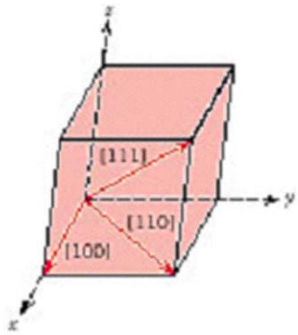
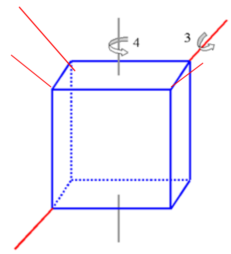
Crystallographic Directions And Planes





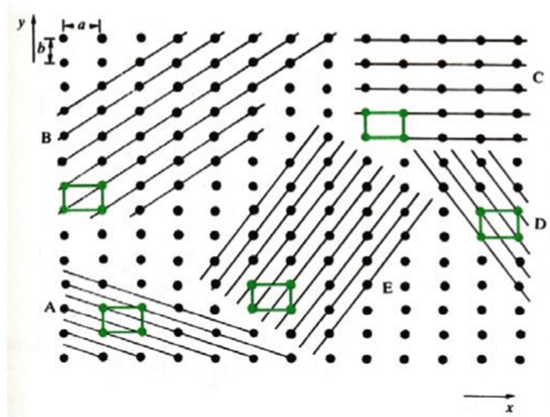
Lattice Directions

Individual directions: [uvw]

Symmetry-related directions: <uvw>

Lattice planes

- It is possible to describe certain directions and planes with respect to the crystal lattice using a set of three integers referred to as Miller Indices



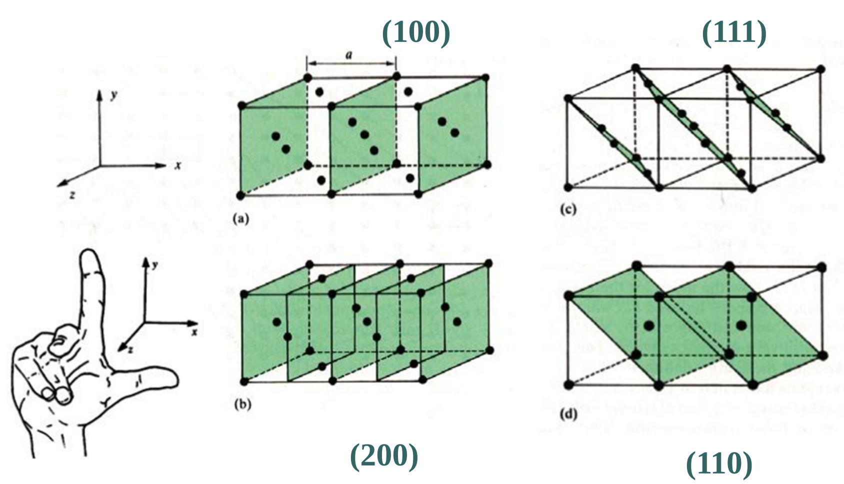
Crystallographic Directions And Planes

Miller Indices:

1. Find the intercepts on the axes in terms of the lattice constant a, b, c
2. Take the reciprocals of these numbers, reduce to the three integers having the same ratio
   (hkl)

Set of symmetry-related planes: {hkl}

Examples of Miller indices

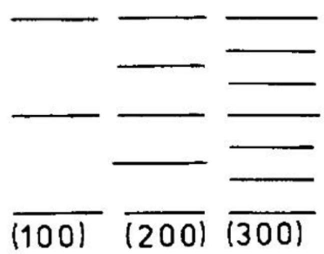


Families of planes

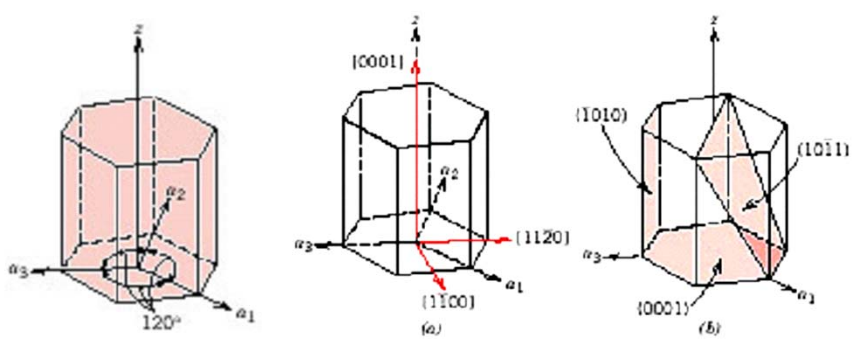
- Miller indices describe the orientation a spacing of a family of planes
  - The spacing between adjacent planes in a family is referred to as a "d-spacing"

Three different families of planes

d-spacing between (300) planes is one third of the (100) spacing



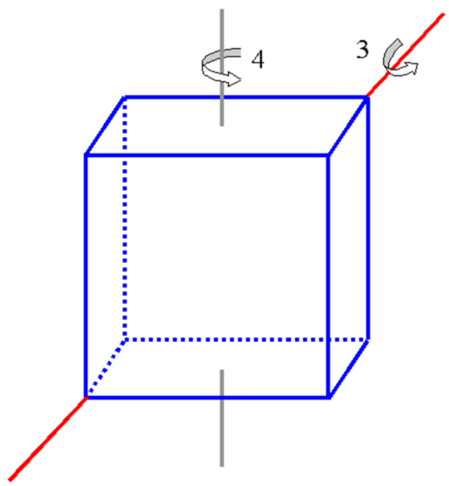
Crystallographic Directions And Planes



Miller-Bravais indices

[uvtw], (hkil)

t=-(u+v) *i=-(h+k)*



In cubic system,

[hkl] direction
perpendicular to (hkl) plane

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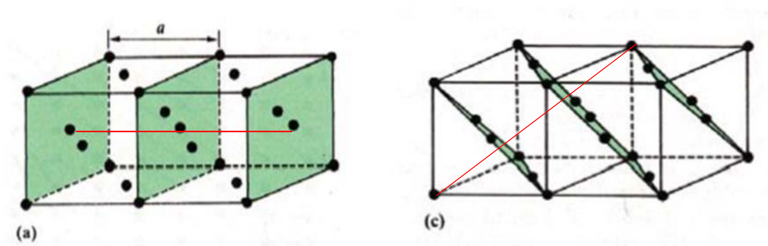
Lattice spacing

