Chapter 12 Diffraction

Reading Assignment:

1. D. Sherwood, Crystals, X-rays, and Proteins-chapter 8

Contents

Diffraction by 3-D Lattice

- diffraction pattern of a crystal

amplitude function of a crystal

$$f(crystal) = f(motif) * [f(infinite\ lattice) \bullet f(shape\ function)]$$

fourier transform

$$Tf(crystal) = Tf(motif) \bullet [Tf(infinite\ lattice) * Tf(shape\ function)]$$

diffraction pattern intensity

$$= \left|Tf(crystal)\right|^2$$

$$= \left|Tf(motif)\right|^2 \bullet \left|Tf(infinite\ lattice) * Tf(shape\ function)\right|^2$$

- diffraction pattern of an infinite, 1-D array of δ-function

in real space $\rightarrow$ an infinite, 1-D array of δ-function

in Fourier, or reciprocal space

Diffraction by 3-D Lattice

- infinite crystal- infinite 3-D array of δ-function
  diffraction pattern- infinite 3-D array of δ-function
- real lattice vs. reciprocal lattice
- real crystal- finite $\rightarrow$ infinitely sharp peak blurred
  by shape function
- intensity of main peak- motif- information of structure
  of unit cell
- 1D- scattering angle $\sin\theta$
  3D- wave vector $\vec{k}$- spatial coordinates

Diffraction by 3-D Lattice

- non-normal incident waves

$$F(\vec{k}) = \int_{\text{all } \vec{r}} f(\vec{r}) e^{i\vec{k}\bullet\vec{r}} d\vec{r}$$

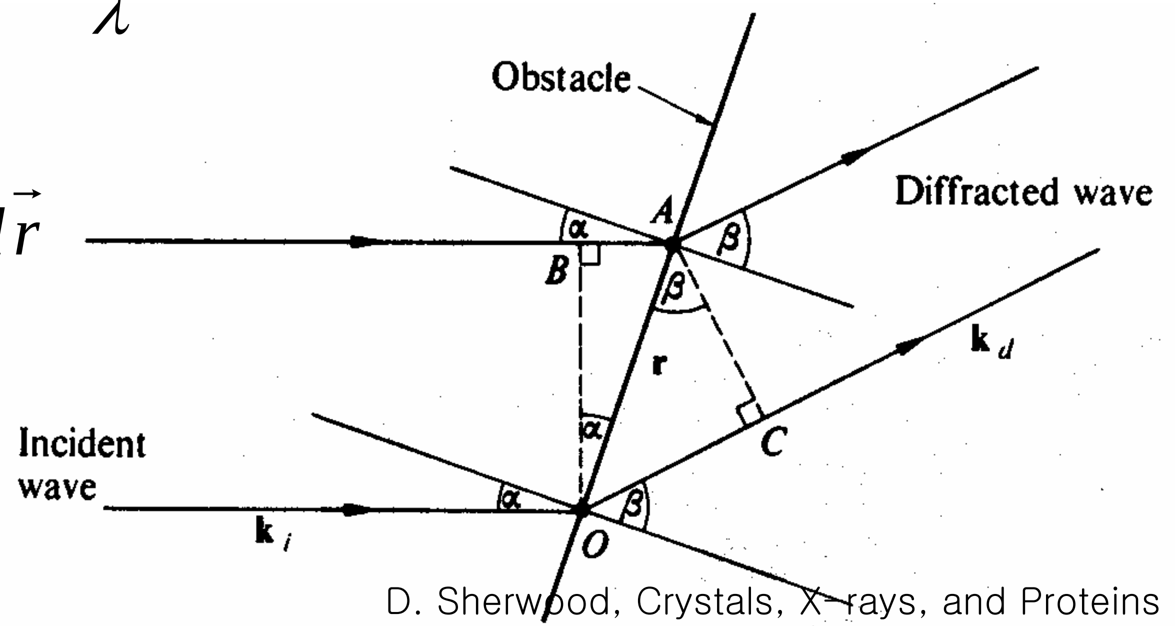
normal incidence- $\vec{k}\bullet\vec{r}$: phase difference

- path difference $= OC - BA = r\sin\beta - r\sin\alpha$

phase difference$= \dfrac{2\pi(r\sin\beta - r\sin\alpha)}{\lambda}$

$$= (\vec{k}_d - \vec{k}_i)\bullet\vec{r} = \Delta\vec{k}\bullet\vec{r}$$

- $F(\Delta\vec{k}) = \int_{\text{all } \vec{r}} f(\vec{r}) e^{i\Delta\vec{k}\bullet\vec{r}} d\vec{r}$



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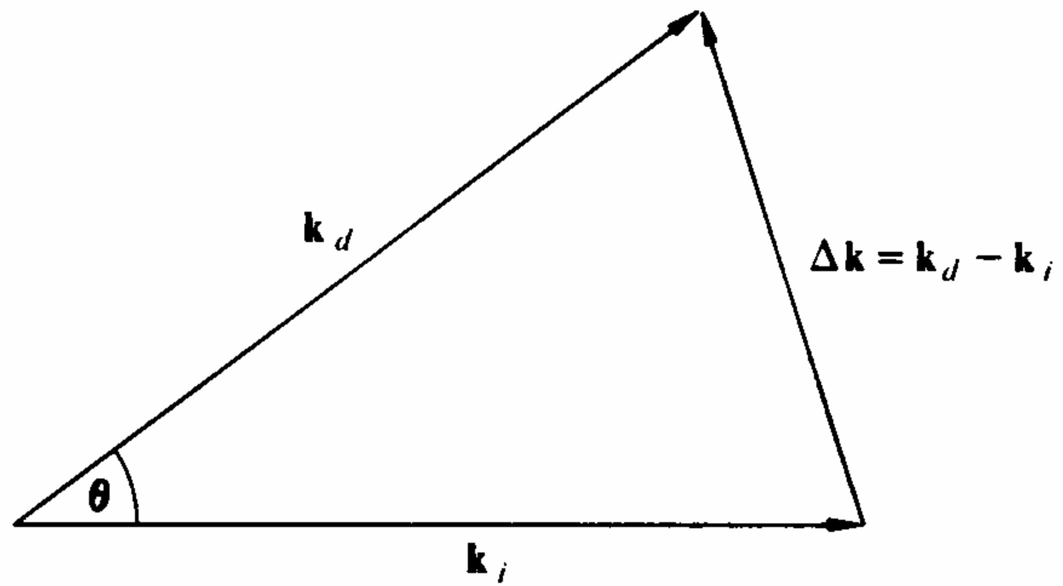
Diffraction by 3-D Lattice

- non-normal incident waves

$\Delta\vec{k} = \vec{k}_d - \vec{k}_i$: scattering vector

θ : scattering angle



Diffraction by 3-D Lattice

- diffraction pattern of finite 3-D lattice

$$F(\Delta\vec{k}) = \int_{\text{all } \vec{r}} f(\vec{r}) e^{i\Delta\vec{k}\cdot\vec{r}} d\vec{r}$$

- for a lattice, unit vectors $\vec{a},\ \vec{b},\ \vec{c}$

lattice point $\vec{r} = p\vec{a} + q\vec{b} + r\vec{c}$

amplitude function $f(\vec{r}) = \sum_{all\ p,\ q,\ r} \delta(\vec{r} - [p\vec{a} + q\vec{b} + r\vec{c}])$

- $F(\Delta\vec{k}) = \int_{all\ \vec{r}} \sum_{all\ p,\ q,\ r} \delta(\vec{r} - [p\vec{a} + q\vec{b} + r\vec{c}]) e^{i\Delta\vec{k}\cdot\vec{r}} d\vec{r}$

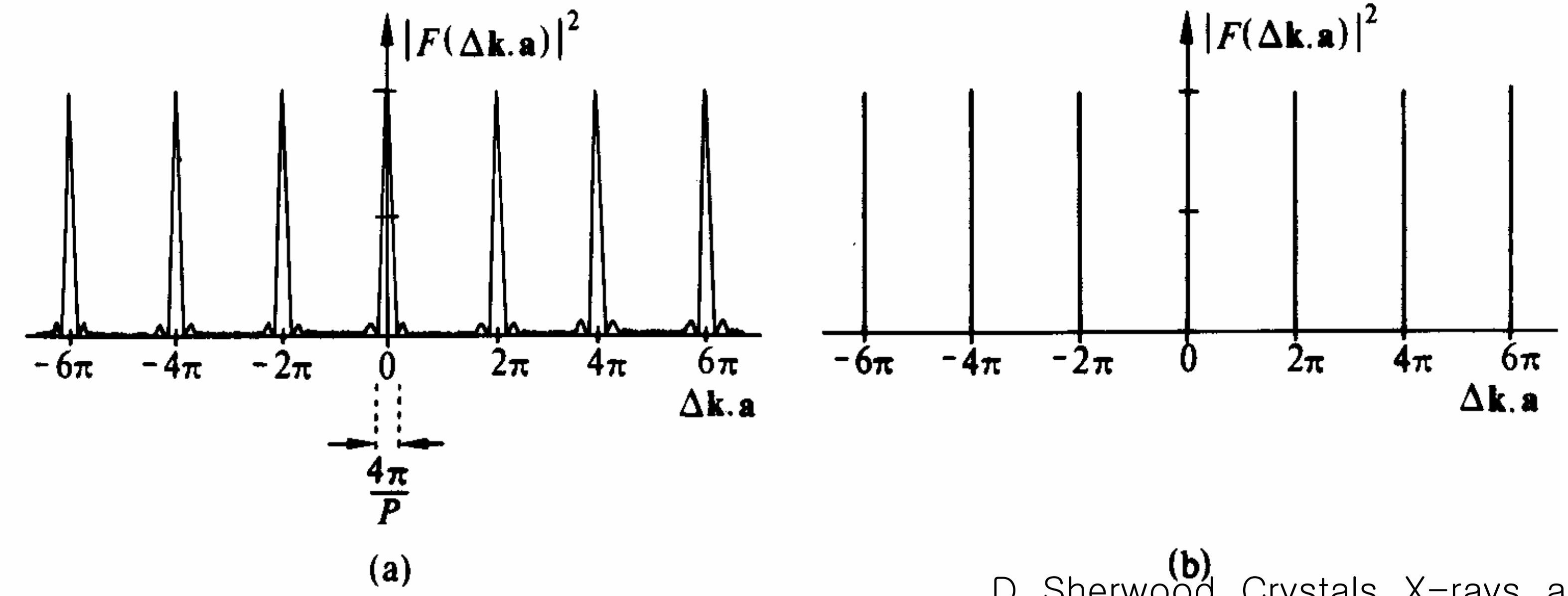
$$= \sum_{all\ p,\ q,\ r} e^{i\Delta\vec{k}\cdot(p\vec{a}+q\vec{b}+r\vec{c})}$$

$$= \sum_{all\ p} e^{i\Delta\vec{k}\cdot p\vec{a}} \sum_{all\ q} e^{i\Delta\vec{k}\cdot q\vec{b}} \sum_{all\ r} e^{i\Delta\vec{k}\cdot r\vec{c}}$$

Diffraction by 3-D Lattice

- $F(\Delta\vec{k}) = \sum_{all\ p} e^{i\Delta\vec{k}\bullet p\vec{a}} \sum_{all\ q} e^{i\Delta\vec{k}\bullet q\vec{b}} \sum_{all\ r} e^{i\Delta\vec{k}\bullet r\vec{c}}$

- $\left|F(\Delta\vec{k})\right|^2 = \dfrac{\sin^2 \dfrac{P\Delta\vec{k}\bullet\vec{a}}{2}}{\sin^2 \dfrac{\Delta\vec{k}\bullet\vec{a}}{2}} \dfrac{\sin^2 \dfrac{Q\Delta\vec{k}\bullet\vec{a}}{2}}{\sin^2 \dfrac{\Delta\vec{k}\bullet\vec{a}}{2}} \dfrac{\sin^2 \dfrac{R\Delta\vec{k}\bullet\vec{a}}{2}}{\sin^2 \dfrac{\Delta\vec{k}\bullet\vec{a}}{2}}$



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Diffraction by 3-D Lattice

- $$\left|F(\Delta\vec{k})\right|^2 = \frac{\sin^2\frac{P\Delta\vec{k}\bullet\vec{a}}{2}}{\sin^2\frac{\Delta\vec{k}\bullet\vec{a}}{2}}\frac{\sin^2\frac{Q\Delta\vec{k}\bullet\vec{a}}{2}}{\sin^2\frac{\Delta\vec{k}\bullet\vec{a}}{2}}\frac{\sin^2\frac{R\Delta\vec{k}\bullet\vec{a}}{2}}{\sin^2\frac{\Delta\vec{k}\bullet\vec{a}}{2}}$$

- first term, maximum at $\frac{\Delta\vec{k}\bullet\vec{a}}{2} = 0,\ \pi, 2\pi,\ \cdots$

  $\rightarrow \Delta\vec{k}\bullet\vec{a} = h2\pi$ (h: integer)

- first term, zero at $\frac{P\Delta\vec{k}\bullet\vec{a}}{2} = \pm\pi$

  $\rightarrow$ peak width $\Delta(\Delta\vec{k}\bullet\vec{a}) = \frac{4\pi}{P}$

- $P \rightarrow \infty$, peak becomes narrower $\rightarrow \delta$ function

Diffraction by 3-D Lattice

- infinite crystal

$$\frac{\sin^2 \frac{P\Delta\vec{k}\bullet\vec{a}}{2}}{\sin^2 \frac{\Delta\vec{k}\bullet\vec{a}}{2}} \rightarrow \left[\sum_{all\ h} \delta(\Delta\vec{k}\bullet\vec{a} - 2h\pi)\right]^2$$

- $$\left|F(\Delta\vec{k})\right|^2 = \left[\sum_{all\ h} \delta(\Delta\vec{k}\bullet\vec{a} - 2h\pi)\right]^2 \left[\sum_{all\ k} \delta(\Delta\vec{k}\bullet\vec{b} - 2k\pi)\right]^2 \times \left[\sum_{all\ l} \delta(\Delta\vec{k}\bullet\vec{c} - 2l\pi)\right]^2$$

