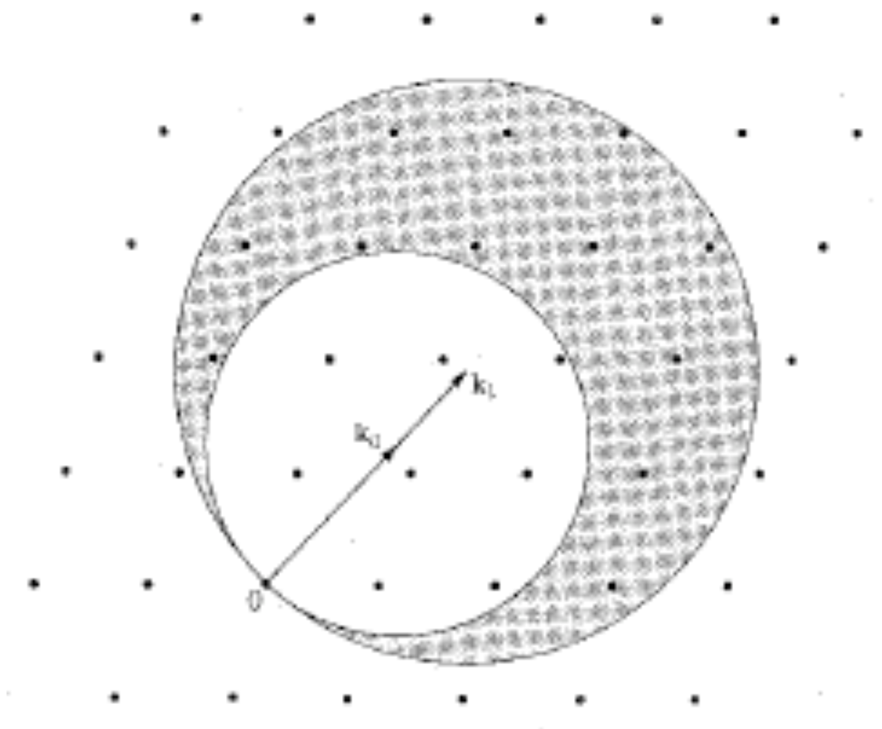




The Laue Method

sample position and incident beam (direction) - unchanged

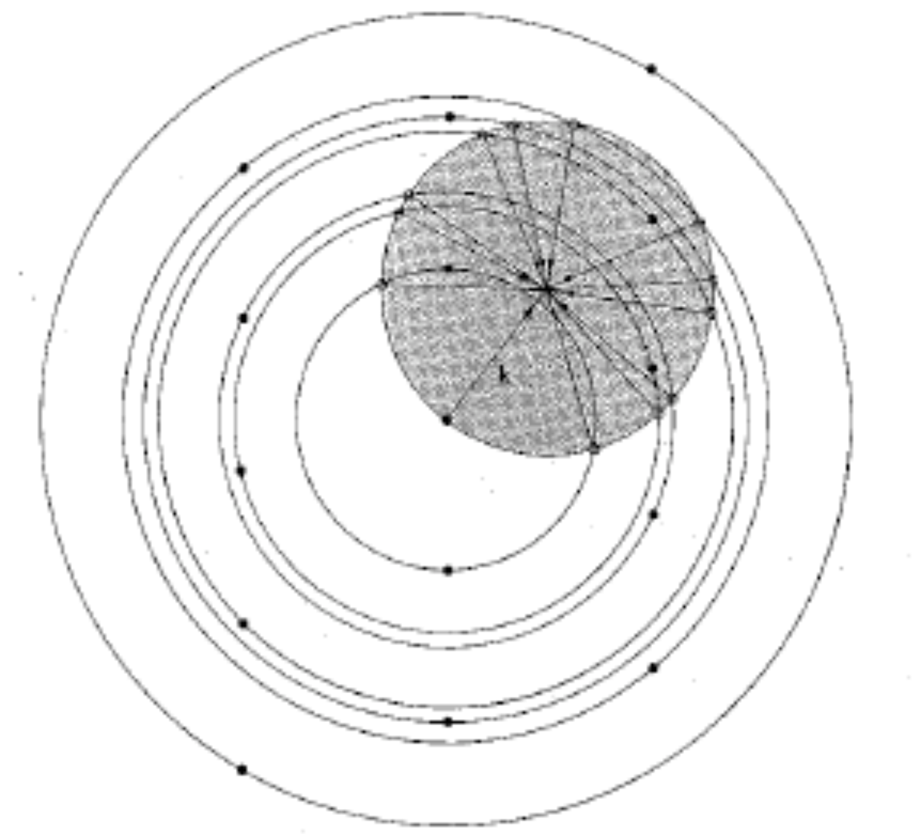
wave length - from λ_1 to λ_0



The Rotating - Crystal Method