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

For cubic system



d-spacing formulae

- For a unit cell with orthogonal axes
  - $(1 / d^2_{hkl}) = (h^2/a^2) + (k^2/b^2) + (l^2/c^2)$
- Hexagonal unit cells
  - $(1 / d^2_{hkl}) = (4/3)([h^2 + k^2 + hk]/ a^2) + (l^2/c^2)$

Crystal Structure Analysis

X-ray diffraction

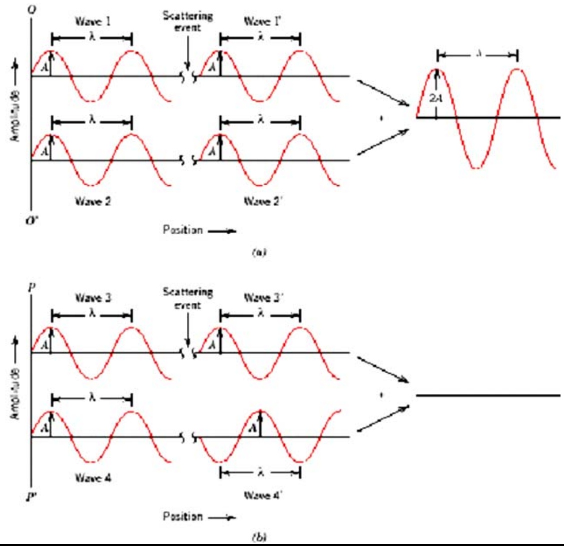
Electron Diffraction

Neutron Diffraction

Essence of diffraction: Bragg Diffraction

Light

Interference fringes

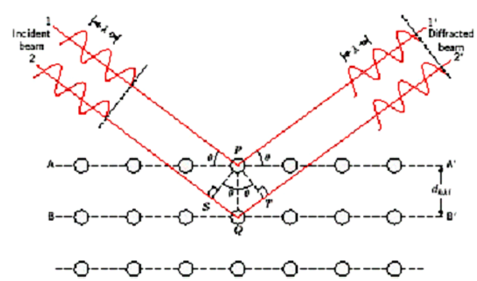


Constructive

Destructive

Bragg's Law

$$n\lambda = \overline{SQ} + \overline{QT}$$
$$= d_{hkl}\sin\theta + d_{hkl}\sin\theta$$
$$= 2d_{hkl}\sin\theta$$



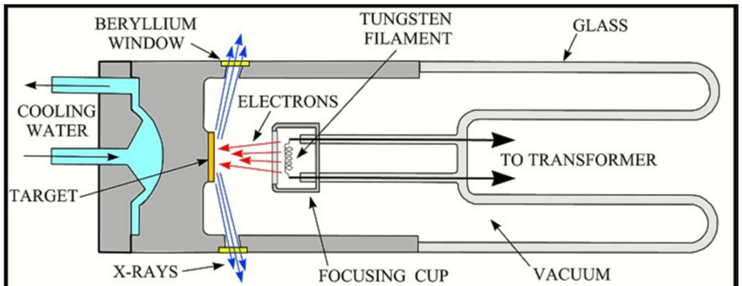
For cubic system:

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

But not all planes have the diffraction !!!

X-Ray Diffraction

$$E = h\nu = hc/\lambda$$



SCHEMATIC CROSS SECTION OF AN X-RAY TUBE

Mo: *35KeV ~ 0.1-1.4Å*
Cu K 1.54 A

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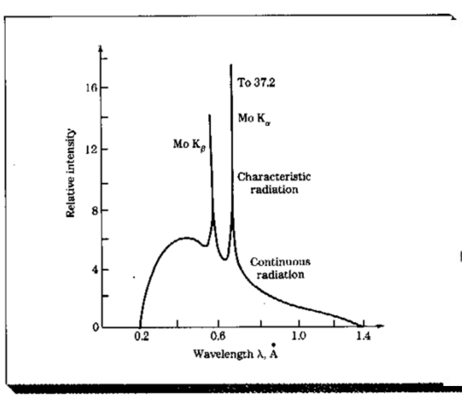
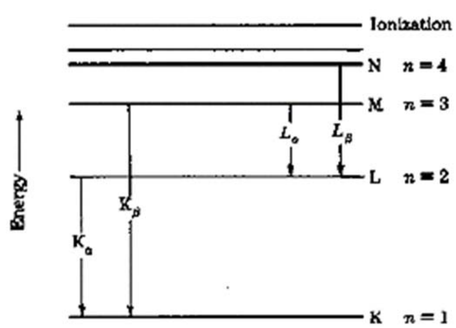
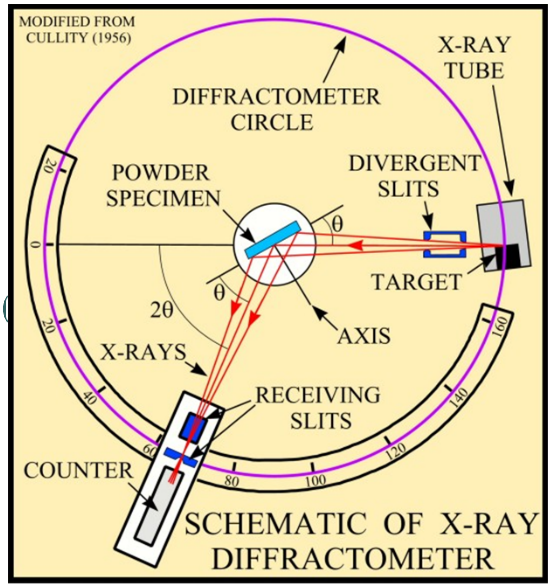
X-Ray Diffraction