- real lattice vs. reciprocal lattice

Diffraction by 3-D Lattice

- $\sum_{all\ h} \delta(\Delta\vec{k}\bullet\vec{a} - 2h\pi) \rightarrow \sum_{all\ n} \delta(\vec{r}\bullet\vec{x} - nx_0)$ $\quad \vec{x}$: unit vector

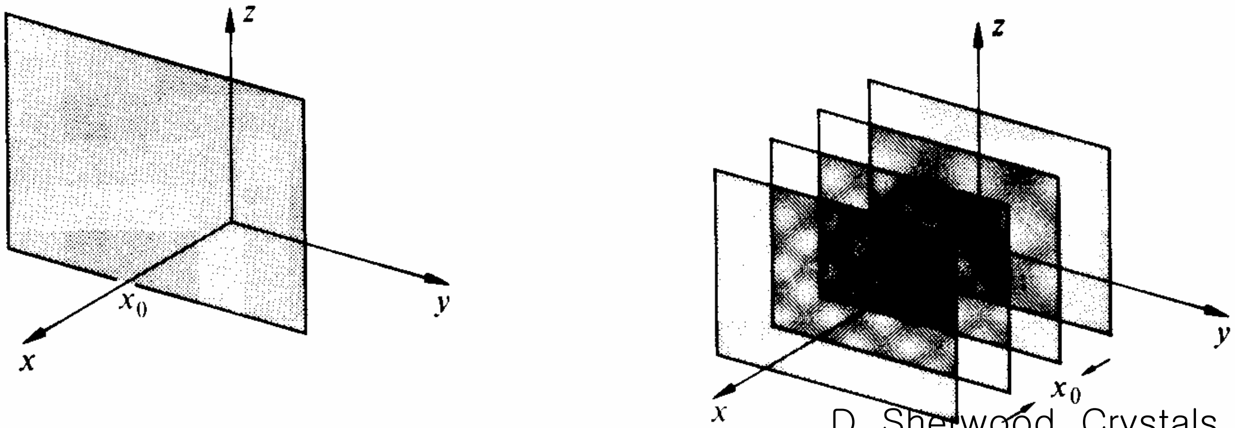
- $\delta(\vec{r} - \vec{r_0})$ refers to the point located at $\vec{r} = \vec{r_0}$

- what does $\delta(\vec{r}\bullet\vec{x} - x_0)$ represent?

  finite only when $\vec{r}\bullet\vec{x} = x_0 \rightarrow$ projection of $\vec{r}$ along $\vec{x}$ is constant

  equal to $x_0 \Rightarrow$ plane

  a stack of planes, all parallel to *yz* plane, separated by x_0



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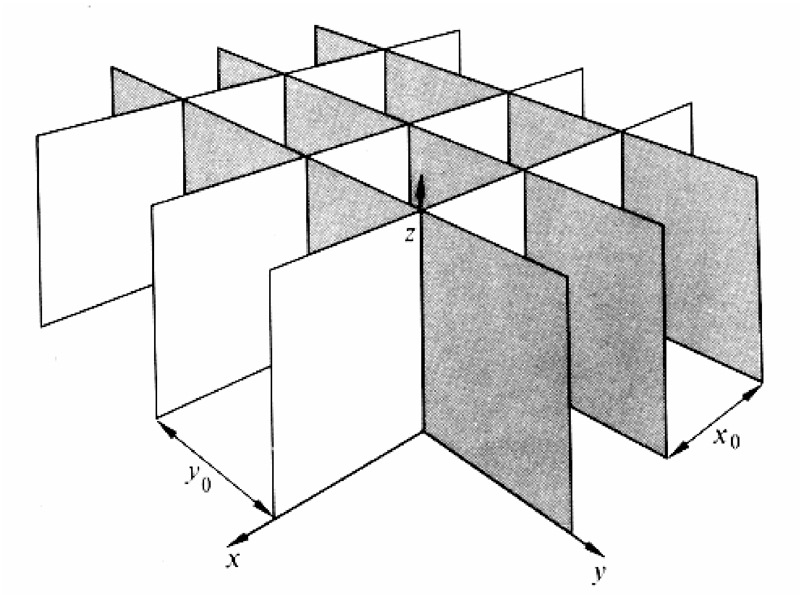
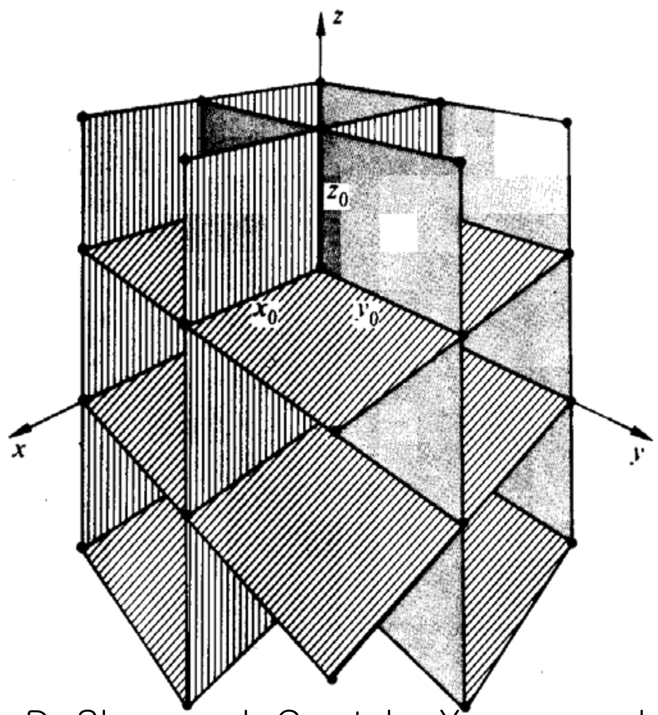
Diffraction by 3-D Lattice

- $\sum_{all\ n} \delta(\vec{r} \bullet \vec{x} - nx_0) \rightarrow$ plane, $\quad \sum_{all\ m} \delta(\vec{r} \bullet \vec{y} - my_0) \rightarrow$ plane
- $\sum_{all\ n} \delta(\vec{r} \bullet \vec{x} - nx_0) \sum_{all\ m} \delta(\vec{r} \bullet \vec{y} - my_0) \rightarrow$ line
- $\sum_{all\ n} \delta(\vec{r} \bullet \vec{x} - nx_0) \sum_{all\ m} \delta(\vec{r} \bullet \vec{y} - my_0) \sum_{all\ s} \delta(\vec{r} \bullet \vec{z} - sz_0) \rightarrow$ point





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Diffraction by 3-D Lattice

- $\sum_{all\ h} \delta(\Delta\vec{k} \bullet \vec{a} - 2h\pi)$: a set of planes in $\Delta\vec{k}$ space, perpendicular

  to the direction defined by $\vec{a}$ and separated by a distance $2\pi/a$

- $$\left|F(\Delta\vec{k})\right|^2 = \left[\sum_{all\ h} \delta(\Delta\vec{k} \bullet \vec{a} - 2h\pi)\right]^2 \left[\sum_{all\ k} \delta(\Delta\vec{k} \bullet \vec{b} - 2k\pi)\right]^2 \times \left[\sum_{all\ l} \delta(\Delta\vec{k} \bullet \vec{c} - 2l\pi)\right]^2$$

  three sets of planes $\rightarrow$ define space lattice

  reciprocal lattice

Laue Equations

- $\Delta\vec{k}\bullet\vec{a} = 2h\pi, \quad \Delta\vec{k}\bullet\vec{b} = 2k\pi, \quad \Delta\vec{k}\bullet\vec{c} = 2l\pi$
- what we seek is that value or those values, of the scattering vector $\Delta\vec{k}$ which satisfy all three equations simultaneously.
- $\Delta\vec{k} = \vec{k}_d - \vec{k}_i$
- real space $\vec{r} = p\vec{a} + q\vec{b} + r\vec{c}$

  Fourier space (reciprocal space) $\Delta\vec{k} = \chi(\mathrm{h}\vec{a}^* + \mathrm{k}\vec{b}^* + \mathrm{l}\vec{c}^*)$
- $\Delta\vec{k}\bullet\vec{a} = \chi(\mathrm{h}\vec{a}^* + \mathrm{k}\vec{b}^* + \mathrm{l}\vec{c}^*)\bullet\vec{a} = 2h\pi$

$$\chi\mathrm{h}\vec{a}^*\bullet\vec{a} + \chi\mathrm{k}\vec{b}^*\bullet\vec{a} + \chi\mathrm{l}\vec{c}^*\bullet\vec{a} = 2h\pi$$

$$\chi\mathrm{h}\vec{a}^*\bullet\vec{b} + \chi\mathrm{k}\vec{b}^*\bullet\vec{b} + \chi\mathrm{l}\vec{c}^*\bullet\vec{b} = 2k\pi$$

$$\chi\mathrm{h}\vec{a}^*\bullet\vec{c} + \chi\mathrm{k}\vec{b}^*\bullet\vec{c} + \chi\mathrm{l}\vec{c}^*\bullet\vec{c} = 2l\pi$$

Laue Equations

- $\chi = 2\pi$
- $h\vec{a}^* \bullet \vec{a} + k\vec{b}^* \bullet \vec{a} + l\vec{c}^* \bullet \vec{a} = h$

  $h\vec{a}^* \bullet \vec{b} + k\vec{b}^* \bullet \vec{b} + l\vec{c}^* \bullet \vec{b} = k$

  $h\vec{a}^* \bullet \vec{c} + k\vec{b}^* \bullet \vec{c} + l\vec{c}^* \bullet \vec{c} = l$
- $\vec{a}^* \bullet \vec{a} = 1 \quad \vec{b}^* \bullet \vec{a} = 0 \quad \vec{c}^* \bullet \vec{a} = 0 \Rightarrow \vec{a}^*$ perpendicular to $\vec{b}$ & $\vec{c}$

  $\vec{a}^* \bullet \vec{b} = 0 \quad \vec{b}^* \bullet \vec{b} = 1 \quad \vec{c}^* \bullet \vec{b} = 0 \qquad \vec{a}^* = \xi \vec{b} \times \vec{c}$

  $\vec{a}^* \bullet \vec{c} = 0 \quad \vec{b}^* \bullet \vec{c} = 0 \quad \vec{c}^* \bullet \vec{c} = 1 \qquad \vec{a} \bullet \vec{a}^* = \xi \vec{a} \bullet \vec{b} \times \vec{c} = 1$

- h=h, k=k, l=l

$$\vec{a}^* = \frac{\vec{b} \times \vec{c}}{\vec{a} \bullet \vec{b} \times \vec{c}}$$

- $\Delta\vec{k} = 2\pi(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)$

Laue Equations

- $\vec{a}^* = \dfrac{\vec{b}\times\vec{c}}{\vec{a}\bullet\vec{b}\times\vec{c}}, \quad \vec{b}^* = \dfrac{\vec{c}\times\vec{a}}{\vec{a}\bullet\vec{b}\times\vec{c}}, \quad \vec{c}^* = \dfrac{\vec{a}\times\vec{b}}{\vec{a}\bullet\vec{b}\times\vec{c}}$
- $\Delta\vec{\mathrm{k}} = 2\pi(h\vec{a}^* + k\vec{b}^* + l\vec{c}^*)$