Monochromic beam (same λ)

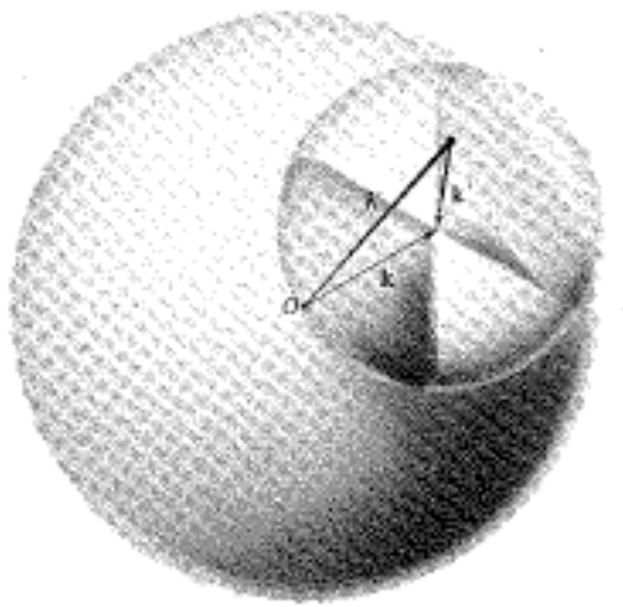
Rotate sample: change angle Θ



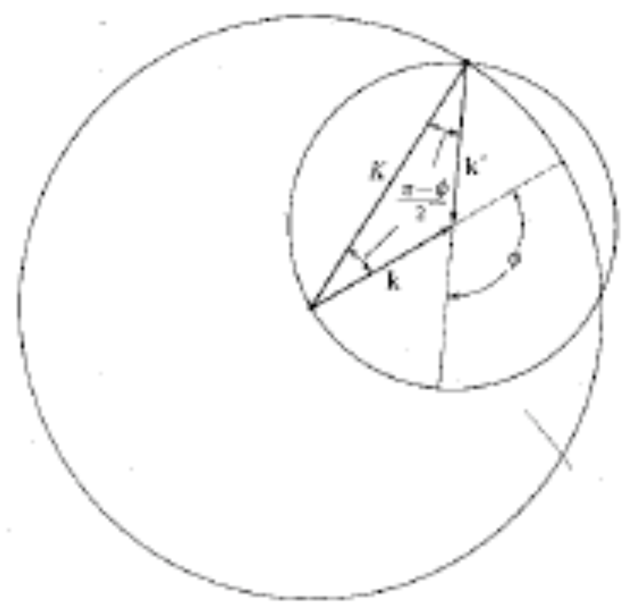
The Debye -Scherrer Method
-- for Powder X-ray Diffraction

Monochromic beam (same λ)