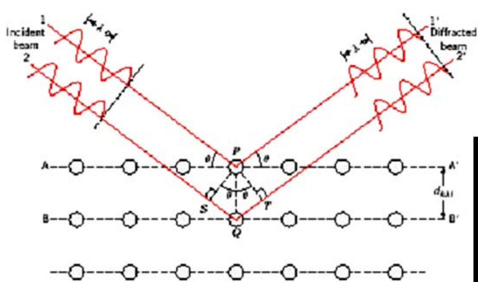




Powder diffraction



Powder diffraction



BRAGG LAW

$$2d(\sin\theta) = \lambda_o$$

where:

d = lattice interplanar spacing of the crystal
θ = x-ray incidence angle (Bragg angle)
λ = wavelength of the characteristic x-rays

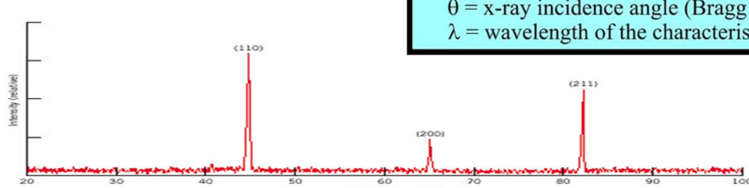
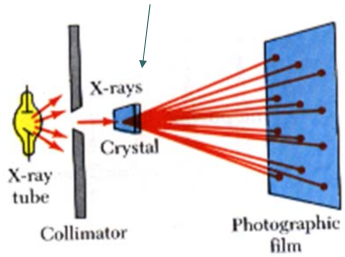
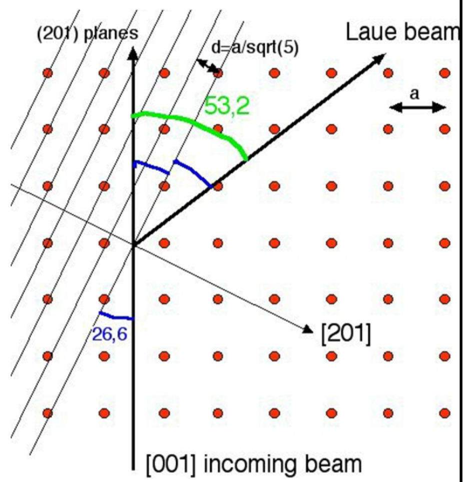


FIGURE 3.20 Diffraction pattern for polycrystalline α-iron.

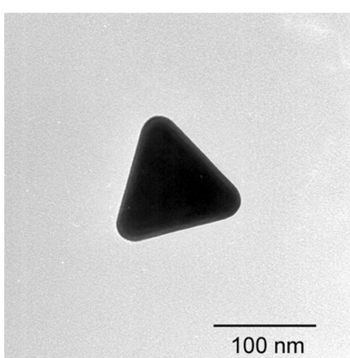
Laue Diffraction

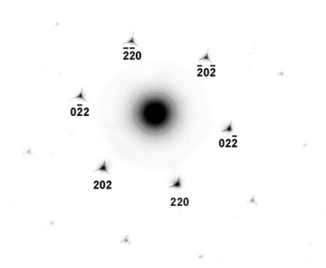
Single crystal





Electron Diffraction





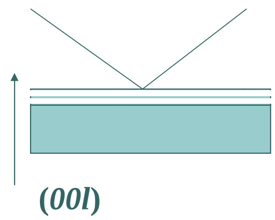
Example: La_2CuO_2

Layered Cuprates
Thin film, growth oriented along c axis

Cu K 1.54 A

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

2*theta	d	(hkl)
7.2	12.1	(001)
14.4	6.1	(002)
22	4.0	(003)



c=12.2 A

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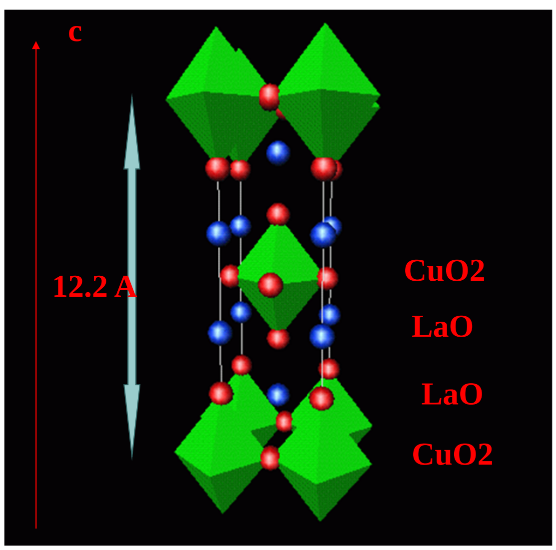
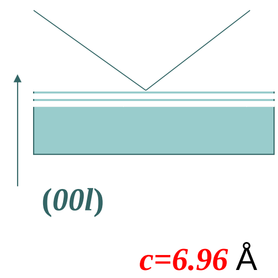