$$\vec{\mathrm{G}} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

$$\Delta\vec{\mathrm{k}} = 2\pi\vec{\mathrm{G}}$$

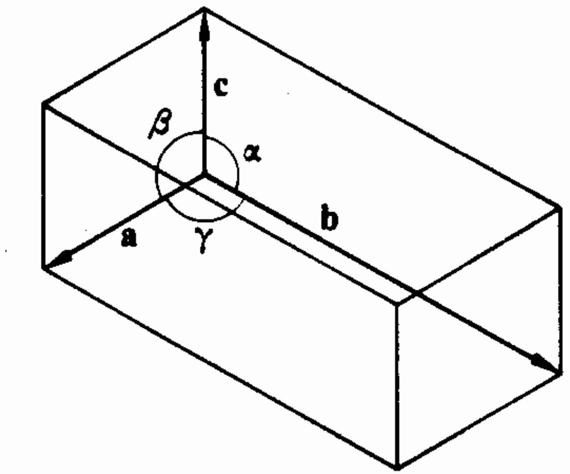
Reciprocal Lattice

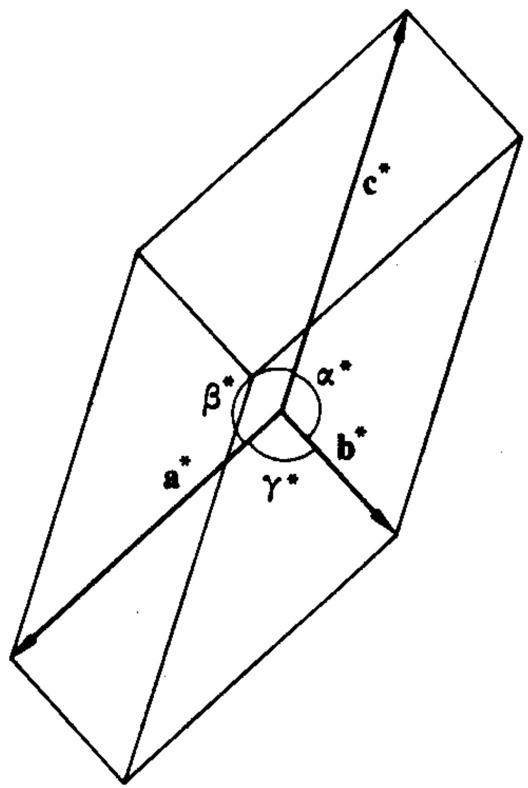
- real lattice is primitive

  direction

  length

  angle





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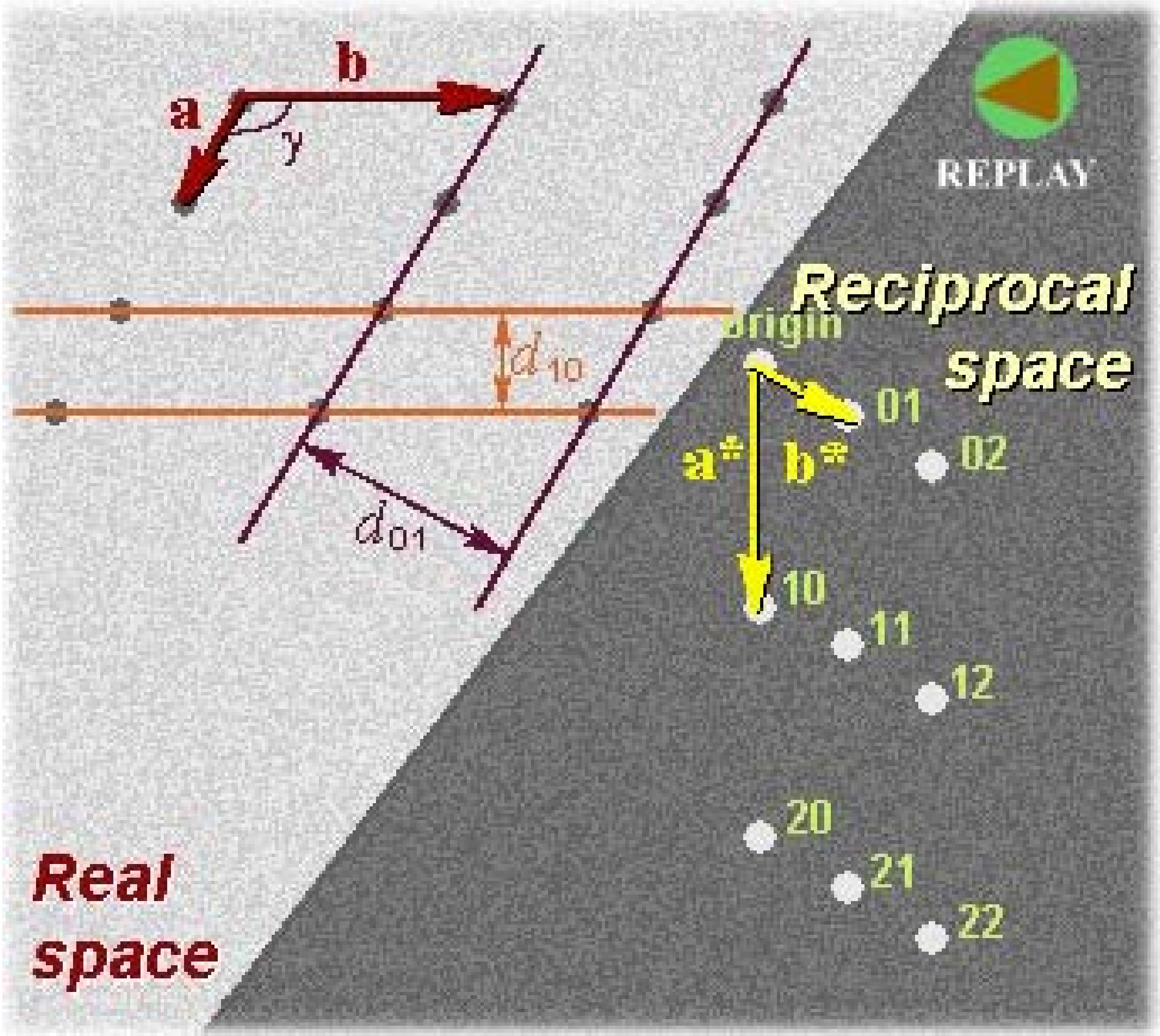


http://www.matter.org.uk/diffraction/geometry/2D_reciprocal_lattices.htm

Reciprocal Lattice

- monoclinic P $a \neq b \neq c \quad \alpha = \gamma = 90^o \neq \beta$

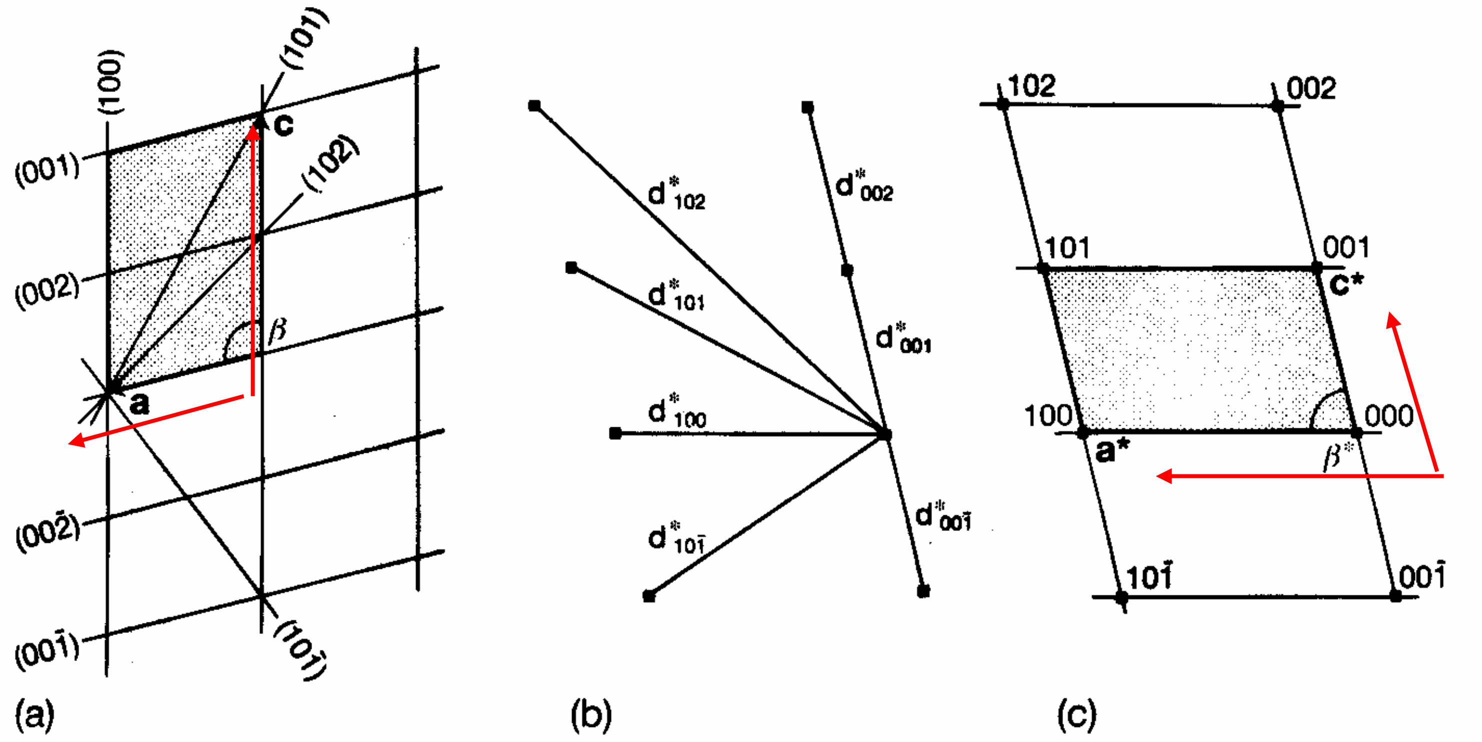
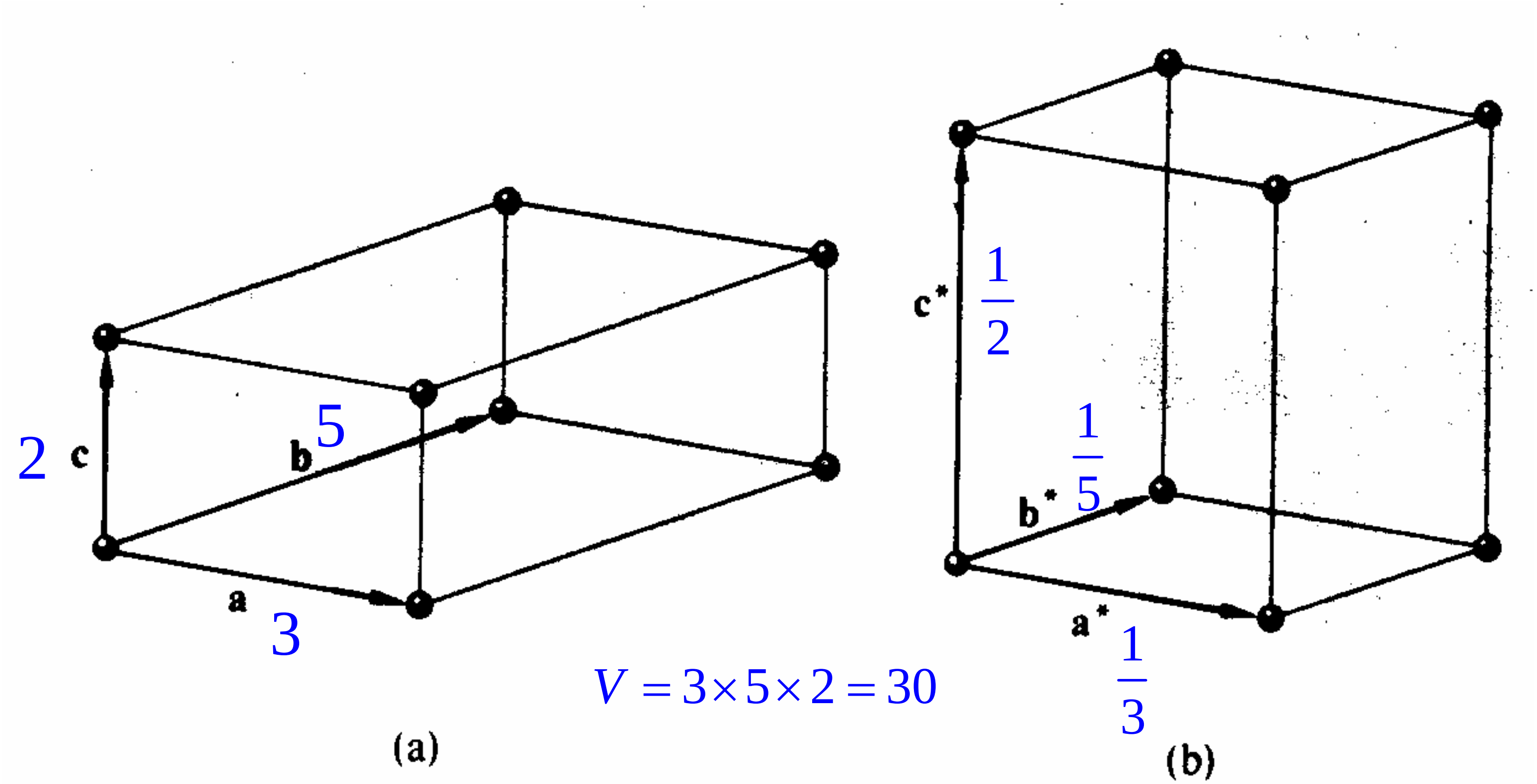


Fig. 6.2. (a) Plan of a monoclinic *P* unit cell perpendicular to the *y*-axis with the unit cell shaded. The traces of some planes of type $\{h0l\}$ (i.e. parallel to the *y*-axis) are indicated, (b) the reciprocal (lattice) vectors, $\mathbf{d}^*_{hkl}$ for these planes and (c) the reciprocal lattice defined by these vectors. Each reciprocal lattice point is labelled with the indices of the plane it represents and the unit cell is shaded. The angle β^* is the complement of β.

Reciprocal Lattice

- primitive orthorhombic lattice



$$V = 3 \times 5 \times 2 = 30$$

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Reciprocal Lattice

- real lattice- non-primitive

  if we use the conventional crystallographic base vectors,

  the reciprocal lattice so generated is not complete

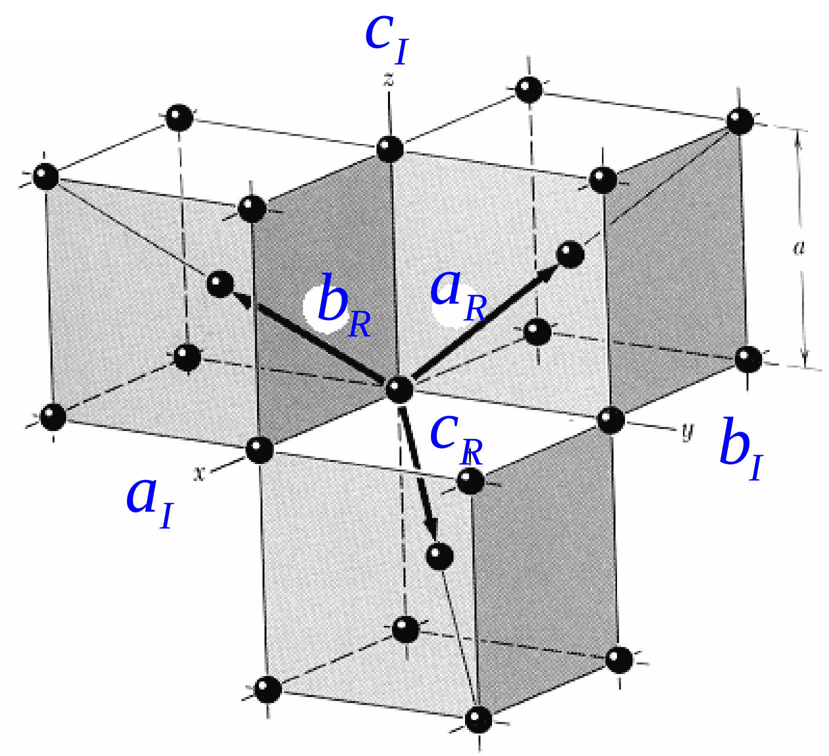
  as we have not taken into account those lattice sites