change angle Θ



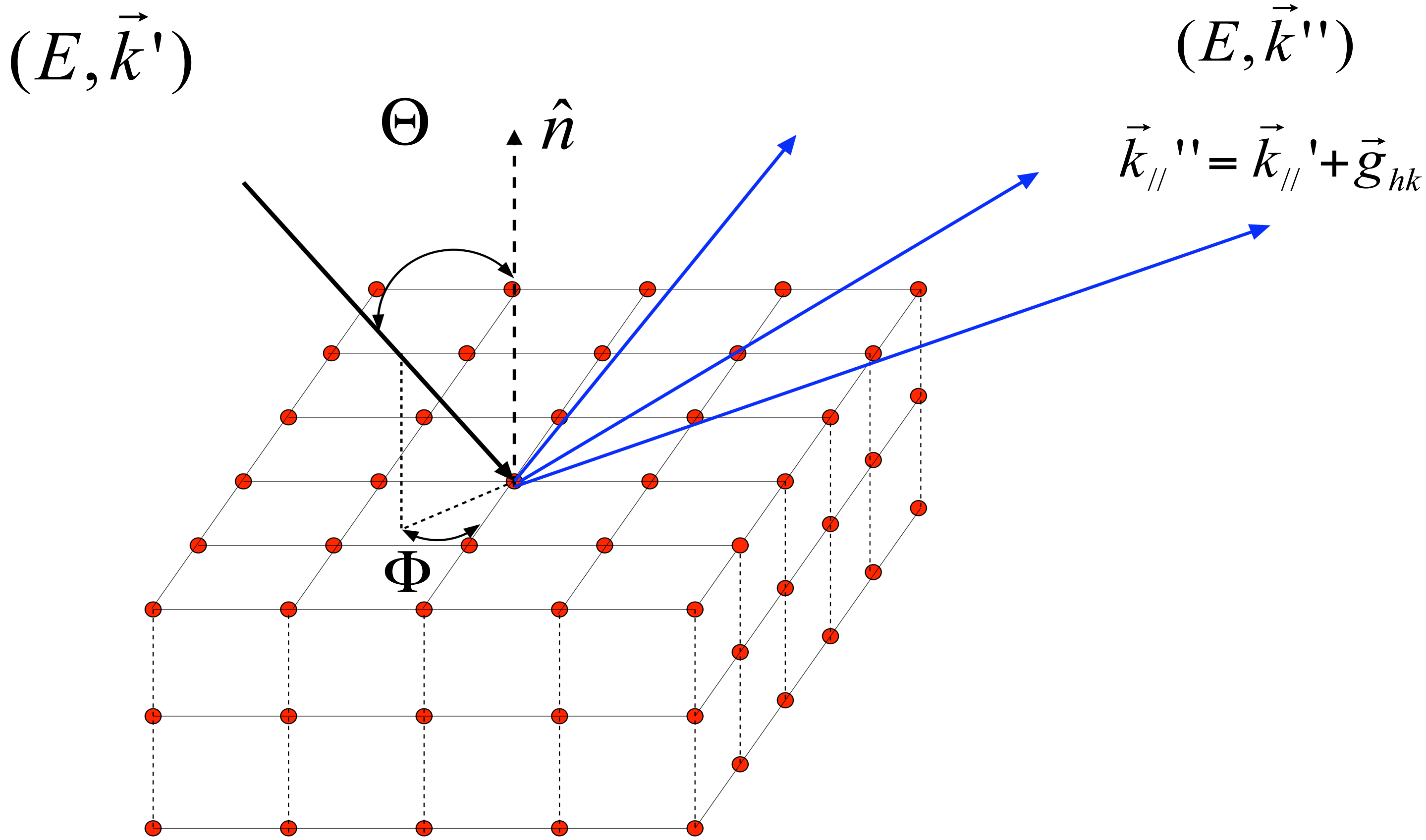
(a)