Example: $Ca_{0.5}Sr_{0.5}CuO_2$

Layered Cuprates
Thin film, growth oriented along c axis

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

2*theta	d	(hkl)
12.7	6.96	(001)
26	3.42	(002)
42.2	2.15	(003)



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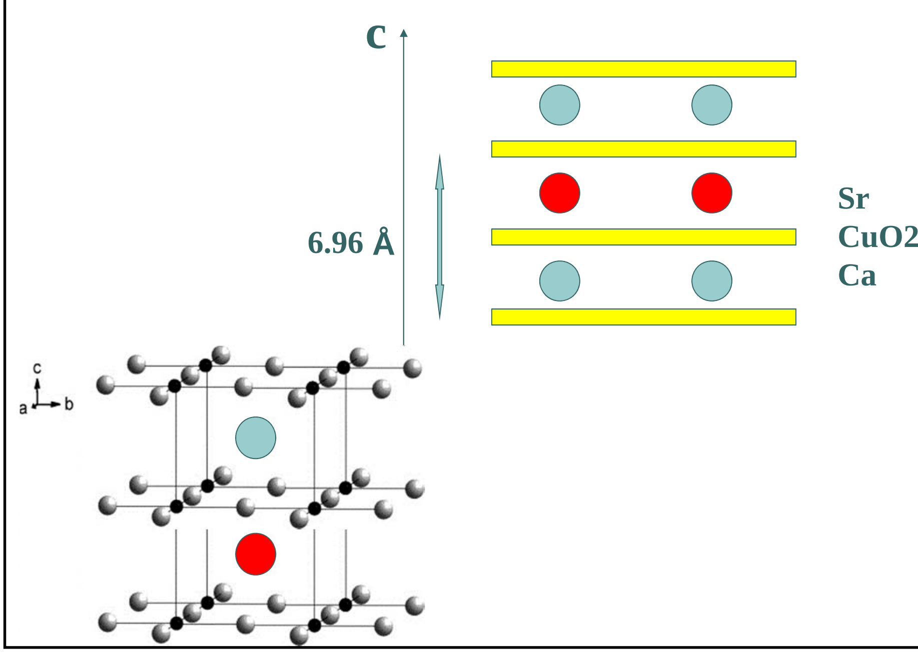


What we will see in XRD of simple cubic, BCC, FCC?

$$\frac{\sin^2\theta_A}{\sin^2\theta_B} = 0.5\,(BCC); = 0.75\ (FCC)$$

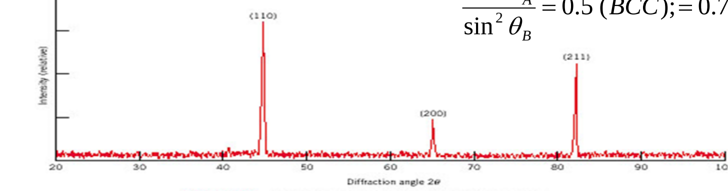
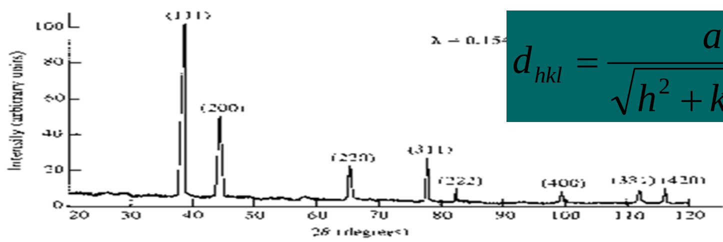


FIGURE 3.20 Diffraction pattern for polycrystalline α-iron.



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

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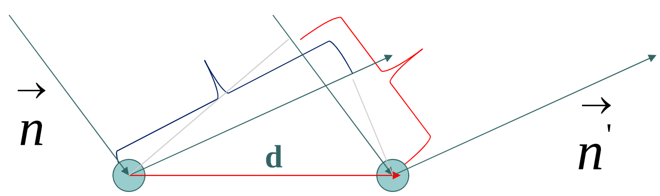
Reciprocal Lattice



$\vec{n}$ $\vec{n}'$ $\vec{R}$

$$\vec{R} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

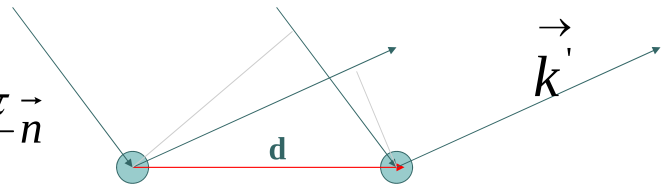
Path Difference:

$$\Delta = \vec{R}\bullet\vec{n} - \vec{R}\bullet\vec{n}' = \vec{R}(\vec{n}-\vec{n}') = m\lambda$$

$$\vec{R}\bullet\frac{2\pi}{\lambda}(\vec{n}-\vec{n}') = 2\pi m$$

Reciprocal Lattice

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



$\vec{k}'$

$\vec{R}$

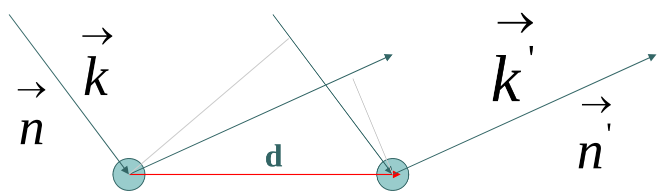
$$\vec{R} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

$$\vec{R} \bullet \frac{2\pi}{\lambda}(\vec{n} - \vec{n}') = 2\pi m$$

$$\vec{R} \bullet (\vec{k} - \vec{k}') = 2\pi m$$

Correspond to plane wave: $e^{i\vec{R}\bullet(\vec{k}-\vec{k}')} = e^{i2\pi m} = 1$