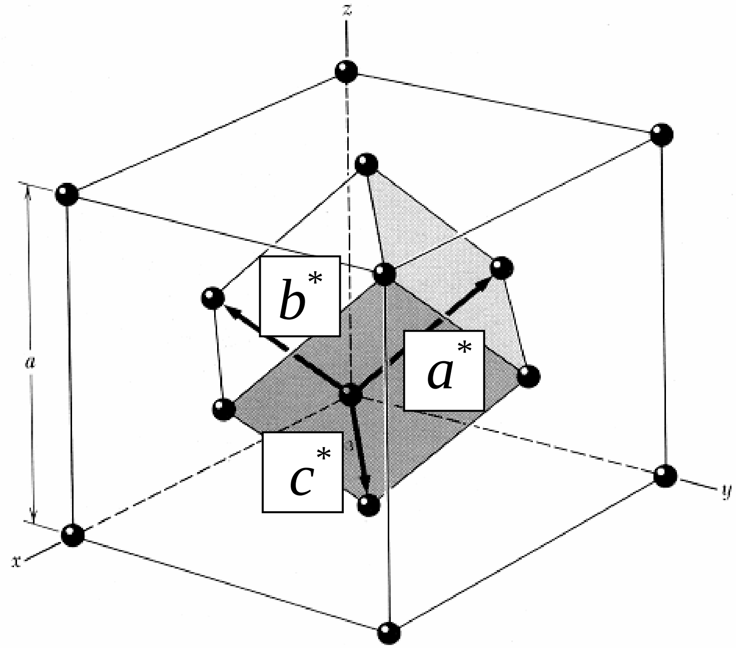
  at fractional distance within the unit cell

- choose three vectors which are compatible with given

  real lattice but which define a primitive unit cell

Reciprocal Lattice





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

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

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

$$a^* = \frac{2\pi}{a}(\vec{y}+\vec{z})$$

$$b^* = \frac{2\pi}{a}(\vec{z}+\vec{x})$$

$$c^* = \frac{2\pi}{a}(\vec{x}+\vec{y})$$

C. Kittel, Introduction to Solid State Physics

Reciprocal Lattice

- cubic I $\quad a = b = c$

$$\alpha = \beta = \gamma = 90^o$$

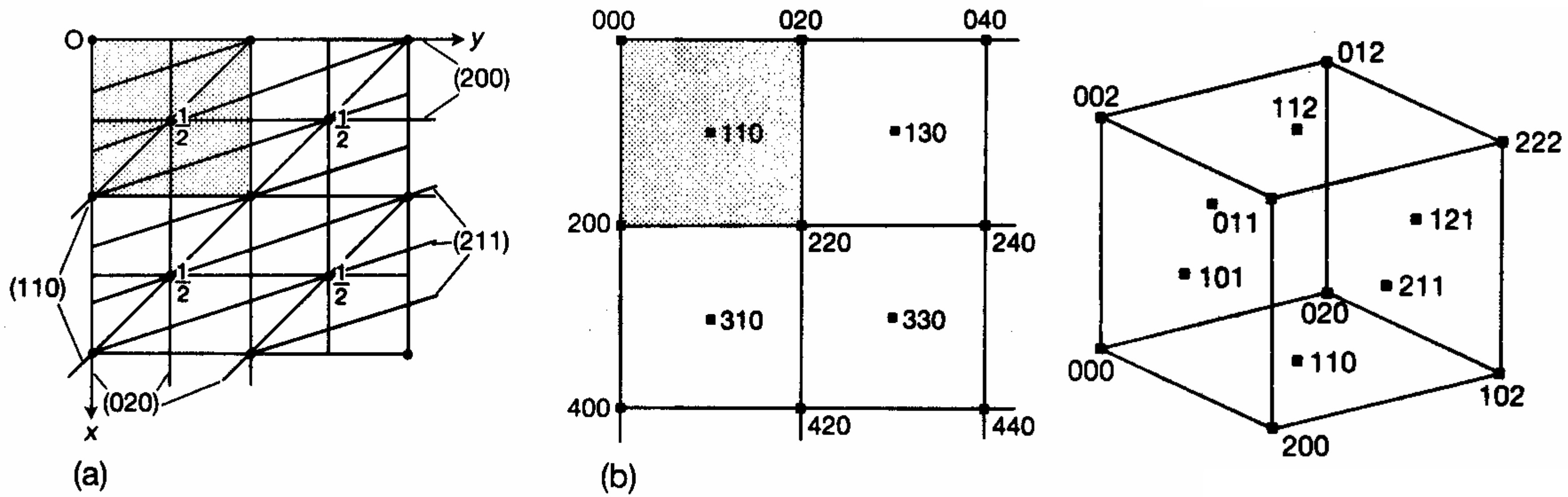


Fig. 6.4. (a) Plan of a cubic *I* crystal perpendicular to the *z*-axis and (b) pattern of reciprocal lattice points perpendicular to the *z*-axis. Note the cubic *F* arrangement of reciprocal lattice points in this plane.

Reciprocal Lattice Direction vs. Real Lattice Plane

- Theorem 1

The reciprocal lattice vector

$$\vec{G}_{hkl} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

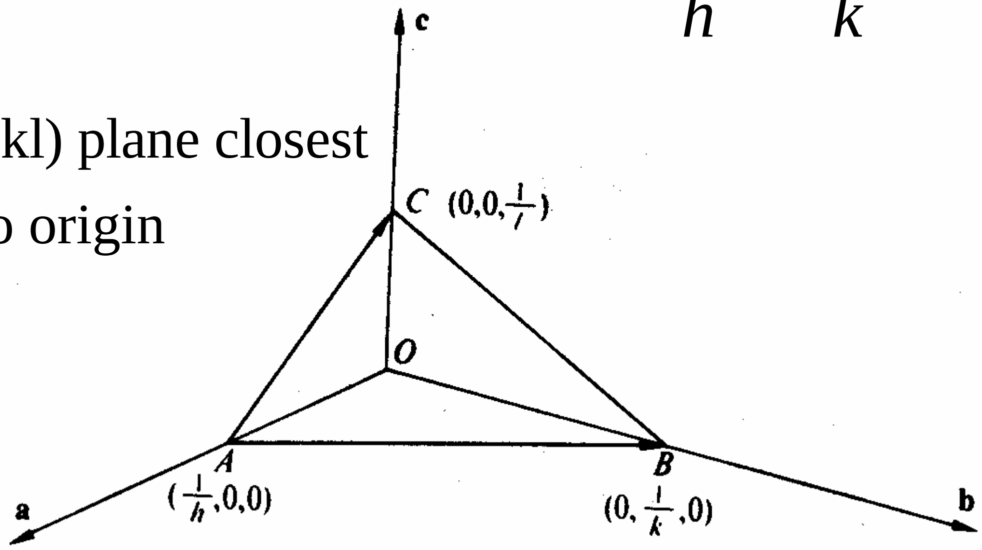
is perpendicular to the (*hkl*) set of planes in real lattice.

- proof $\overrightarrow{AB} = (-\frac{1}{h}, \frac{1}{k}, 0)$ $\quad \vec{G}_{\alpha\beta\gamma} = \alpha\vec{a}^* + \beta\vec{b}^* + \gamma\vec{c}^*$

$$\overrightarrow{AB} \bullet \vec{G}_{\alpha\beta\gamma} = (-\frac{1}{h}\vec{a} + \frac{1}{k}\vec{b}) \bullet (\alpha\vec{a}^* + \beta\vec{b}^* + \gamma\vec{c}^*) = -\frac{\alpha}{h} + \frac{\beta}{k}$$

=0 if perpendicular

(hkl) plane closest to origin



$$\therefore \frac{\alpha}{h} = \frac{\beta}{k}$$

$$\overrightarrow{\mathrm{AC}} \Rightarrow \frac{\alpha}{h} = \frac{\gamma}{l}$$

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Reciprocal Lattice Direction vs. Real Lattice Plane

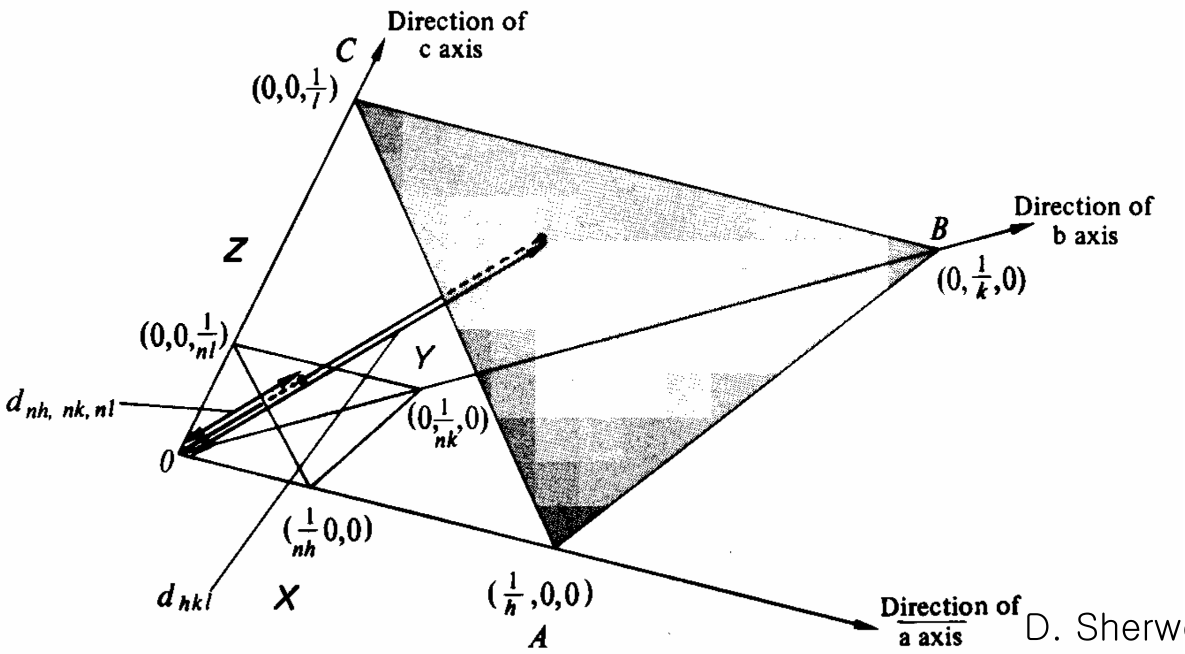
- $\vec{G}_{\alpha\beta\gamma}$ is perpendicular to (hkl) plane if $\dfrac{\alpha}{h} = \dfrac{\beta}{k} = \dfrac{\gamma}{l}$

- one solution $\alpha = h,\ \beta = k,\ \gamma = l$

- $\vec{G}_{hkl} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$ is normal to (hkl) set of planes

- another solution

$$\alpha = nh,\ \beta = nk,\ \gamma = nl \ \Rightarrow\ \vec{G}_{nhnknl} = nh\vec{a}^* + nk\vec{b}^* + nl\vec{c}^*$$



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Reciprocal Lattice Direction vs. Real Lattice Plane

- Theorem 2

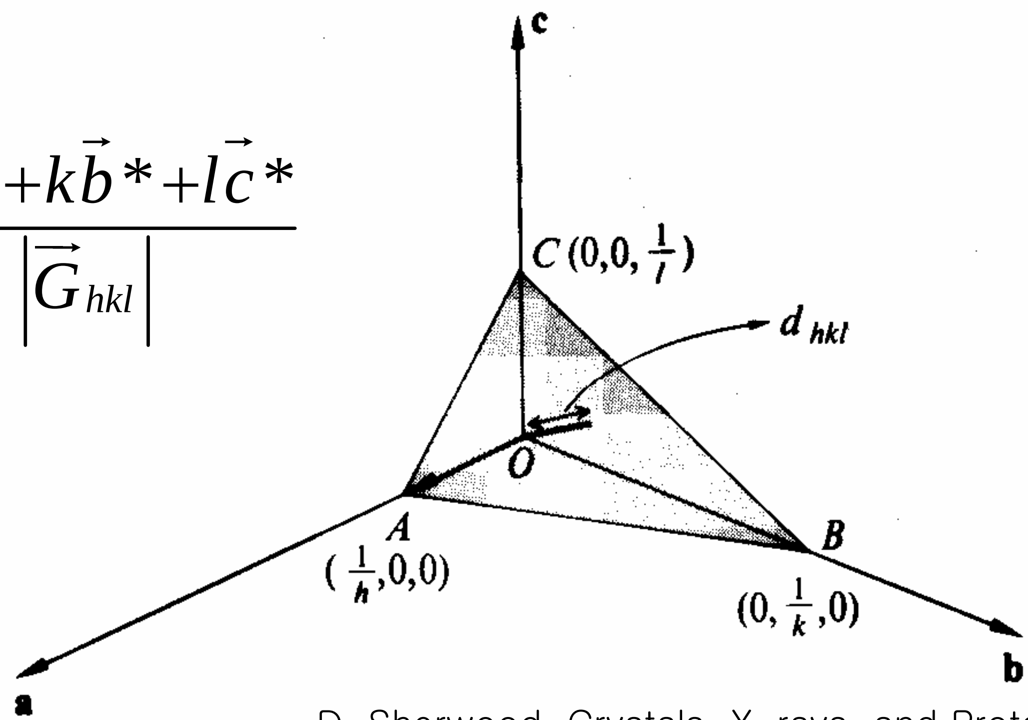
The magnitude G_{hkl} of the reciprocal vector $\vec{G}_{hkl}$ is related to the spacing d_{hkl} between the (hkl) set of planes by

$$G_{hkl} = \frac{1}{d_{hkl}}$$

- proof

$$d_{hkl} = \frac{\vec{a}}{h} \bullet \frac{\vec{G}_{hkl}}{\left|\vec{G}_{hkl}\right|} = \frac{\vec{a}}{h} \bullet \frac{h\vec{a}^* + k\vec{b}^* + l\vec{c}^*}{\left|\vec{G}_{hkl}\right|}$$