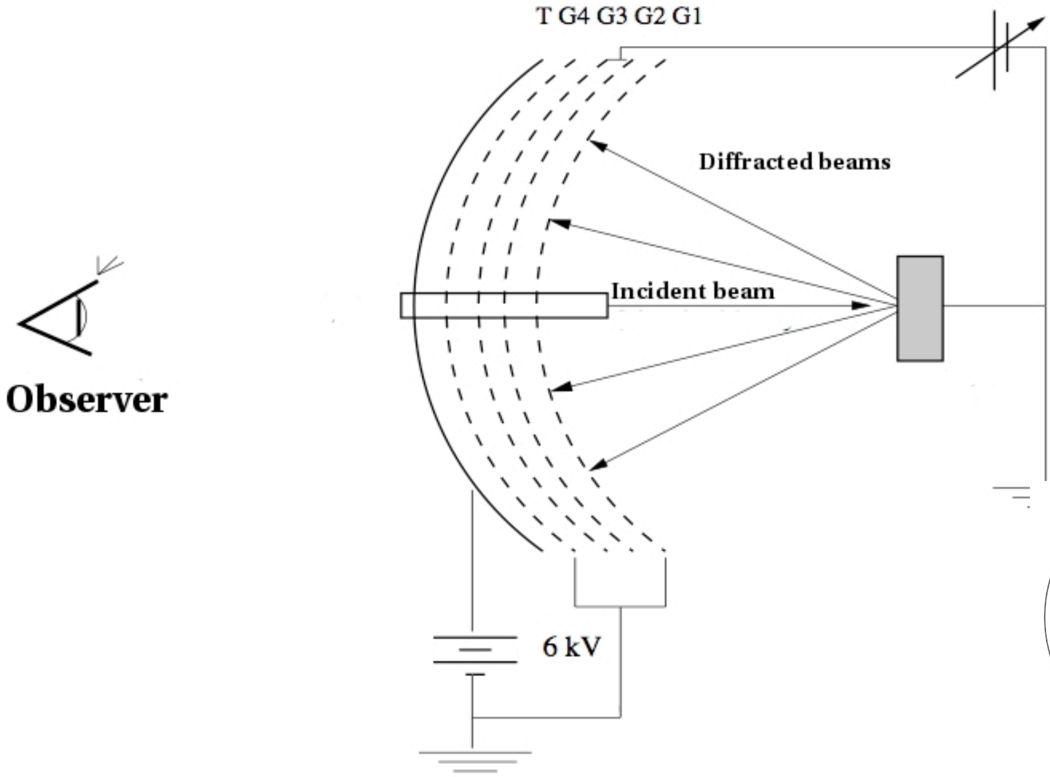
(b)