Reciprocal Lattice



$\vec{n}$ $\vec{k}$ $\vec{k}'$ $\vec{n}'$

$\vec{R}$

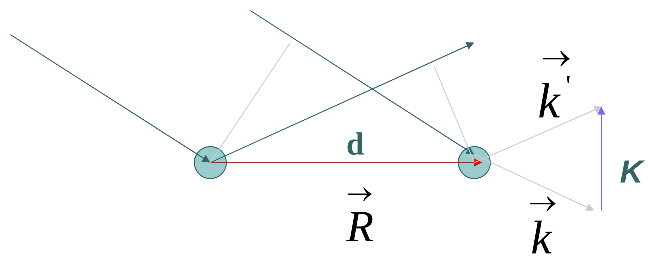
$$\vec{R} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

$$\boxed{e^{i\vec{R}\bullet(\vec{k}-\vec{k}')} = 1}$$ **Laue Condition**

$$\boxed{\vec{K} = \vec{k}' - \vec{k}}$$ **Reciprocal lattice vector**

$e^{-iK\cdot R} = 1$ **For all R in the Bravais Lattice**

Reciprocal Lattice



$$e^{i\vec{R}\bullet(\vec{k}-\vec{k}')}=1$$ **Laue Condition**

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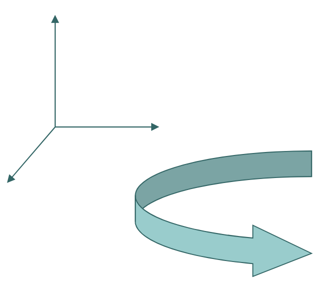
$$e^{-iK\cdot R}=1$$ **For all R in the Bravais Lattice**

Reciprocal Lattice

$$e^{-iK\cdot R}=1$$ **For all R in the Bravais Lattice**

A reciprocal lattice is defined with reference to a particular Bravias Lattice.



$$\vec{a} \quad \vec{b} \quad \vec{c}$$ **Primitive vectors**

$$\vec{a}^*=2\pi\frac{b\times c}{a\cdot(b\times c)}$$
$$\vec{b}^*=2\pi\frac{c\times a}{a\cdot(b\times c)}$$
$$\vec{c}^*=2\pi\frac{a\times b}{a\cdot(b\times c)}$$

Reciprocal Lattice

$$\boxed{e^{-iK\cdot R} = 1 \quad \text{For all R in the Bravais Lattice}}$$

$$\vec{a}^* = 2\pi \frac{b\times c}{a\cdot(b\times c)}$$

$$\vec{b}^* = 2\pi \frac{c\times a}{a\cdot(b\times c)}$$

$$\vec{c}^* = 2\pi \frac{a\times b}{a\cdot(b\times c)}$$

Verify:

$$a^*\cdot a = 2\pi$$

$$a^*\cdot b = 0$$

$$a^*\cdot c = 0$$

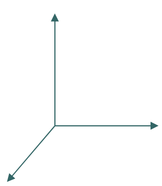
For any $K = k_1 a^* + k_2 b^* + k_3 c^*$

$$\vec{R} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

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

Reciprocal Lattice

Reciprocal lattice is always one of 14 Bravais Lattice.



$$\vec{a} = a\cdot\vec{x}$$

$$\vec{b} = a\cdot\vec{y}$$

$$\vec{c} = a\cdot\vec{z}$$

Simple cubic

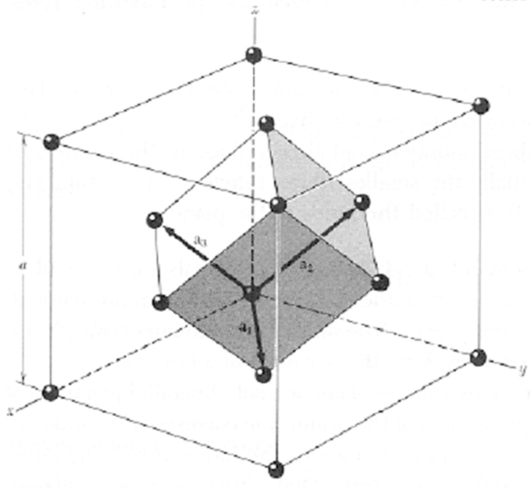
$$\vec{a}^* = 2\pi \frac{b\times c}{a\cdot(b\times c)} = \frac{2\pi}{a}\vec{x}$$

$$\vec{b}^* = 2\pi \frac{c\times a}{a\cdot(b\times c)} = \frac{2\pi}{a}\vec{y}$$

$$\vec{c}^* = 2\pi \frac{a\times b}{a\cdot(b\times c)} = \frac{2\pi}{a}\vec{z}$$

Simple cubic

Primitive Cell of FCC



$$a_1 = \frac{1}{2}a(\vec{x}+\vec{y})$$

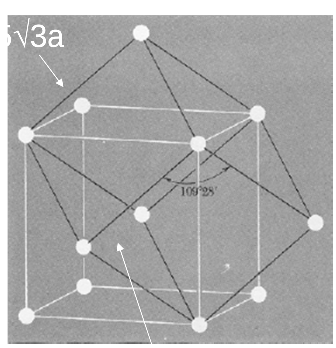
$$a_2 = \frac{1}{2}a(\vec{z}+\vec{y})$$

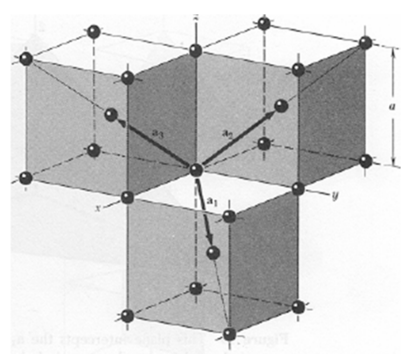
$$a_3 = \frac{1}{2}a(\vec{z}+\vec{x})$$

- Angle between a_1, a_2, a_3: 60^o

Primitive Cell of BCC

- Rhombohedron primitive cell





- Primitive Translation Vectors:

