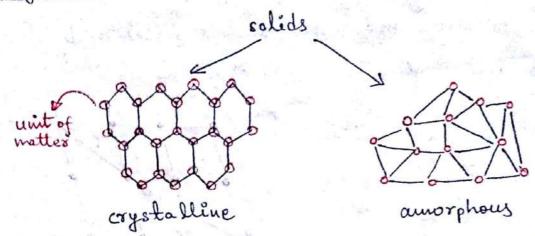
#### SOLID STATE PHYSICS

Crystal structure, direct lattice & (un) holy grail



(i) Auwophous solid: no order in arrangement of unit of matter ( atoms, molecules etc). XRD shows Liquid like property.

what's "solid"? -> elasticity stress  $\sigma = K \frac{\chi}{L}$ 

but 
$$\frac{1}{2}kx^2 = \frac{1}{2}keT$$

Cequipartition)

 $f = -kx$ 
 $f = -kx$ 

$$F = -k R \frac{\pi}{L}$$

$$= -k R \alpha = -k \alpha$$

$$\therefore \vec{\alpha}^2 = \frac{k_B T}{R} = \frac{k_B T}{K \ell}$$

amorphous solids \rightarrow highly viscous, supercooled liquids.

Example pitch, plastie, (
silicate glass.

(i) molecular motion is irregular but distance is more or less same with dastie solid.

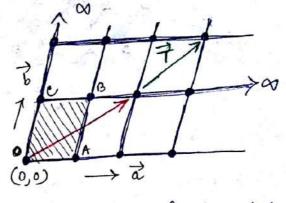
SALIENT FEATURES

- (ii) no regular stope > conductivity, elasticity tensile strength is isotropic
- (in) no long range order. short range / medium rauge order possible.
- (iv) no storp melting point.

There are polycrystalline substances which are composed of many small domains/regions of single crystals. Crystalline substances are distinguished from amorphous solids by their anisotropic behaviour (direction dependent).

Ideal crystal : infinite repetition of identical structure in space.

Periodic arrangement of unit (atoms, molecules, ions) in a



orystal is alled the lattice, defined by three fundamental translation vectors  $\vec{a}$ ,  $\vec{b}$ ,  $\vec{c}$ . / basis vectors

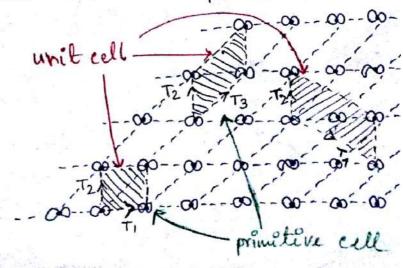
Atomie position vector 
$$\vec{r}' = \vec{r} + \vec{T}$$
  
=  $\vec{r} + n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$ 

where n, u2, u3 are integers.

# primitive lattice & Unit cell

Unit cell is volume from which entire crystal can be constructed by translational repitition. (OABC parallelogram)

primitive cell is a type of unit cell that contain 1 lettier point at corners & minimum in volume =  $|(\vec{a} \times \vec{b}) \cdot \vec{c}|$ 



Basis in coystal stoucture, every lattice point is associated with an unit assembly of atoms/molecules/ions. This unit is called basis.

Basis can contain even hundreds & thousands of molecules.

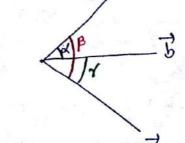
A translation operation leaves the crystal invariant.  $f(\vec{r}) = f(\vec{r} + \vec{T})$ 

$$f(\vec{r}) = f(\vec{r} + T)$$
physical: number density  $n(\vec{r}) = \sum_{\vec{r}} S(\vec{r} - \vec{T})$ 
significance (point mass atom)
$$density \quad p(\vec{r}) = \sum_{\vec{r}, d} m_d S(\vec{r} - \vec{T} - \vec{c}_d)$$

where my is man of atom at lattice sile Ex.