2D Structure Determination

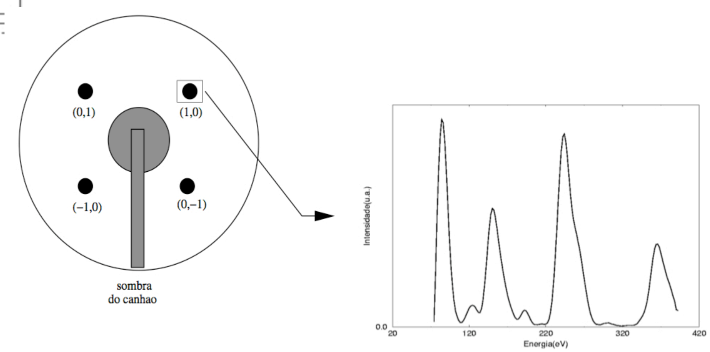
Low-Energy Electron Diffraction



Retarding Field Analyzer

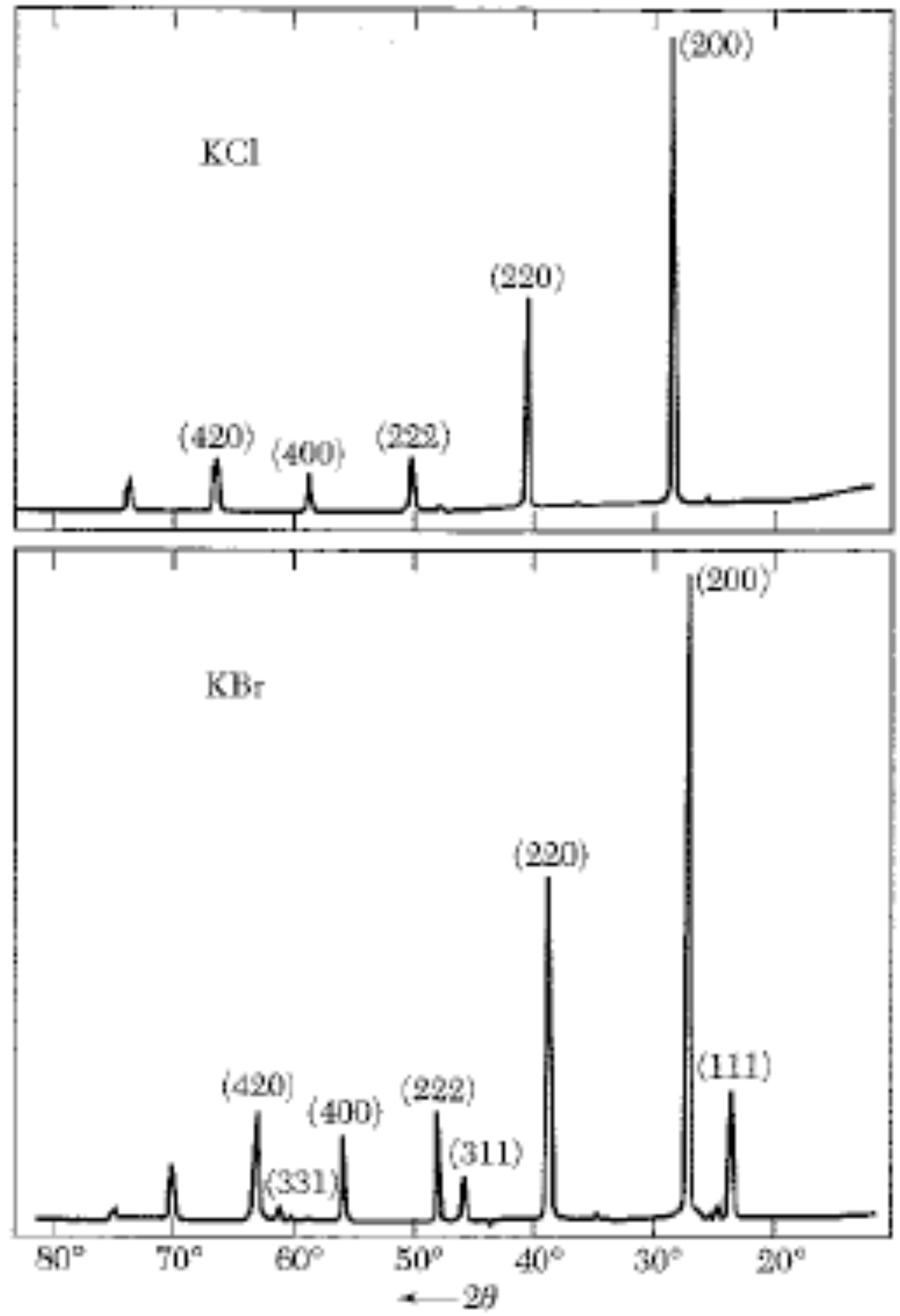


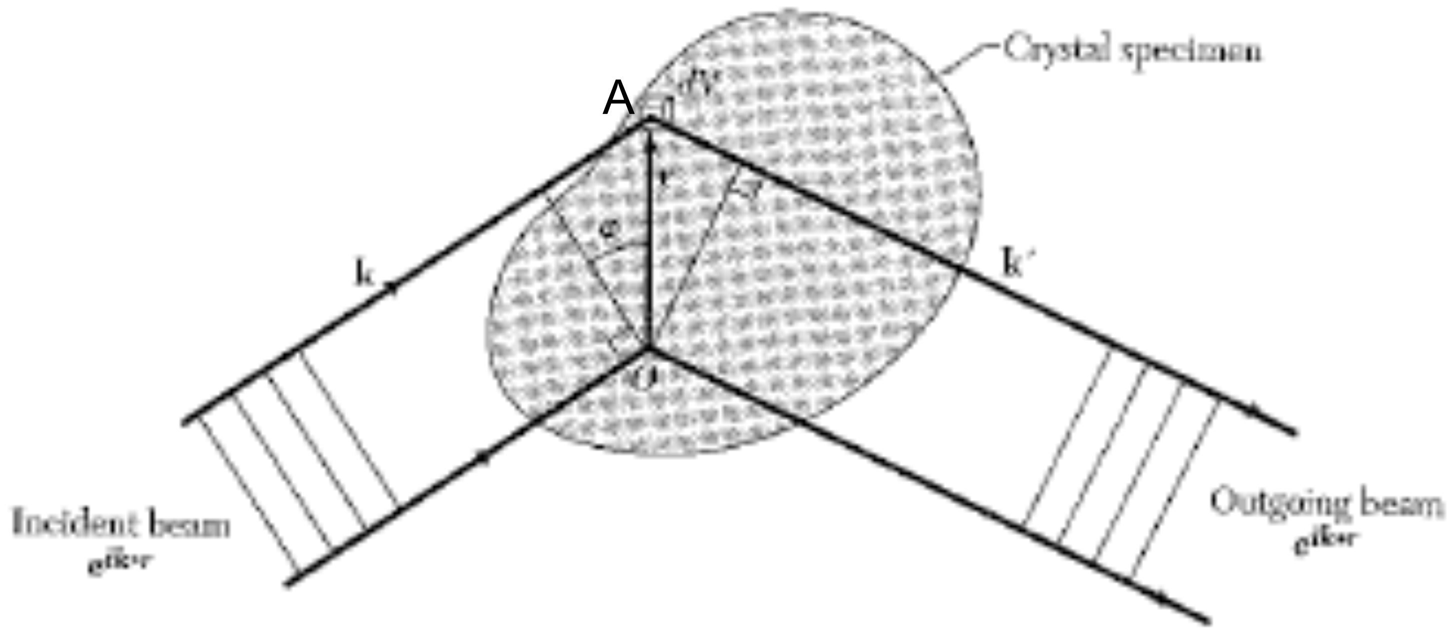
I(V) curves collection



Are all Bragg peaks revealed in the x-ray diffraction pattern?

Why?





phase factor: $e^{i(\mathbf{k}-\mathbf{k}')\bullet\mathbf{r}}$

Scattering amplitude: $F = \int dV n(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\bullet\mathbf{r}}$

$= NS_K$