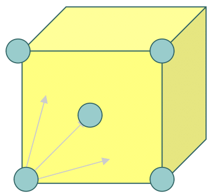
$$a_1 = \frac{1}{2}a(\vec{x}+\vec{y}-\vec{z})$$

$$a_2 = \frac{1}{2}a(-\vec{x}+\vec{y}+\vec{z})$$

$$a_3 = \frac{1}{2}a(\vec{x}-\vec{y}+\vec{z})$$

Reciprocal Lattice

Reciprocal lattice is always one of 14 Bravais Lattice.



$$\vec{a} = \frac{a}{2}\cdot(\vec{y}+\vec{z})$$

$$\vec{b} = \frac{a}{2}\cdot(\vec{x}+\vec{z})$$

$$\vec{c} = \frac{a}{2}\cdot(\vec{x}+\vec{y})$$

FCC

$$\vec{a}^* = 2\pi\frac{b\times c}{a\cdot(b\times c)} = \frac{4\pi}{a}\frac{1}{2}(\vec{y}+\vec{z}-\vec{x})$$

$$\vec{b}^* = 2\pi\frac{c\times a}{a\cdot(b\times c)} = \frac{4\pi}{a}\frac{1}{2}(\vec{x}+\vec{z}-\vec{y})$$

$$\vec{c}^* = 2\pi\frac{a\times b}{a\cdot(b\times c)} = \frac{4\pi}{a}\frac{1}{2}(\vec{x}+\vec{y}-\vec{z})$$

BCC

Reciprocal Lattice

- BCC → FCC
- Simple hexagonal → Simple hexagonal

The reciprocal lattice

Case studies:

I) **Orthorhombic crystal system**: (*includes* ***tetragonal*** *and* ***cubic***)

Orientations:

$\vec{a}^* \perp$ (1, 0, 0), the b,c-plane. => $\vec{a}^* \parallel \vec{a}$

$\vec{b}^* \perp$ (0, 1, 0), the a,c-plane. => $\vec{b}^* \parallel \vec{b}$

$\vec{c}^* \perp$ (0, 0, 1), the a,b-plane. => $\vec{c}^* \parallel \vec{c}$

$$\vec{a}^* = 2\pi \frac{b\times c}{a\cdot(b\times c)}$$

$$\vec{b}^* = 2\pi \frac{c\times a}{a\cdot(b\times c)}$$

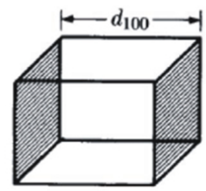
$$\vec{c}^* = 2\pi \frac{a\times b}{a\cdot(b\times c)}$$

Lengths: generally $a^* = 1/d_{100}$, $b^* = 1/d_{010}$, $c^* = 1/d_{001}$

here: $d_{100} = a$, $d_{010} = b$, $d_{001} = c$;

thus: **$a^* = 1/a$, $b^* = 1/b$, $c^* = 1/c$**,

$\boxed{V^* = a^*b^*c^* = 1/V.}$



(100)

Example:

$a = \sqrt{2} = 1.414$

$b = 1/\sqrt{2} = 0.707$

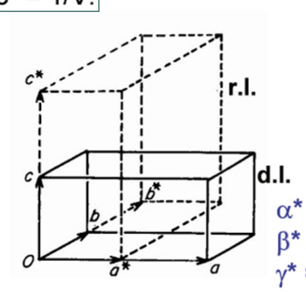
$c = 1/\sqrt{2} = 0.707$

Then:

$a^* = 1/a = 0.707$

$b^* = 1/b = 1.414$

$c^* = 1/c = 1.414$



$\alpha^* = \alpha = 90^o$

$\beta^* = \beta = 90^o$

$\gamma^* = \gamma = 90^o$

The reciprocal lattice

Similar: **hexagonal/trigonal**, i.e. **$\gamma^* = 180^o - \gamma$**

Case studies:

II) **Monoclinic crystal system**:

Orientations:

$\vec{a}^* \perp$ (1, 0, 0), the b,c-plane. => $\vec{a}^*$ **NOT** $\parallel \vec{a}$

$\vec{b}^* \perp$ (0, 1, 0), the a,c-plane. => $\vec{b}^* \parallel \vec{b}$

$\vec{c}^* \perp$ (0, 0, 1), the a,b-plane. => $\vec{c}^*$ **NOT** $\parallel \vec{c}$

Lengths: generally $a^* = 1/d_{100}$, $b^* = 1/d_{010}$, $c^* = 1/d_{001}$

here: $d_{100} = a\sin\beta$, $d_{010} = b$, $d_{001} = c\sin\beta$;

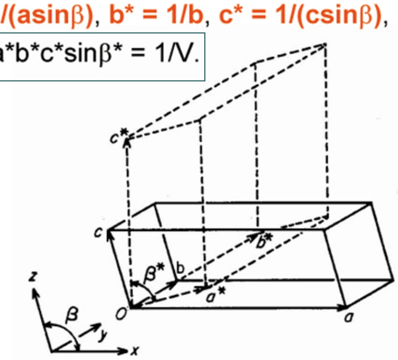
thus: **$a^* = 1/(a\sin\beta)$, $b^* = 1/b$, $c^* = 1/(c\sin\beta)$**,