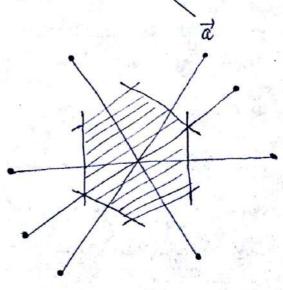
$$p(\vec{r}) = p(\vec{r} + \vec{T})$$

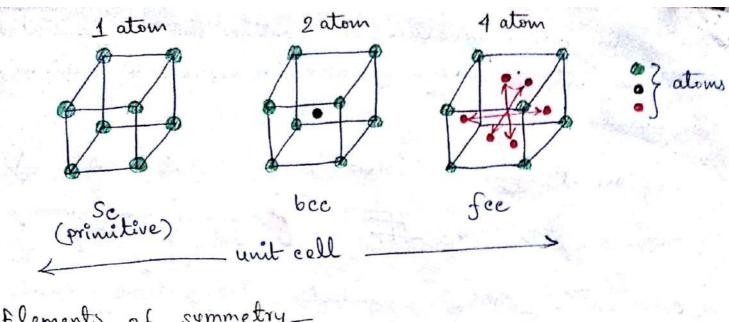
For cubie structure  $|\vec{\alpha}| = |\vec{b}| = |\vec{c}|$  $\alpha = \beta = \delta = \frac{\pi}{2}$ 



# Wigner\_Sielz primitive cell

- 1. Draw lines connecting near by lattice points.
- 2. Draw planes/lines at midpoint of line I perpendicular to it.
  This is WS primitive cell.



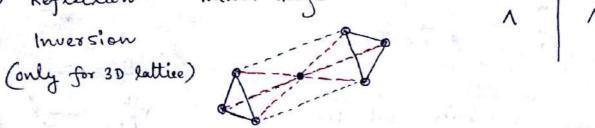


Elements of symmetry A symmetry operation transforms the crystal to itself. Robotion  $N\beta = 2\pi$  N = multiplicity of robotion axis.  $\sum_{r=0}^{r=0} \phi = 60^{\circ}$   $\sum_{r=0}^{r=0} \phi = 60^{\circ}$ 

= 1,2,3,4,×,6. A 2D square lattice has 4-fold rotational symmetry.

(iii) Reflection mirror image

(in) Inversion



Symmetry operation performed about a point/line are called point group symmetry. 3 type of point group (i) plane of symmetry (reflection), (ii) axis of symmetry (rotation), (iii) centre of symmetry (inversion)

5-fold rotational symmetry: quasicrystals. But why 5-fold rotational symmetry is not permissible in onestal structure?

A' chand B'  $AB = a = |\vec{a}| = |\vec{r}_1 - \vec{r}_2|$ = AA' = BB'Suppose AB = qlal (q=integer) LA'AC' = LD'BB' = 0- 7/2 A'e' = D'B' = 1 al  $\cos \theta$ :. A'B' = 1 al + 1 al cos 0 + 1 al cos 0 VIal = (a) + 21 a) wio  $cr |cor\theta| = |\frac{\psi^{-1}}{2}|$ as cost <1, allowed values of q are -1,0,1,2,3  $\{q=-1, \theta=\frac{2\pi}{2}\}, \{q=0, \theta=\frac{2\pi}{3}\}, \{q=1, \theta=\frac{2\pi}{4}\}$ { q= 2, 0= 2√3, 2 q= 5, 0= 2√3 So,  $n = 1, 2, 3, 4, 6 \longrightarrow hexad$ diad triad telrad Point group & space group [translation, rotation, reflection] (point) point group. Total 32 point groups. Group of all symmetry elements is space group. In 20: 17, 30: 230. Bravais lattie: Tat, 161, & 5combination: symmetry operations are P primitive reelangular Centered sectangular I square I heragonal 1前=1前, 中=3 は1+1前, 中=う はまは, ゆ=至  $|\vec{a}| \neq |\vec{b}|, \phi \neq \frac{\pi}{2}$   $|\vec{a}| = |\vec{b}|, \phi = \frac{\pi}{2}$ {2<sup>2</sup>} {<sup>2</sup>/<sub>2</sub>} 多一个,一个 reflection rotation rotation rotation Scanned by CamScanner

length of primitive Angle Type & number Clan a=b=c++ 00 d= p= 7 = 90° P, F, ICubie a=b # c d= p= 1= 50 PI Tetragonal a=b#c d= B= 90, 7=120 Hexagonal asbsc d=p=1+ 90 4120 Rhombohedral/ Trigonal a + b + c d= = = = 90 P, F, I, C ( Orthorhombie a + b + c d=7=90 7 p Monodinie a+b+c d # B # d Triclinie

#### Altours per unit cell

(i) Eight corner atoms in cubic unit cell 18th atom
(ii) Six face atoms in unit cell 1th atom.

(iii) If on edge then stared latween 4 unit, 14th atom

(iv) If inside cell, then (off course) I atom as whole.