Structural factor: $$S_K = \sum_{j=1}^{n} e^{i\Delta\mathbf{K}\bullet\mathbf{d}_j}$$

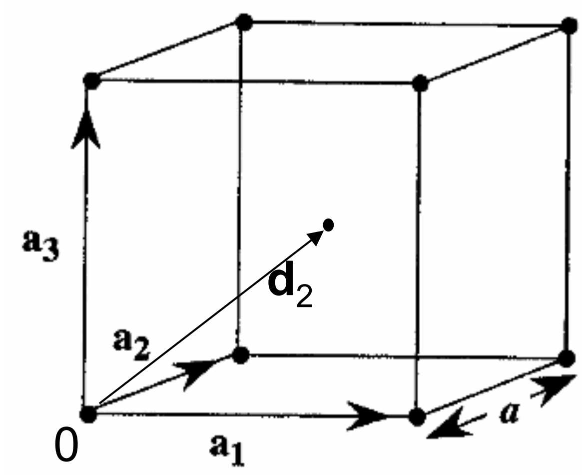
$\Delta\mathbf{K} = \mathbf{k} - \mathbf{k}'$ - vector of reciprocal lattice

$\mathbf{d}_j$ - j^{th} basis point in Bravais lattice

Bragg peak intensity $\propto |S_K|^2$

Can predict when the peak vanishes

Body-centered cubic
Bravais lattice



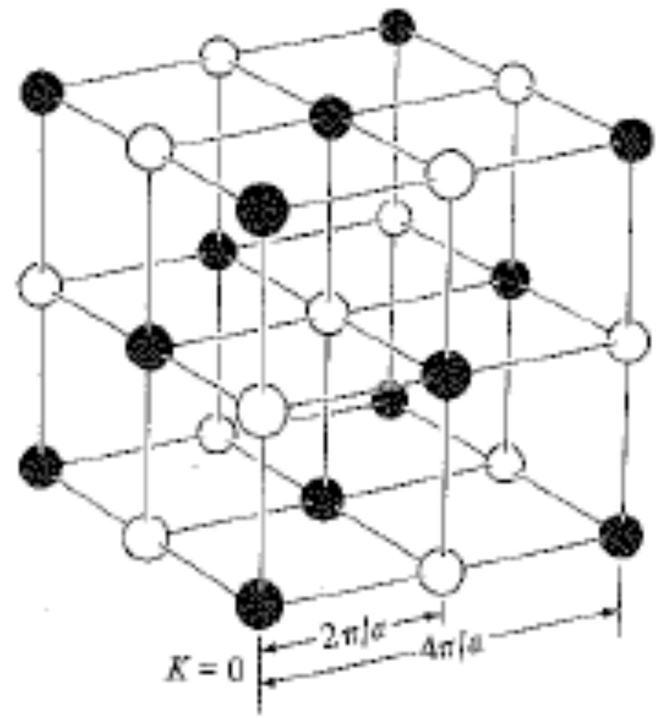
$\mathbf{a}_1 = a\mathbf{x}$, $\mathbf{a}_2 = a\mathbf{y}$, $\mathbf{a}_3 = a\mathbf{z}$