$$= \frac{1}{\left|\vec{G}_{hkl}\right|}$$



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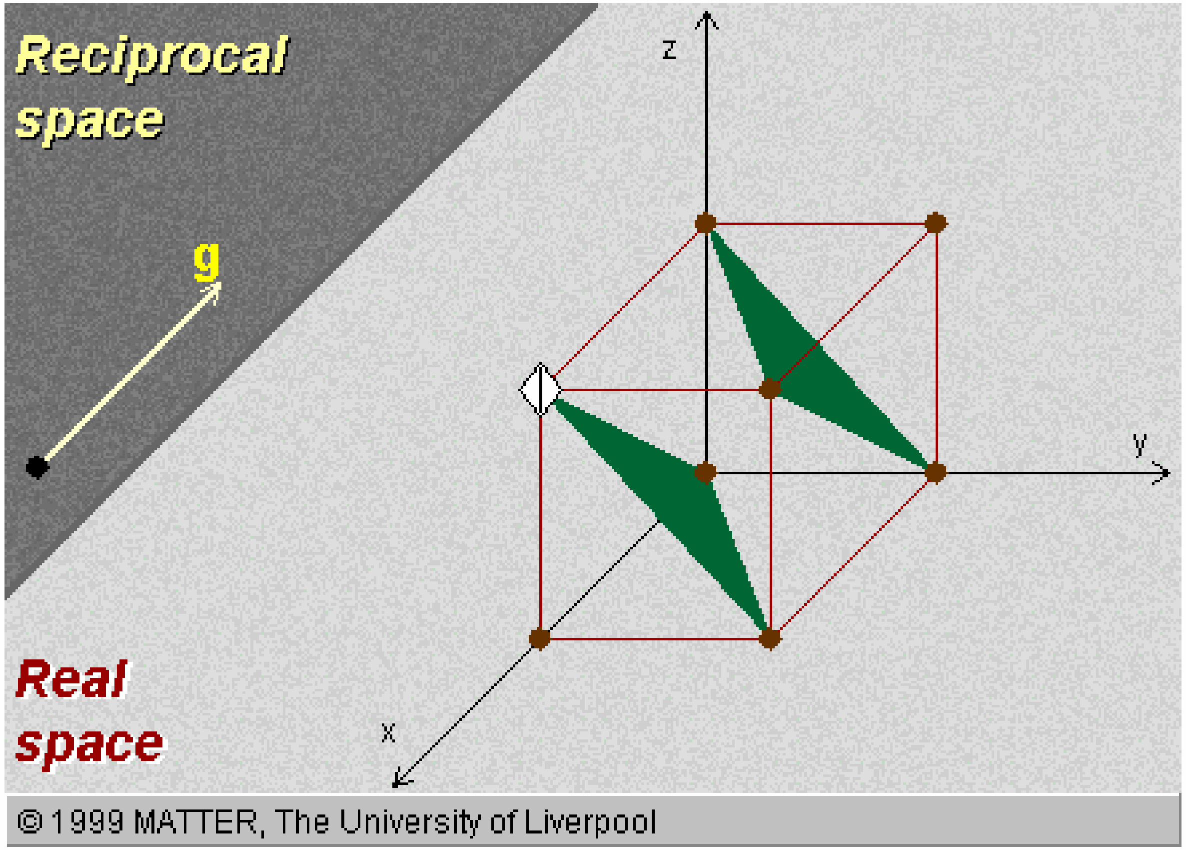


http://www.matter.org.uk/diffraction/geometry

Bragg's Law

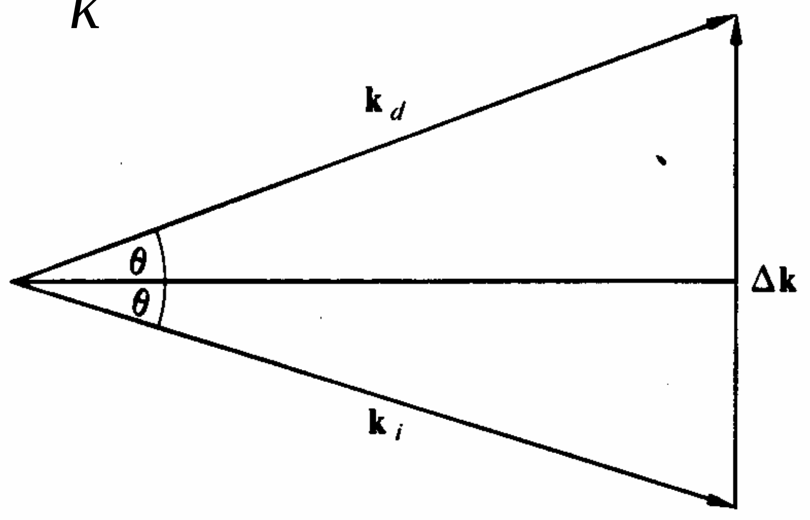
- $\Delta\vec{k} = \vec{k}_d - \vec{k}_i$

$$\left|\Delta\vec{k}\right| = 2k\sin\theta, \qquad k = \frac{2\pi}{\lambda}$$

$$\left|\Delta\vec{k}\right| = 2\pi\left|\vec{G}_{hkl}\right| = \frac{2\pi}{d_{hkl}}$$

$$\Rightarrow 2k\sin\theta = \frac{2\pi}{d_{hkl}} \Rightarrow 2d_{hkl}\sin\theta = \frac{2\pi}{k} = \lambda$$

- Bragg's law



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e.g. X-rays with wavelength 1.54Å are reflected from planes with d=1.2Å. Calculate the Bragg angle, θ, for constructive interference.

$\lambda = 1.54 \times 10^{-10}$ m, $d = 1.2 \times 10^{-10}$ m, $\theta = ?$

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

$$\theta = \sin^{-1}\left(\frac{n\lambda}{2d}\right)$$

n=1 : $\theta = 39.9°$

n=2 : X (nλ/2d)>1

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

We normally set n=1 and adjust Miller indices, to give

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

Example of equivalence of the two forms of Bragg's law:

Calculate θ for λ=1.54 Å, cubic crystal, **a**=5Å

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

(1 0 0) reflection, d=5 Å	(2 0 0) reflection, d=2.5 Å
n=1, $\theta=8.86^o$	
n=2, $\theta=17.93^o$	n=1, $\theta=17.93^o$
n=3, $\theta=27.52^o$	
n=4, $\theta=38.02^o$	n=2, $\theta=38.02^o$
n=5, $\theta=50.35^o$	
n=6, $\theta=67.52^o$	n=3, $\theta=67.52^o$
no reflection for $n\geq7$	no reflection for $n\geq4$

Ewald Circle

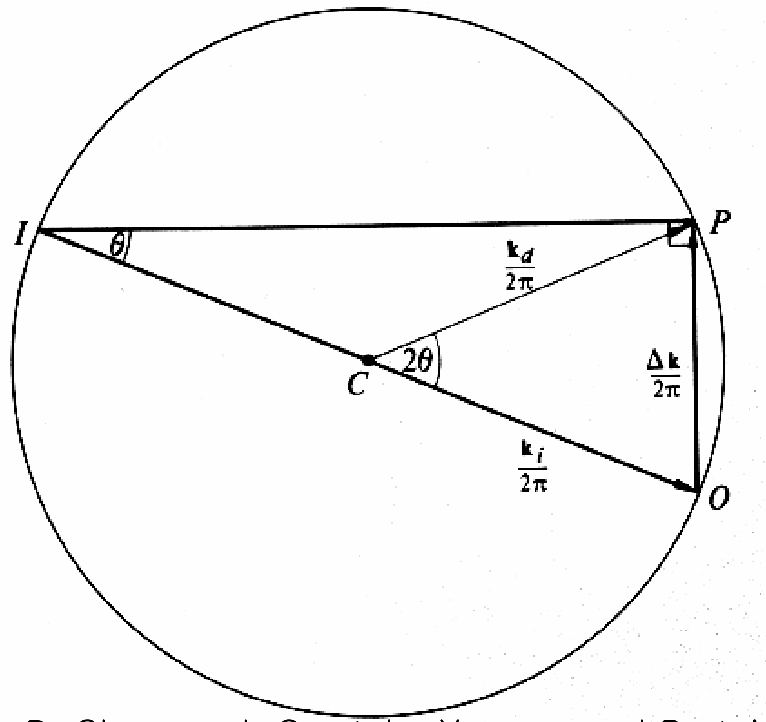
- Bragg's law $2d_{hkl} \sin\theta = \lambda$
- consider a two dimensional system

  crystal- two dimensional real lattice

  $\Rightarrow$ two dimensional reciprocal lattice
- $\vec{k}_i,\ \vec{k}_d,\ \Delta\vec{k}$ confined to a plane
- $\left|\vec{k}_i\right| = \left|\vec{k}_d\right| = \dfrac{2\pi}{\lambda}$
- $r = \dfrac{1}{\lambda}$
- $\overrightarrow{\mathrm{CO}}$: incident wave,

  $\overrightarrow{\mathrm{CP}}$: diffracted wave

  $\overrightarrow{\mathrm{OP}}$: scattering vector



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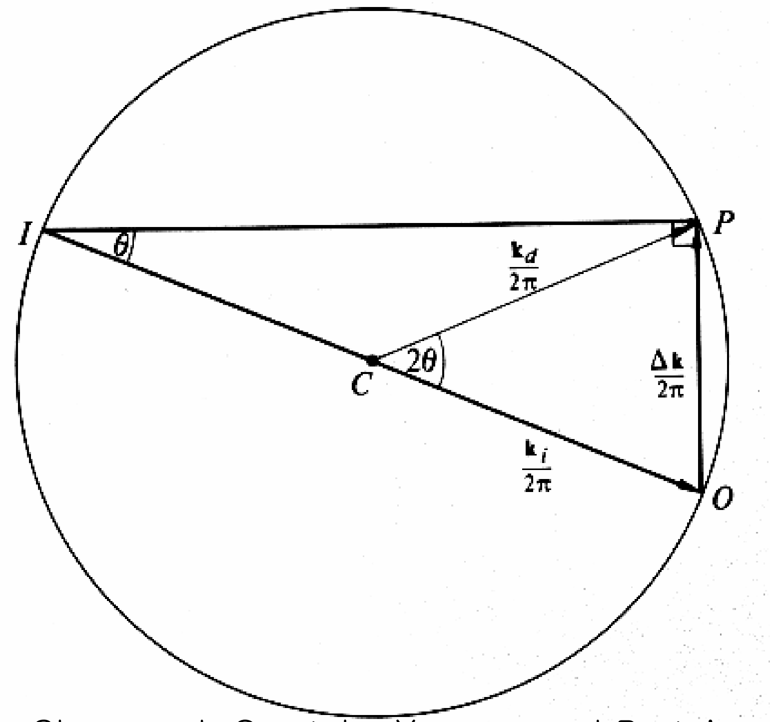
Ewald Circle

- $\overrightarrow{OP} = 2r\sin\theta = 2\dfrac{1}{\lambda}\sin\theta = \dfrac{\left|\Delta\vec{k}\right|}{2\pi}$

- $\Delta\vec{k} = 2\pi\vec{G}_{hl}$

- $\dfrac{2}{\lambda}\sin\theta = \left|\vec{G}_{hk}\right| = \dfrac{1}{d_{hk}} \Rightarrow 2d_{hk}\sin\theta = \lambda$

- Ewald circle or Reflecting circle



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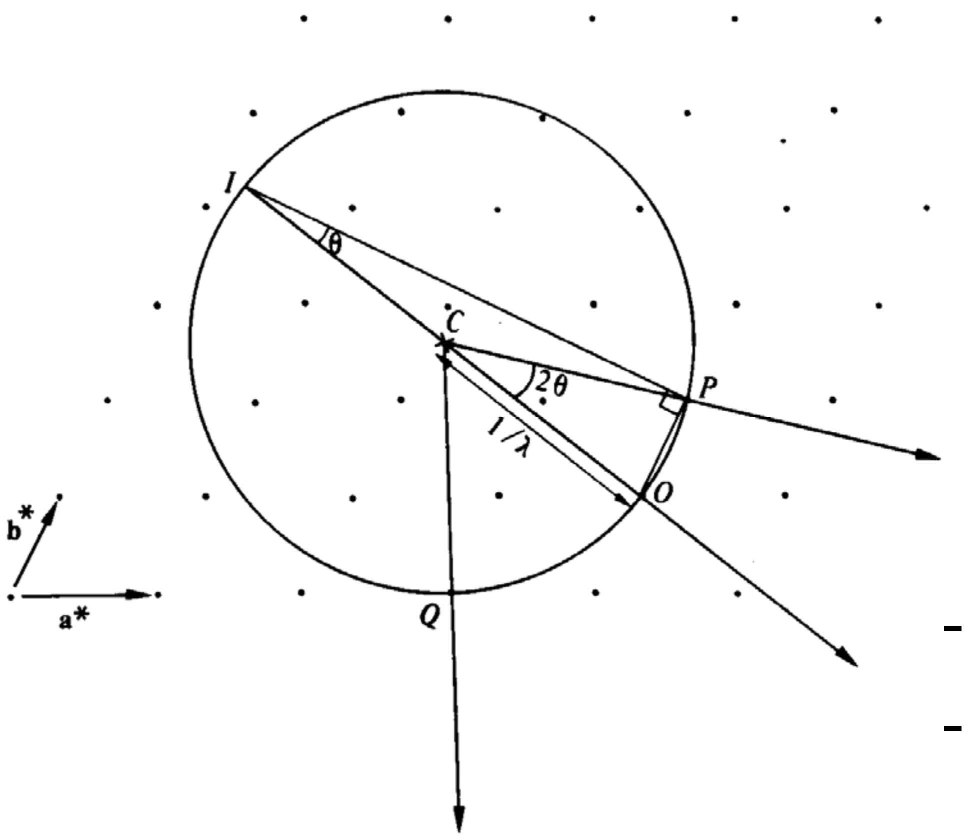
Reciprocal Lattice and Diffraction