Simple cubic cell (se)

# of atoms/ unit cell = 2 = 1.

Body centered cubic cell (bcc)

# of atoms/unit cell = \frac{8}{8} + 1\frac{1}{8} = 2

face centered cubic cell (5cc)

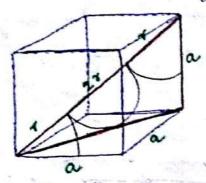
# of atoms / unit cell =  $\frac{8}{8} + \frac{6}{2} = 4$ 

Coordination Number In crystal lattice, the number of nearest neighbours of an atom is called coordination no.

se cell, coord no. = 6.

bcc cell, coord us. = 8

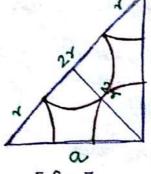
fee cell, word no. =  $4 \times 3 = 12$  $6 \times 7, 72, \times 2$  plane Atomie radius Distance between centre of two touching atoms.



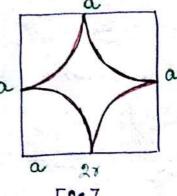
[bee]

$$(4r)^2 = (\sqrt{2}a)^2 + a^2$$

or  $r = \sqrt{\frac{3}{4}} a$ 



[fee ]



[se]

or 
$$r = \frac{\alpha}{2}$$

Atomie packing fraction/factor/ relative packing density

P. F. (3) = volume of atoms in unit cell volume of unit cell.

[bec] 2 atoms/ unil cell,  $\gamma = A \frac{13}{4}a$ 

: vol. of atomo = 2x \frac{1}{3} \tau \gamma^3, vol. of unit cell = a3.

:. 
$$f = \frac{2 \times \frac{4}{3} \pi \times (\frac{\sqrt{3}}{4} \alpha)^3}{\alpha^3} = \frac{\sqrt{3} \pi}{8} = \frac{68\%}{8}$$

Example: Barium, chromium, sodium, iron, caesium chloride

[fee] 4 atoms/unit cell,  $r = \frac{\alpha}{212}$ 

$$f = \frac{4 \times \frac{4}{3} \pi \times \left(\frac{\alpha_{\nu}}{212}\right)^{3}}{\alpha^{3}} = \frac{\pi}{3\sqrt{2}} = \frac{74\%}{4\%}$$

[se] 1 atom/unt cell,  $v = \frac{a}{2}$ 

$$5. \int = \frac{\frac{4}{3} \pi \left(\frac{\alpha}{2}\right)^3}{\alpha^3} = \frac{\pi}{6} = \frac{52\%}{6}$$

example: polonium, potassium chloride

HW 1. Privitive translation vector of hcp lattice of  $\vec{d} = \frac{13}{2}a\hat{i} + \frac{2}{2}\hat{j}$ ,  $\vec{c} = -\frac{13}{2}a\hat{i} + \frac{2}{2}\hat{j}$ ,  $\vec{c} = c\hat{k}$ . Compute the volume of the primitive cell.

copper, aluminium lithius commun, saduum, saduum,

2. Show that for a fee crystal structure, lattice constant is  $\alpha = \left(\frac{4M}{(PN)}\right)^{3}$  where M is the gram molecular weight of molecules at lattice points, I is the density of N is Avogadro's number.

#### Nacl Structure

ionic crystal Nat S. Cl., fec Bravais

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

Cl (シャシッシ) (0,0,シ) (0,シ,0) (シ,0,0)

4 Nace molecule in unit cube.

Nat (0,0,0)  $\downarrow$  Cl  $(\frac{a}{2},0,0)$   $\rightarrow$  6 neasest neighbour (coordination number).

Miller indices To designate the position of orientation of a crystal plane according to following rule:

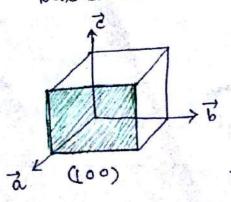
(a) In terms of lattice constant, find the intercept of the plane on crystal axes a, b, c (primitive or nonprimitive)

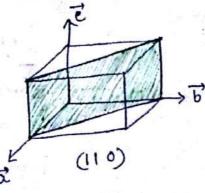
(2,0,0), (0,3,0), (0,0,1) -> 2a,3b, C.