$\mathbf{b}_1 = (2\pi/a)\mathbf{x}$, $\mathbf{b}_2 = (2\pi/a)\,\mathbf{y}$, $\mathbf{b}_3 = (2\pi/a)\mathbf{z}$

Two basis points: $\mathbf{d}_1 = 0$, $\mathbf{d}_2 = (a/2)\,(\mathbf{x}+\mathbf{y}+\mathbf{z})$

$\Delta\mathbf{K} = (2\pi/a)(n\mathbf{x}+m\mathbf{y}+l\mathbf{z})$

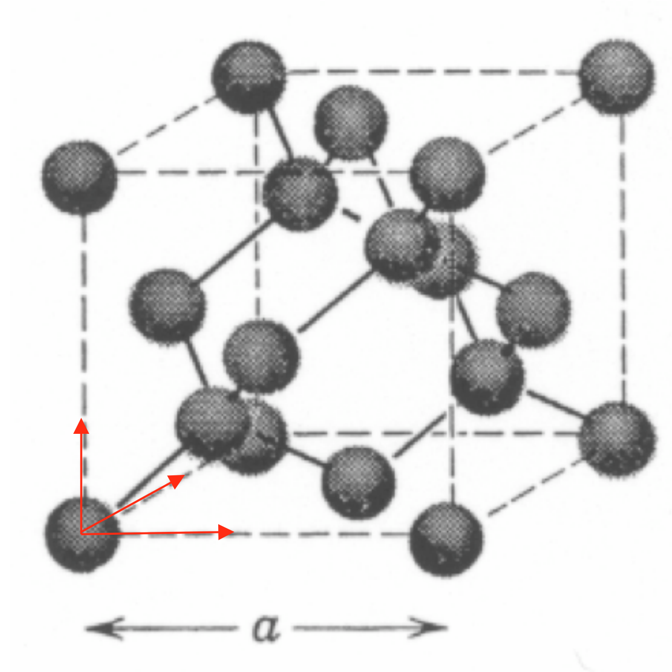
$$S_K = \sum_{j=1}^{n} e^{i\Delta\mathbf{K}\bullet\mathbf{d}_j} = 1+(-1)^{n+m+l} = \begin{cases} 2, & n+m+l = \text{even} \\ 0, & n+m+l = \text{odd} \end{cases}$$



$$S_K = \sum_{j=1}^{n} e^{i\Delta \mathbf{K}\bullet\mathbf{d}_j} = 1 + (-1)^{n+m+l} = \begin{cases} 2, & \text{n+m+l = even} \\ 0, & \text{n+m+l = odd} \end{cases}$$