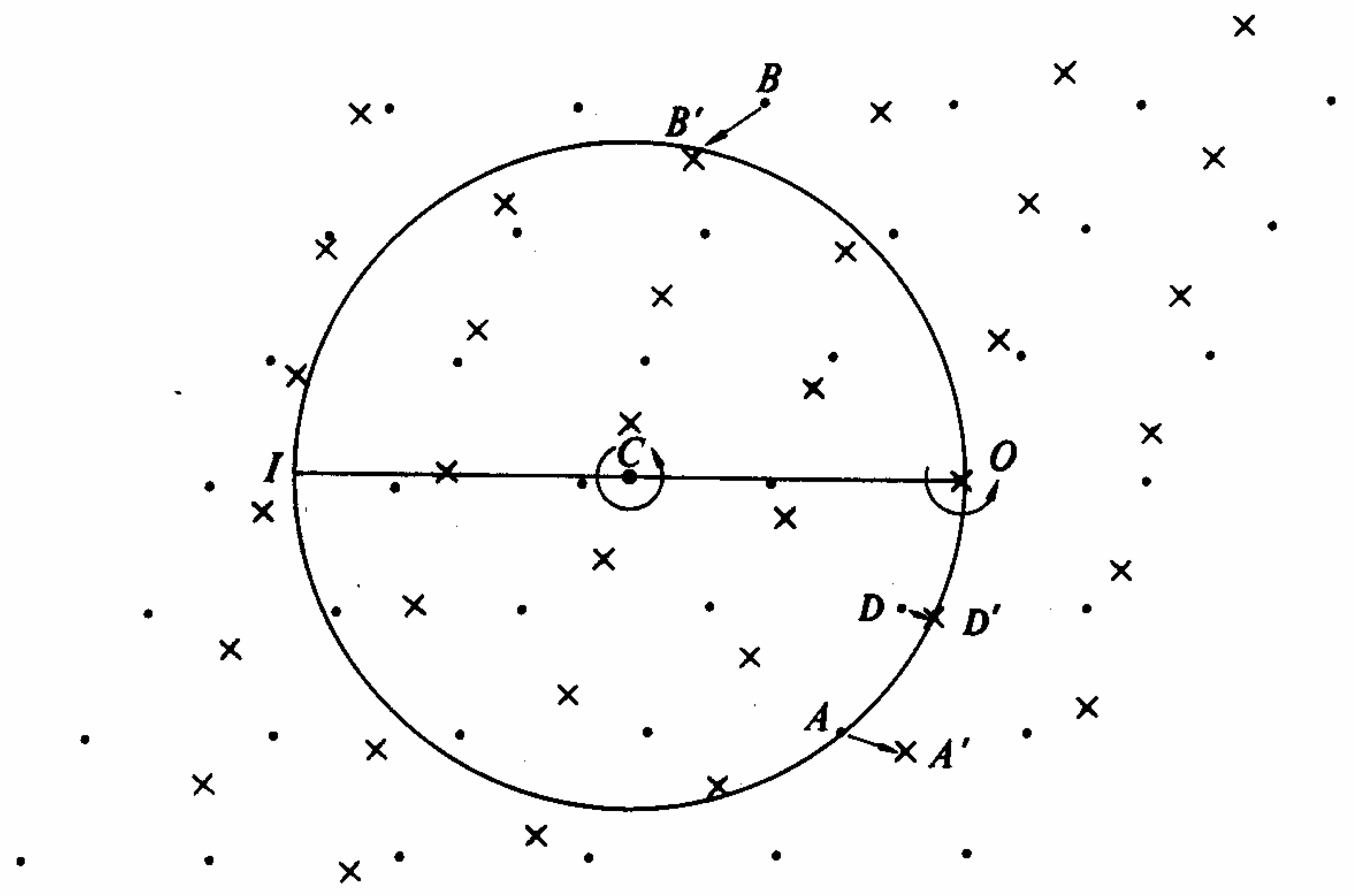
- assume the orientation of the inciddent beam w.r.t. the real lattice, and hence w.r.t. the reciprocal lattice
- O: origin of the reciprocal lattice
- superimpose the reciprocal lattice on the Ewald circle



- reciprocal lattice vector G_{hk}
- Ewald circle, Bragg condition

Reciprocal Lattice and Diffraction

- rotating crystal

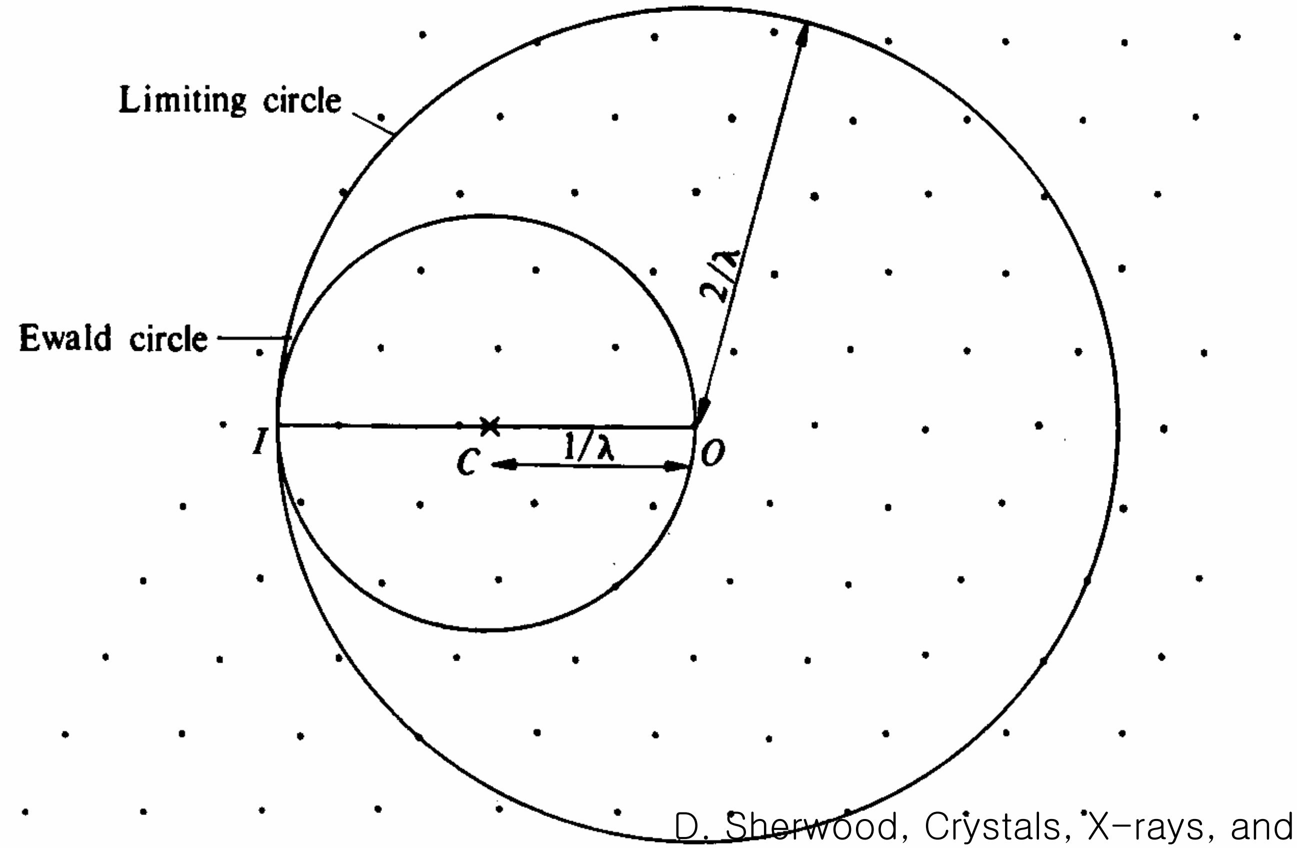


Reciprocal Lattice and Diffraction

- limiting circle

$$G_{hk} \leq 2r = \frac{2}{\lambda}$$

$$G_{hk} = \frac{2}{\lambda}\sin\theta, \quad 0 \leq \sin\theta \leq 1, \quad 0 \leq G_{hk} \leq \frac{2}{\lambda}$$



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Why X-Ray Diffraction Works

- $G_{hk} \leq \frac{2}{\lambda}$

- crystal- length of unit cell: 1 nm (10 $\mathring{A}$)
  magnitude of reciprocal lattice vector: 1 $(nm)^{-1}$

- $\lambda \leq \frac{2}{G_{hk}}, \quad \lambda \leq 2$ nm

- greatest wavelength- 2 nm (20 $\mathring{A}$)

- typical X-ray wavelength- 1 $\mathring{A}$ satisfy the inequality

Ewald Sphere

- 2D $\rightarrow 3D$

  Ewald circle $\rightarrow$ Ewald sphere

- before Ewald sphere construction

  1. direction of incident beam relative to real crystal
  2. geometric property of reciprocal lattice

- rules for Ewald sphere construction

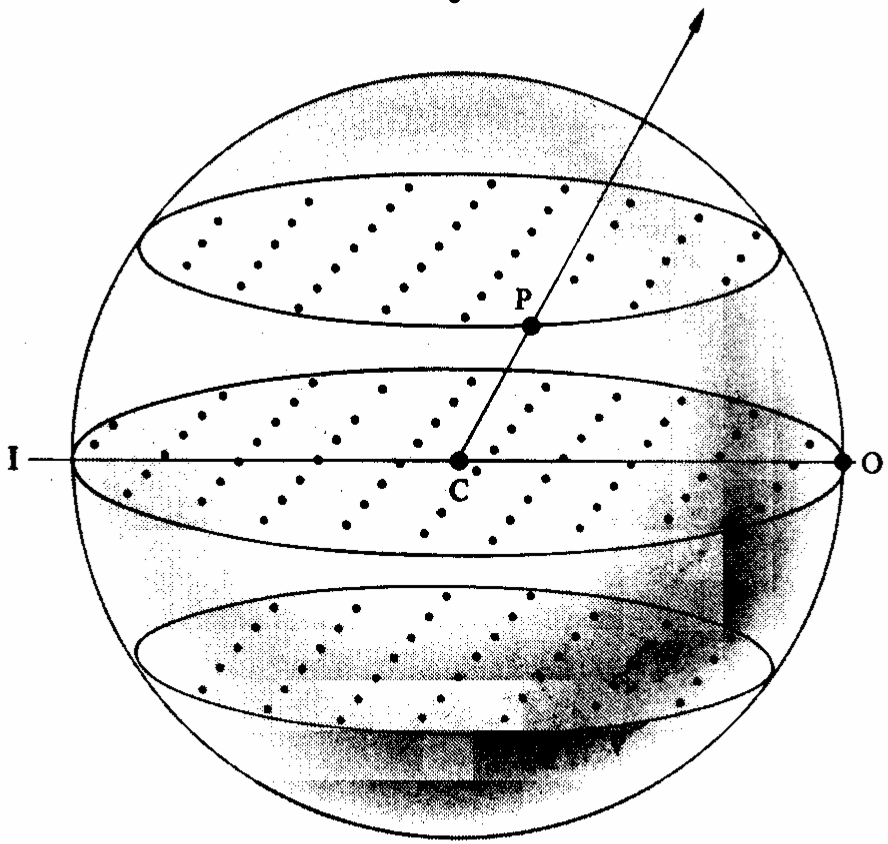
  i) draw a sphere of radius r $(=1/\lambda)$ about C (crystal)