$\boxed{V^* = a^*b^*c^*\sin\beta^* = 1/V.}$

$$\vec{a}^* = 2\pi \frac{b\times c}{a\cdot(b\times c)}$$

$$\vec{b}^* = 2\pi \frac{c\times a}{a\cdot(b\times c)}$$

$$\vec{c}^* = 2\pi \frac{a\times b}{a\cdot(b\times c)}$$



$\alpha^* = \alpha = 90^o$

$\beta^* = 180^o - \beta$

$\gamma^* = \gamma = 90^o$

The reciprocal lattice

Case studies:

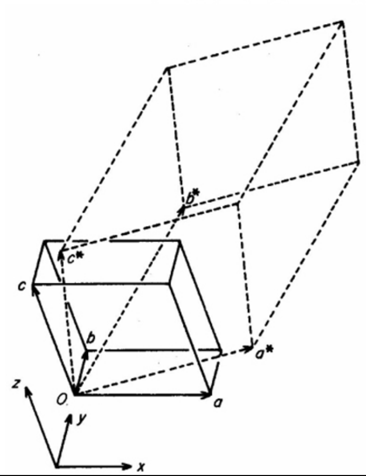
III) **Triclinic crystal system**:

Orientations:

$\vec{a}^* \perp$ (1, 0, 0), the b,c-plane. => $\vec{a}^*$ **NOT** $||$ $\vec{a}$

$\vec{b}^* \perp$ (0, 1, 0), the a,c-plane. => $\vec{b}^*$ **NOT** $||$ $\vec{b}$

$\vec{c}^* \perp$ (0, 0, 1), the a,b-plane. => $\vec{c}^*$ **NOT** $||$ $\vec{c}$



Lengths/angles:
quite complex;
see next slide.

The reciprocal lattice

Case studies:

III) **Triclinic crystal system**:

Formulas correct for all systems!
But often much simpler, when
e.g. α = 90º => sinα = 1, cosα = 0

$$a^* = \frac{bc \sin\alpha}{V} \qquad a = \frac{b^* c^* \sin\alpha^*}{V^*}$$

$$b^* = \frac{ac \sin\beta}{V} \qquad b = \frac{a^* c^* \sin\beta^*}{V^*}$$

$$c^* = \frac{ab \sin\gamma}{V} \qquad c = \frac{a^* b^* \sin\gamma^*}{V^*}$$

$$\boxed{V = \frac{1}{V^*}} = abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$$

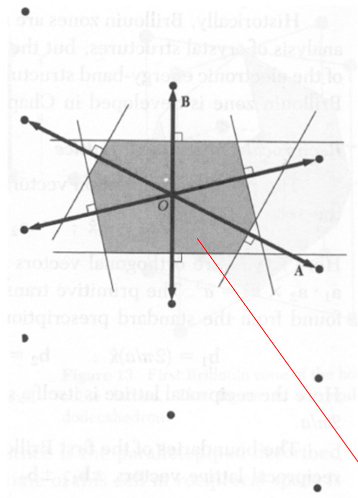
$$\boxed{V^* = \frac{1}{V}} = a^* b^* c^* \sqrt{1 - \cos^2\alpha^* - \cos^2\beta^* - \cos^2\gamma^* + 2\cos\alpha^*\cos\beta^*\cos\gamma^*}$$

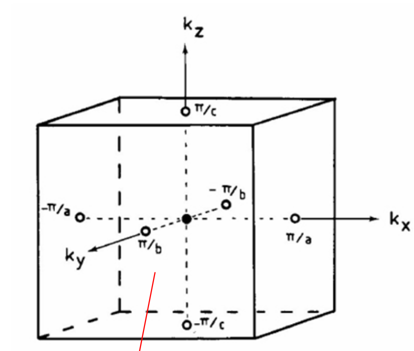
$$\cos\alpha^* = \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma} \qquad \cos\alpha = \frac{\cos\beta^*\cos\gamma^* - \cos\alpha^*}{\sin\beta^*\sin\gamma^*}$$

$$\cos\beta^* = \frac{\cos\alpha\cos\gamma - \cos\beta}{\sin\alpha\sin\gamma} \qquad \cos\beta = \frac{\cos\alpha^*\cos\gamma^* - \cos\beta^*}{\sin\alpha^*\sin\gamma^*}$$

$$\cos\gamma^* = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta} \qquad \cos\gamma = \frac{\cos\alpha^*\cos\beta^* - \cos\gamma^*}{\sin\alpha^*\sin\beta^*}$$

Examples for Brillouin zones



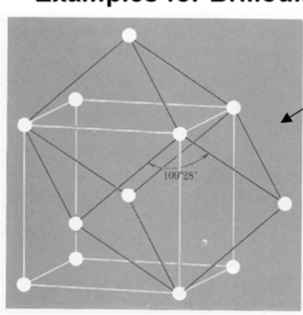


cubic primitive

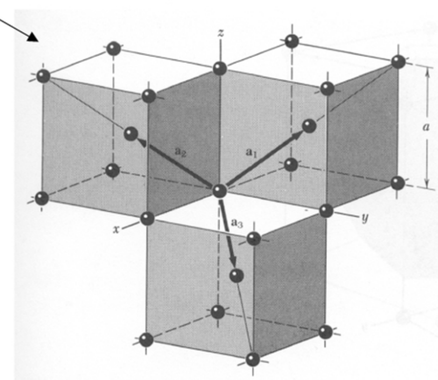
2-D, general

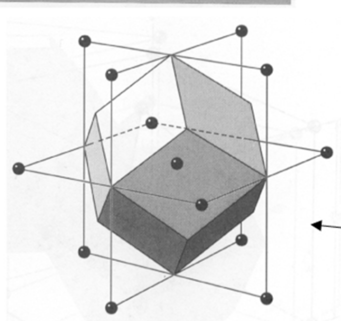
Wigner-Seitz cells of reciprocal lattice