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

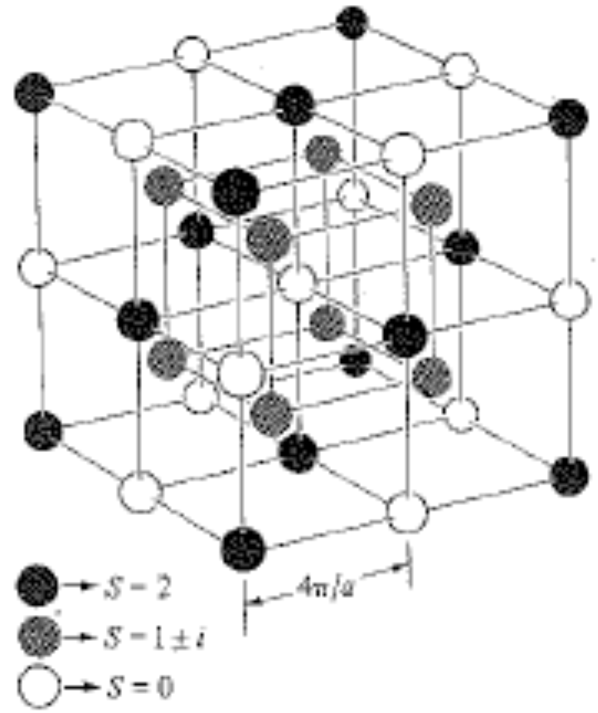
$\mathbf{b}_1 = (2\pi/a)(\mathbf{y}+\mathbf{z}-\mathbf{x})$
$\mathbf{b}_2 = (2\pi/a)(\mathbf{z}+\mathbf{x}-\mathbf{y})$
$\mathbf{b}_3 = (2\pi/a)(\mathbf{x}+\mathbf{y}-\mathbf{z})$



Two basis points: $\mathbf{d}_1 = 0$, $\mathbf{d}_2 = (a/4)(\mathbf{x}+\mathbf{y}+\mathbf{z})$

$\Delta\mathbf{K} = (4\pi/a)(n\mathbf{x}+m\mathbf{y}+l\mathbf{z})$

$$S_K = \sum_{j=1}^{n} e^{i\Delta\mathbf{K}\bullet\mathbf{d}_j} = 1 + e^{[\frac{1}{2}i\pi(n+m+l)]} = \begin{cases} 2, & (n+m+l)/2 = \text{even} \\ 1\pm i, & n+m+l = \text{odd} \\ 0, & (n+m+l)/2 = \text{odd} \end{cases}$$



$$S_K = \sum_{j=1}^{n} e^{i\Delta \mathbf{K} \bullet \mathbf{d}_j} = 1 + e^{[\frac{1}{2} i\pi (n+m+l)]} = \begin{cases} 2, & (n+m+l)/2 = \text{even} \\ 1 \pm i, & n+m+l = \text{odd} \\ 0, & (n+m+l)/2 = \text{odd} \end{cases}$$

Symmetry element	*Reflection affected*	*Systematic-absence condition*
Centred cells		
Body-centred, I	hkl	$h+k+l=2n+1$
Face-centred, F	hkl	$h+k, h+l, k+l=2n+1$
Side-centred, C	hkl	$h+k=2n+1$
Screw axis		
2_1 along a	$h00$	$h=2n+1$
Glide planes $\perp$ *b*		
Translation ($a/2$) (a-glide)	$h0l$	$h=2n+1$
Translation ($a/2+c/2$) (n-glide)	$h0l$	$h+l=2n+1$
Translation ($a/4+c/4$) (d-glide)	$h0l$	$h+l=4n+1, 2, 3$

In case of powder sample:

$$S_K = \sum_{j=1}^{n} f_j\left(\Delta\,\mathbf{K}\right) e^{i\Delta\,\mathbf{K}\bullet\mathbf{d}_{\,j}}$$

↑

Atomic form factor

$$\left|S_K\right| \neq 0$$

Homework today (due on Sept. 9, 2010)

1. Problem 1 in page 93 (Ashcroft/Mermin)
2. Hexagonal space lattice: The primitive translation vectors of the hexagonal space lattice may be taken as: $\mathbf{a}_1 = (3^{1/2}a/2)\mathbf{x} + (a/2)\mathbf{y}$; $\mathbf{a}_2 = -(3^{1/2}a/2)\mathbf{x} + (a/2)\mathbf{y}$; $\mathbf{a}_3 = c\mathbf{z}$.

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

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

   $\mathbf{b}_1 = (3^{1/2}2\pi/a)\mathbf{x} + (2\pi/a)\mathbf{y}$; $\mathbf{b}_2 = -(3^{1/2}2\pi/a)\mathbf{x} + (2\pi/a)\mathbf{y}$; $\mathbf{b}_3 = (2\pi/c)\mathbf{z}$.

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