  ii) draw a diameter ICO (incident beam direction) w.r.t. crystal

  iii) choose the origin of reciprocal lattice as point O

  iv) plot the reciprocal lattice

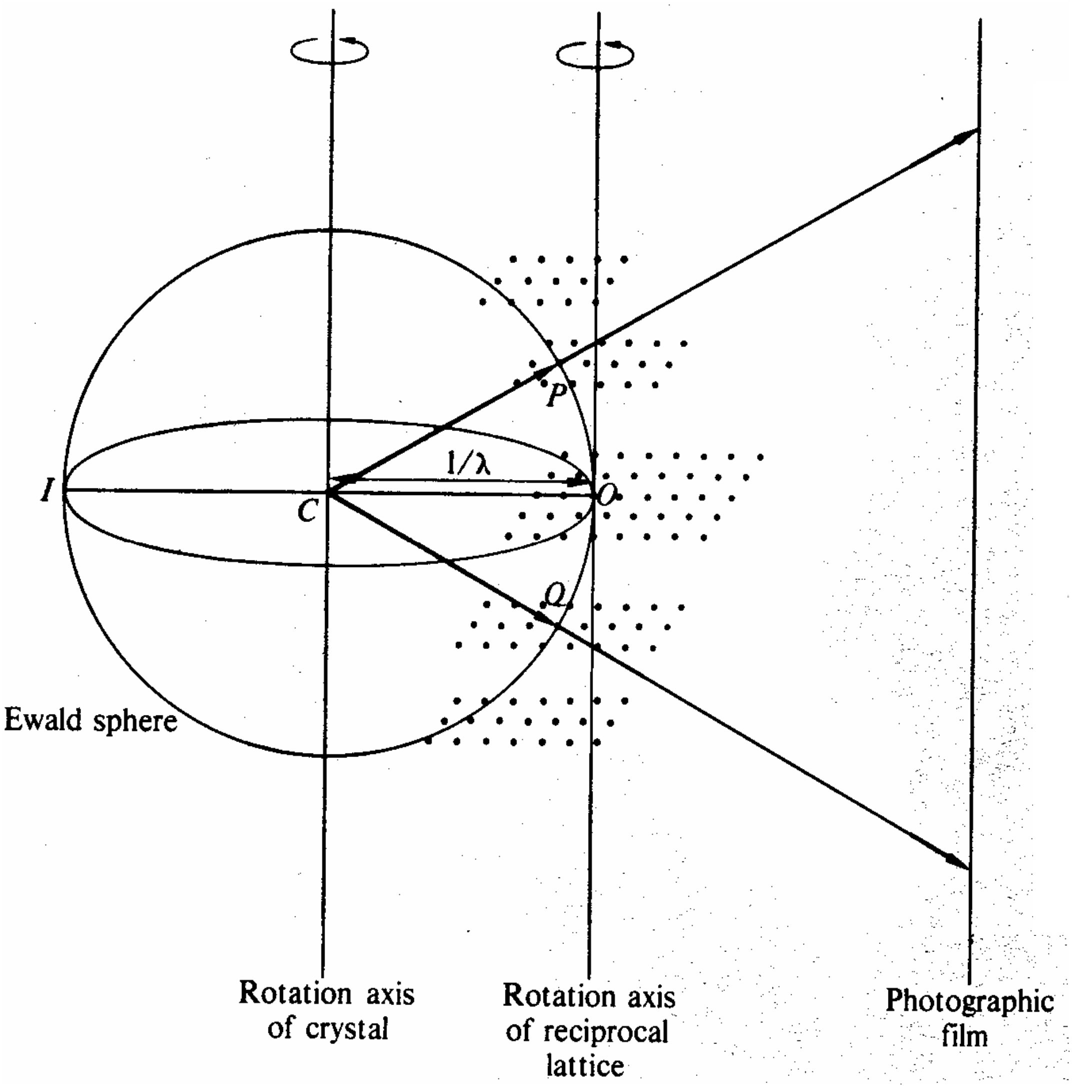
Ewald Sphere

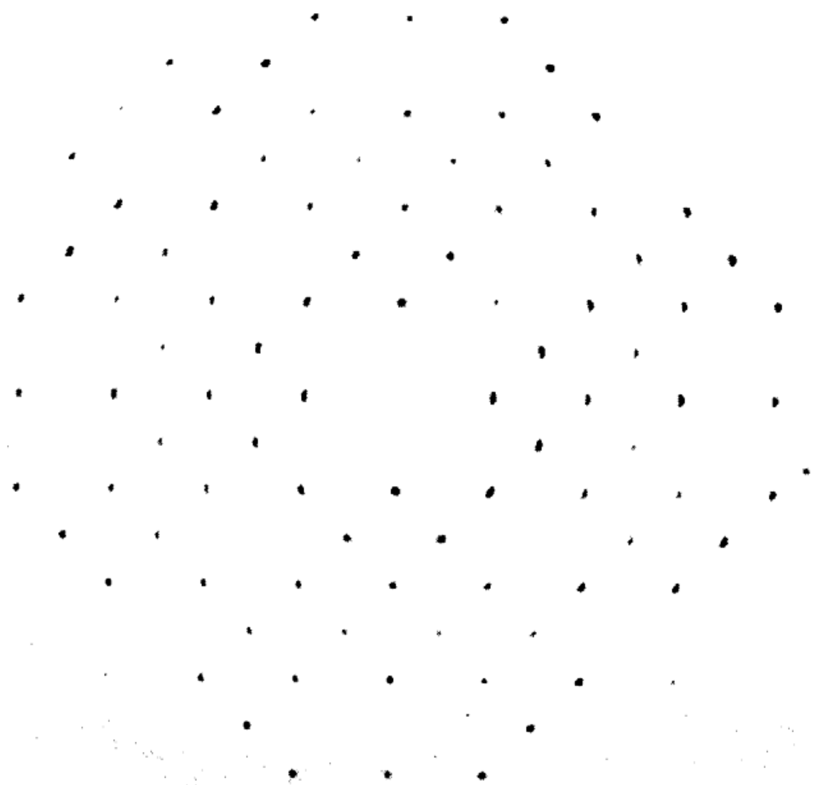


- ensure that the origin of the reciprocal lattice is chosen as that point at which the incident beam leaves the Ewald sphere

ensure that the scale used for the Ewald sphere is same as that used for the reciprocal lattice

Ewald Sphere and Diffraction





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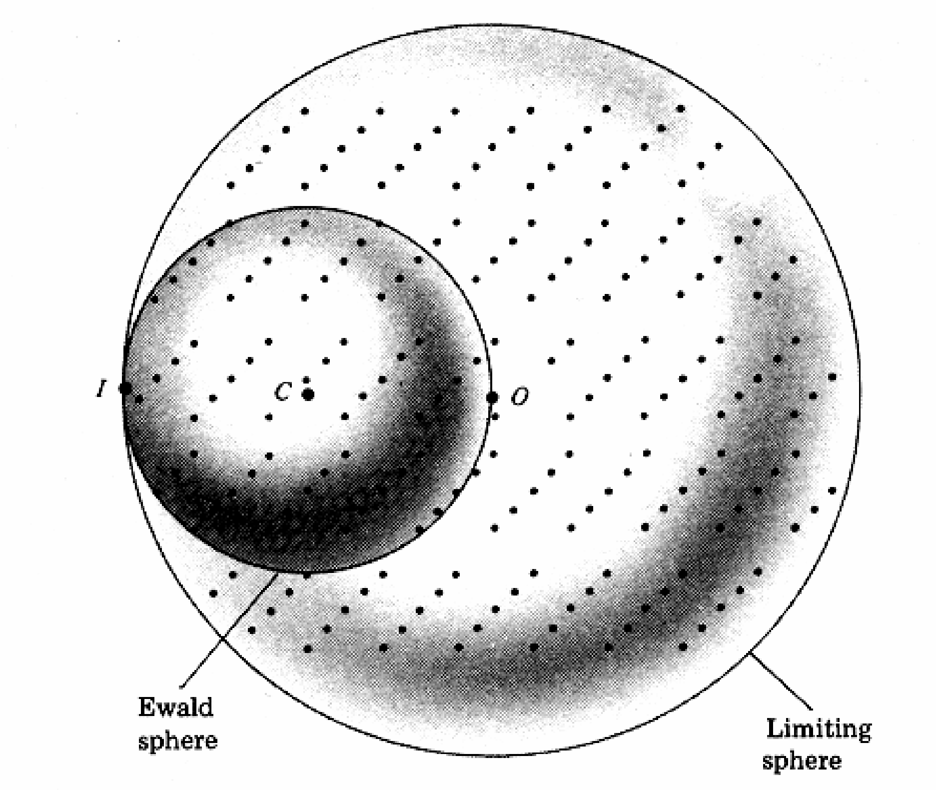
Ewald Sphere and Diffraction

- limiting sphere



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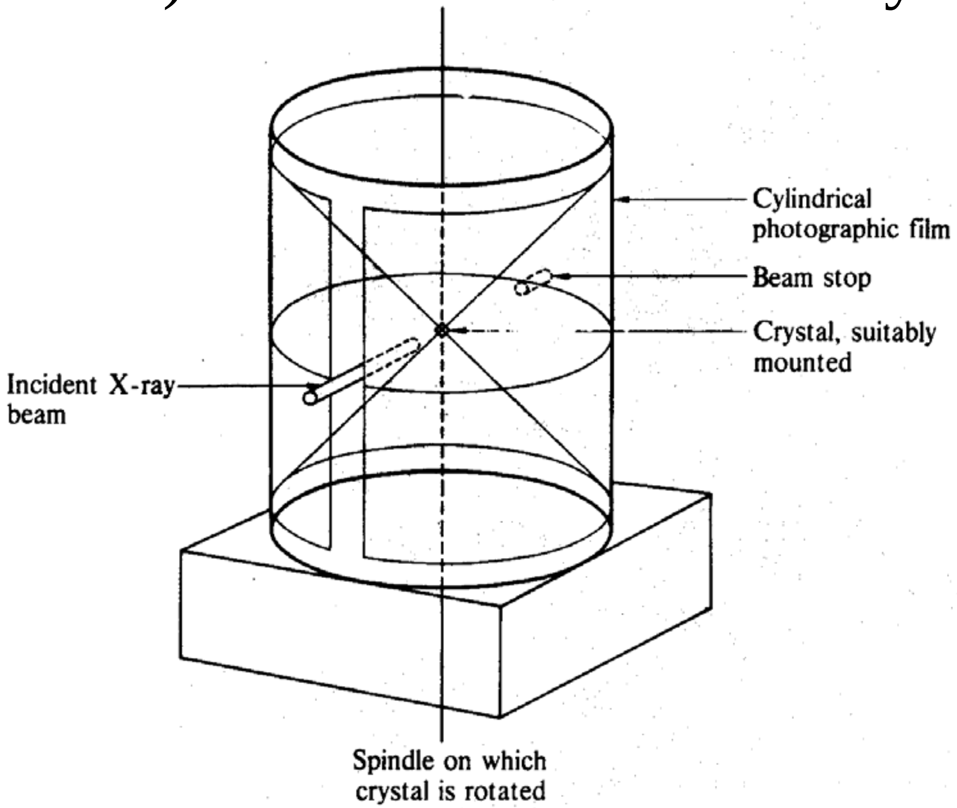
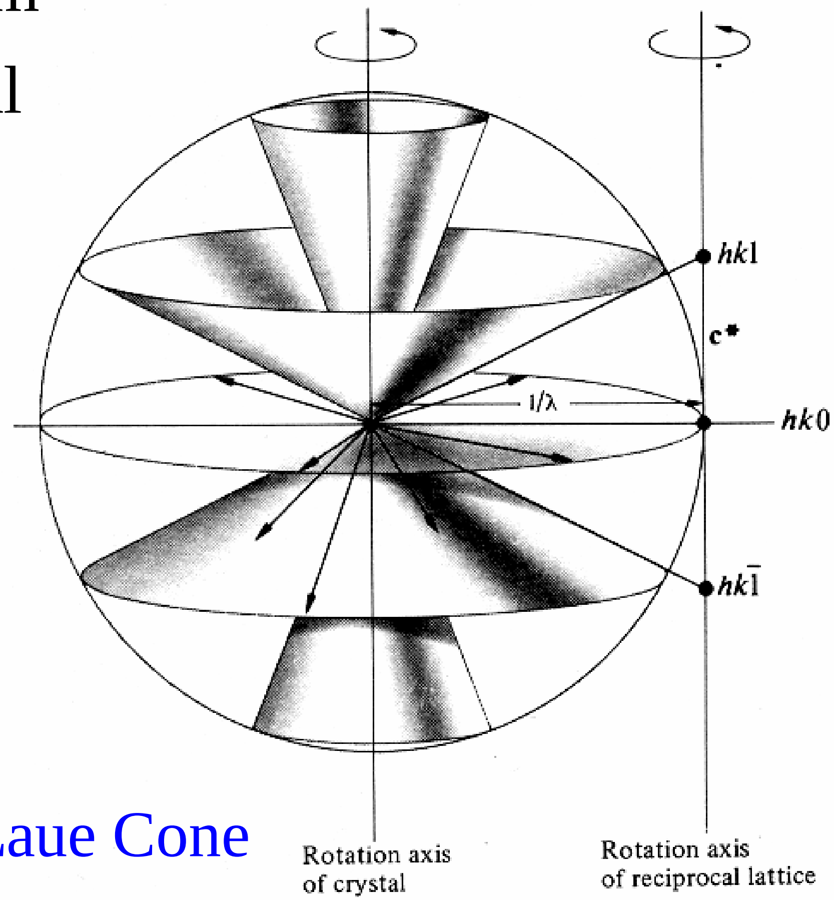
Rotation Camera

- crystal is mounted with crystallographic axis accurately vertical
  crystal rotates about the axis, and diffraction pattern is recorded on the cylinderical film
- ex) c-axis in orthorhombic crystal