Examples for Brillouin zones **body-centered cubic**



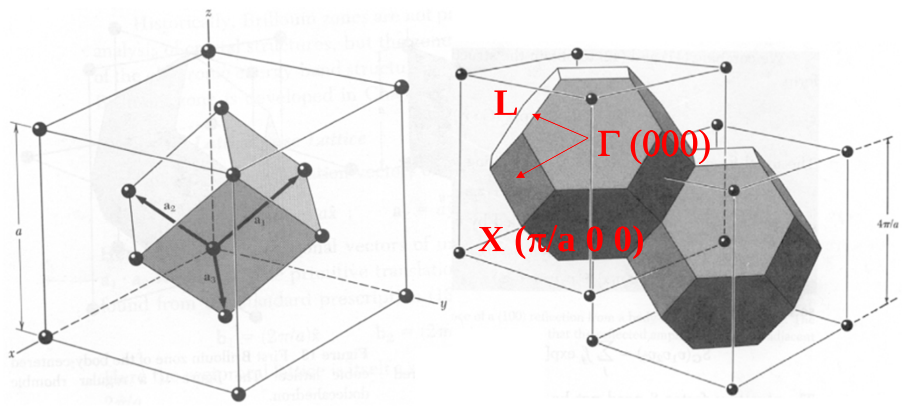
d.l.: centered and primitive celll





r.l.: 1st Brillouin zone:
a rhombic dodecahedron

Examples for Brillouin zones **face-centered cubic**



d.l.: centered and primitive cell

r.l.: 1st Brillouin zone

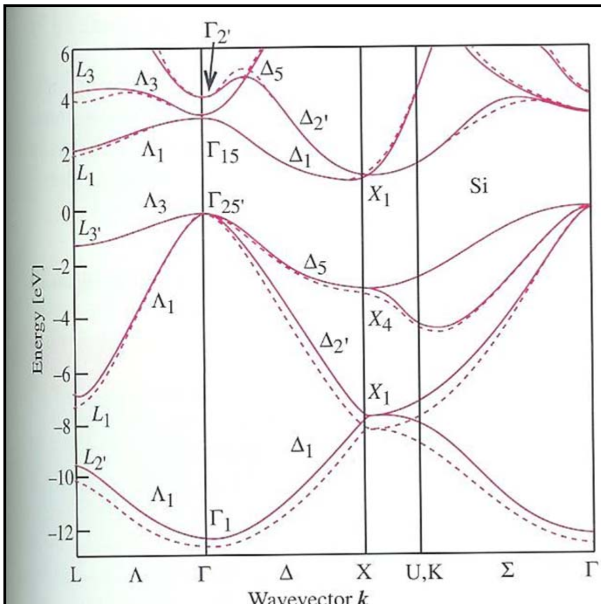
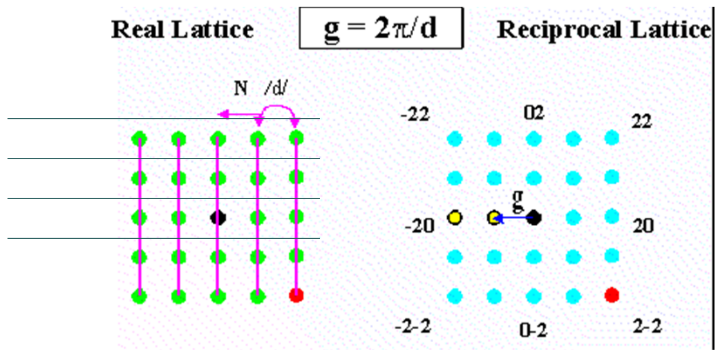


Fig. 2.10. Electronic band structure of Si calculated by the pseudopotential te
solid and the *dotted lines* represent calculations with a **nonlocal** and a **local**]
tial, respectively. [Ref. 2.8, p. 81]



Theorem:

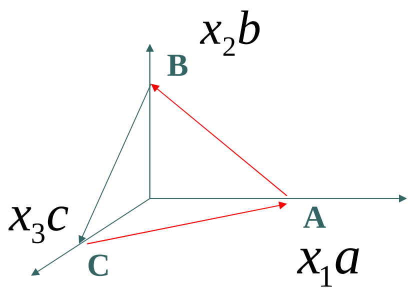
For any family of lattice planes separated by distance d, there are reciprocal lattice vectors perpendicular to the planes, the shortest being $2\pi/d$.

Orientation of plane is determined by a normal vector

The miller indices of a lattice plane are the coordination at the reciprocal lattice vector normal to the plane.

Plane (hkl) →

$$(hkl) = \left(\frac{1}{x_1}, \frac{1}{x_2}, \frac{1}{x_3}\right)$$



$$\boxed{\begin{aligned} K &= ha^* + kb^* + lc^* \\ &= \frac{2\pi}{x_1}a^* + \frac{2\pi}{x_2}b^* + \frac{2\pi}{x_3}c^* \end{aligned}}$$

$$\vec{K} = \vec{AB} \times \vec{AC} = (x_1a - x_2b) \times (x_1a - x_3c)$$
$$= \frac{1}{x_1}a^* + \frac{1}{x_2}b^* + \frac{1}{x_3}c^*$$

$$K = ha^* + kb^* + lc^*$$

$$\vec{a}^* = 2\pi \frac{b \times c}{a \cdot (b \times c)}$$
$$\vec{b}^* = 2\pi \frac{c \times a}{a \cdot (b \times c)}$$
$$\vec{c}^* = 2\pi \frac{a \times b}{a \cdot (b \times c)}$$