Laue Cone



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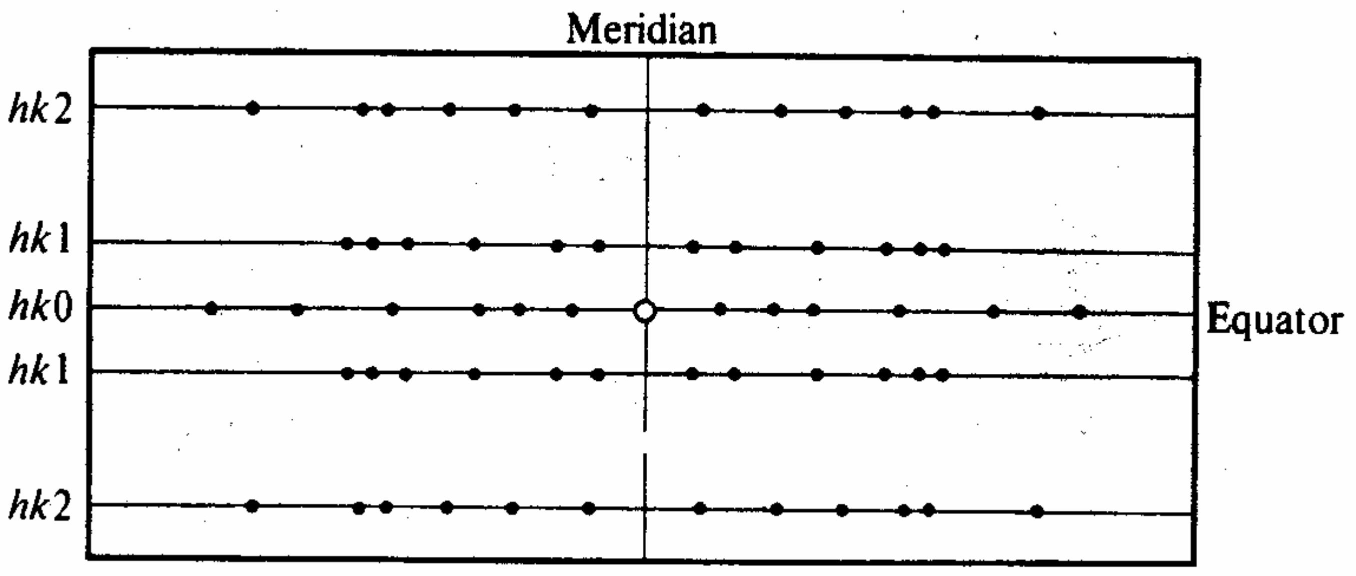
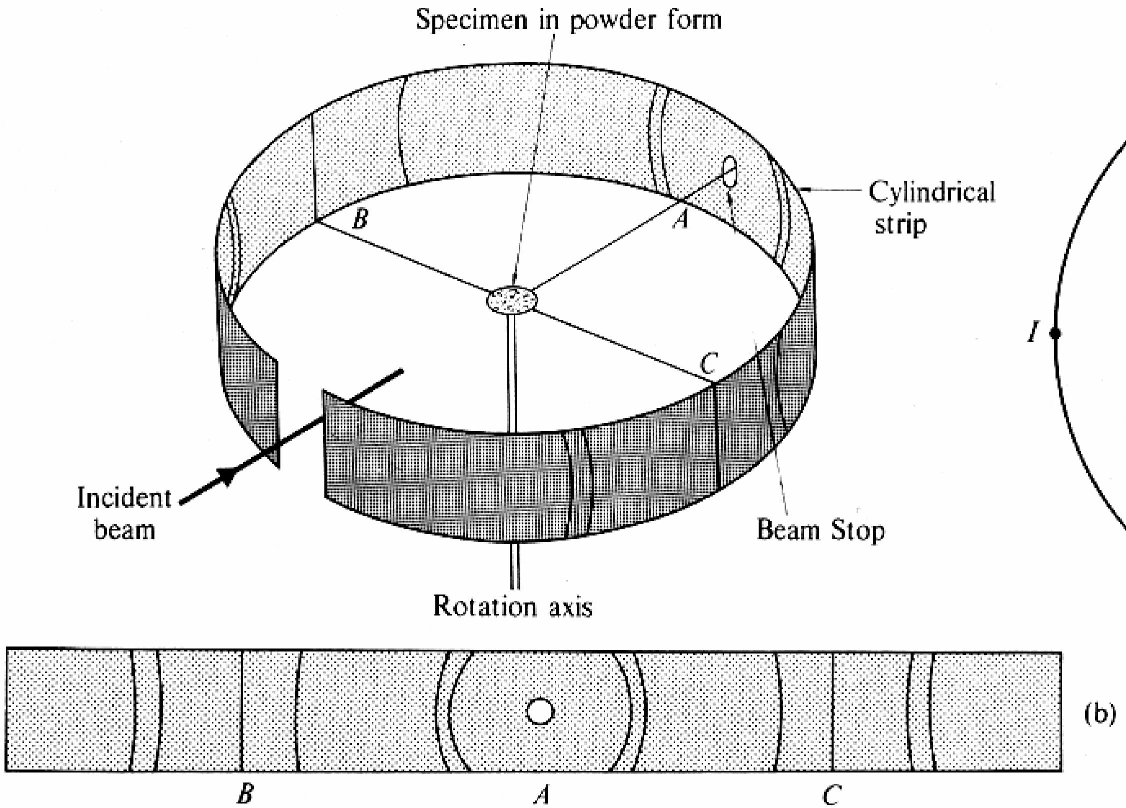
Rotation Camera

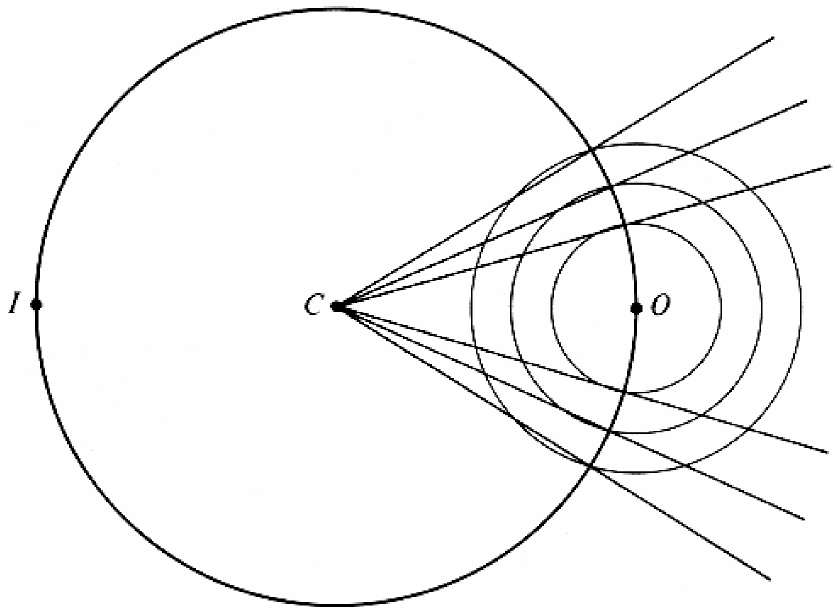
- symmetrical in both position and intensity about equator and also meridian



Powder Camera

- speimen-fine powder- a vrey large number of randomly oriented crystallite
- reciprocal sphere



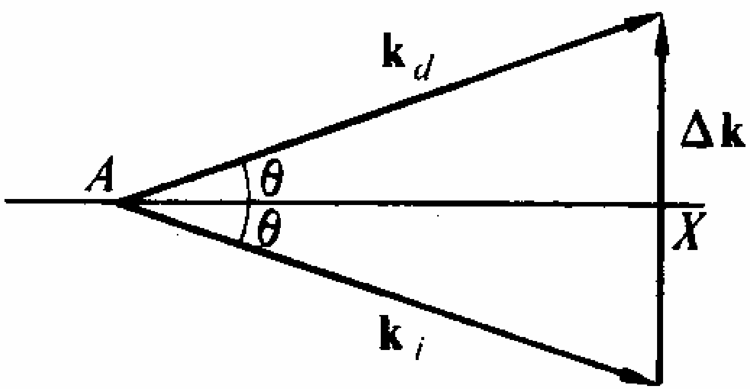


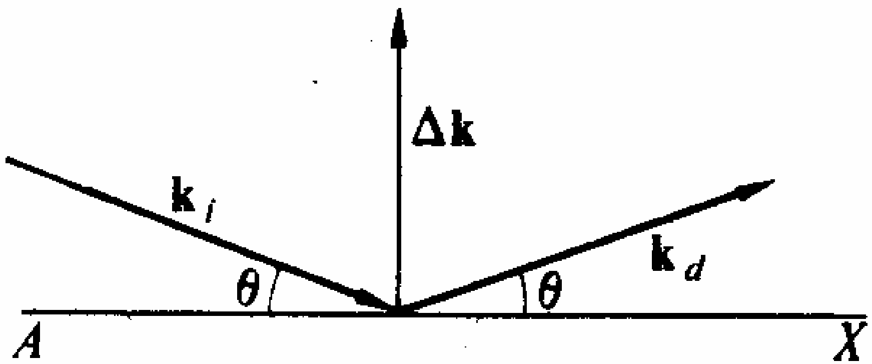
Bragg's Law and Crystal Planes

- Bragg's law $2d_{hkl} \sin\theta = \lambda$
- geometric relationship between $\vec{k}_i,\ \vec{k}_d,\ \Delta\vec{k}$
- $\Delta\vec{k} = 2\pi\vec{G}_{hkl} \Rightarrow \Delta\vec{k} \parallel \vec{G}_{hkl}$

  $\vec{G}_{hkl} \perp (hkl)$ set of planes $\Rightarrow \Delta\vec{k} \perp (hkl)$ set of planes

$\therefore$ line AX is parallel to the (hkl) set of planes

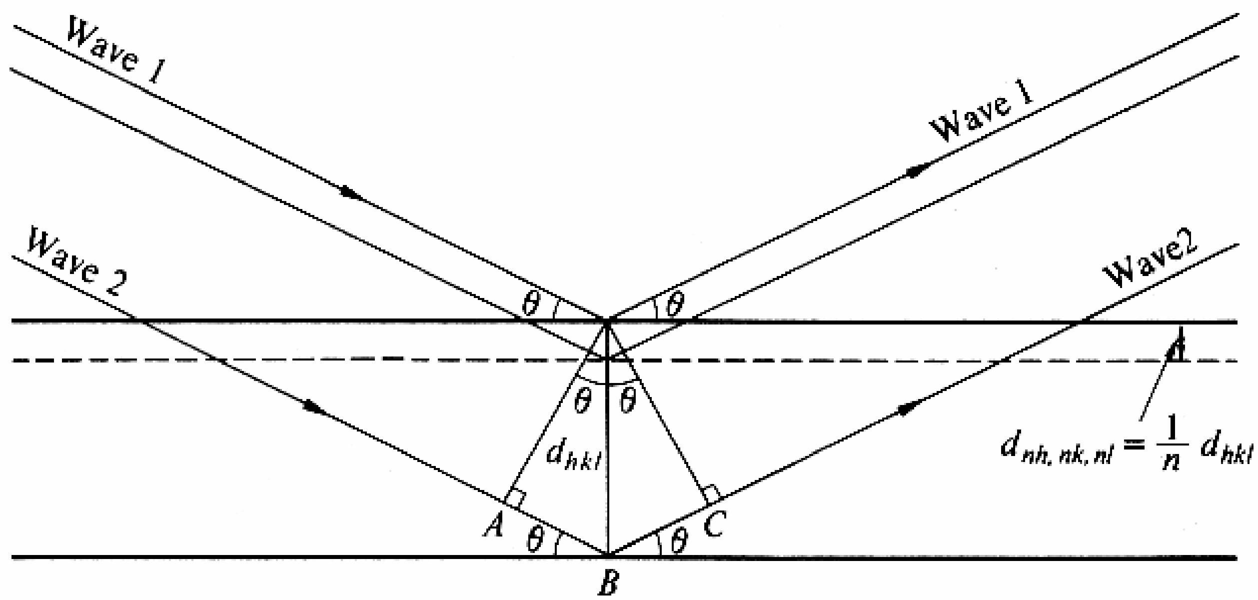




reflection

Bragg's Law and Crystal Planes

- a physical explanation of Bragg's law
- path difference=$2d_{hkl} \sin\theta$
- phase difference=$\dfrac{2\pi}{\lambda} 2d_{hkl} \sin\theta$
- maximum intensity $\dfrac{4\pi d_{hkl} \sin\theta}{\lambda} = n2\pi \Rightarrow 2d_{hkl} \sin\theta = n\lambda$



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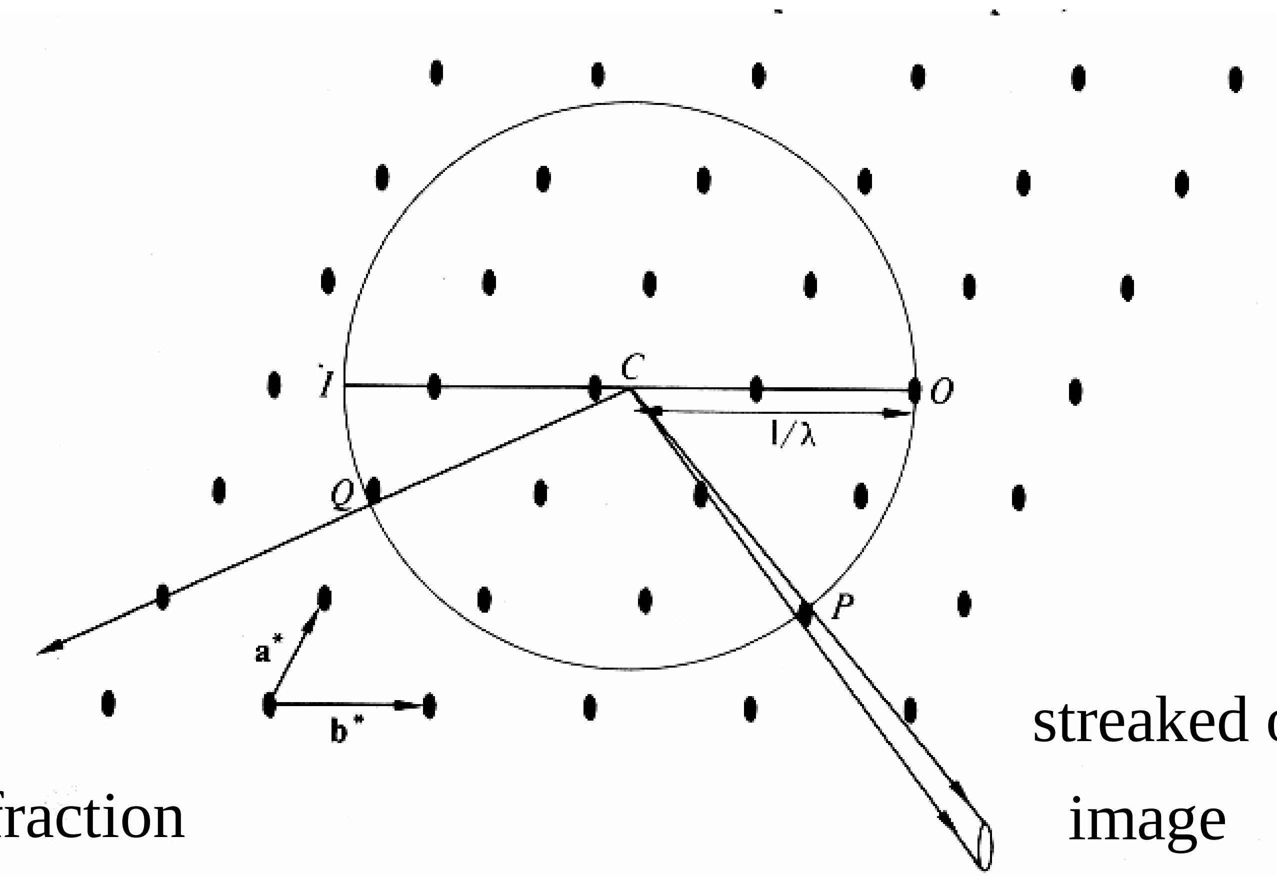
Effect of Finite Crystal Size

- finite size of the crystal- blurring or smearing out diffraction pattern → rather fuzzy, not a point



weak diffraction pattern

streaked or blurred image