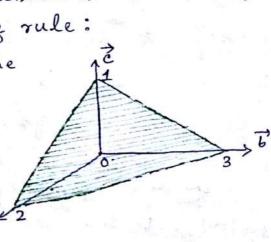
(b) Take reciprocals of them I reduce to smallest 3 integers, Denote with (h, K, L)

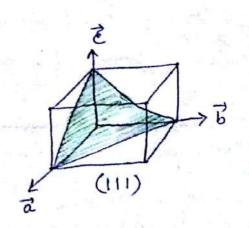
So 20,36, C reciproc 2, 3, 1 smallest

Willer index is (3,2,6) plane









If plane cuts negative side of axis, M. index (h, k, e) 6-faces of cubic crystal, N-index (1,0,0), (0,1,0), (0,0,1) = \$1,0,0
according through rotation, all faces (1,0,0), (0,1,0), (0,0,1) because through rotation, all faces So (2,0,0) plane intercepts on 2,5,2 are 1a, on, or. I parallel are equivalent & written in & 3. to (1,0,0) 1 (1,0,0) plane. Indices of a direction [h, K, E] & direction & peopendicular lo plane (h,k,e). à axis = [1,0p], -6 axis = [0,1,0]
body d'agoral = [1,1,1] Spacing of planes in sc lattice simple unit cell à 1 b 1 è f a plane (n,k,l) (miller index). Intercepts a/h, b/k, c/L on a, b, c axes 7 if d & P OP I (h, k, l) plane I OP=d. 1 LAOP = d, LBOP = B, LCOP = d. L LAPO = LBPO = LCPO = 90.  $\frac{OP}{OA} = \cos d$  or  $OP = OA \cos d$  or  $d = \frac{a}{h} \cos d$  or  $\cos d = \frac{dh}{a}$ Similarly cosp = dk, cost = dl. Law of direction cosines, cost + cost 3+ cost = 1  $c_0 d^2 \left( \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{k^2}{c^2} \right) = 1$ or d = 1 If cubic lattice, a=b=c, d= \( \frac{a}{h+k+1}^2 \)  $d_{100} = \frac{\alpha}{\sqrt{1+6+0}} = \alpha, \quad d_{110} = \frac{\alpha}{\sqrt{1+1+0}} = \frac{\alpha}{\sqrt{2}}, \quad d_{111} = \frac{\alpha}{\sqrt{3}} = \frac{\alpha}{\sqrt{3}}$ 

### Spacing of planes in bee lattice

One atom at each corner + one atom at cube centre.

(portion) (whole)

:  $d_{100} = \frac{a}{2}$  as additional (1,0,0) is there halfway between (100) plane of sc.

 $d_{110} = d_{110} = \frac{a}{\sqrt{2}}$ . but  $d_{111} = \frac{1}{2} \frac{a}{\sqrt{3}}$  on (1,1,1) plane lies midway of (111) plane of se.

## Spacing of planes in fee lattice

one atom at each corner + one atom at each face. (portion) (portion)

:.  $d_{100} = \frac{a}{2}$  as additional (1,0,0) is there halfway

between (1,90) plane of se.

But  $d_{110} = \frac{1}{2} \frac{a}{\sqrt{2}}$  on additional set of (110) is there halfway between (1,1,0) plane.

 $d_{111} = \frac{a}{\sqrt{3}}$  as centre of all face plane without new plane.

$$\Re \vec{r}_1 = \vec{a}_{k_1}, \vec{r}_2 = \vec{b}_{k_2}, \vec{r}_3 = \vec{c}_{k_2}$$

ha+ kb+ le represents [h, k, L]

Now (\$1-\$2). (ha+ kb+le) = (\$-\frac{1}{h}-\frac{1}{k}). (ha+kb+le)

 $= \vec{a} \cdot \vec{a} - \vec{b} \cdot \vec{b} = 0$ . (as  $|\omega| = |b|$ )

Similarly (\$1-\$3). (ha+ kb+ lc) = 0 (as M=1el)

As vectors  $\vec{r}_1 - \vec{r}_2$  &  $\vec{r}_1 - \vec{r}_3$  lie in (h, k, L) plane, so [h,k,l] is perpendicular to plane (h,k,L).

Reciprocal lattice To represent slope & interplanas spacing 5 of crystal plane, each set of parallel plane in a space lettice for a, b, c, we describe reciprocal basis vectors a, b, c\* Cprimitive) such that  $\vec{a} \cdot \vec{a}^* = 2\pi$ ,  $\vec{b} \cdot \vec{a}^* = 0$ ,  $\vec{c} \cdot \vec{a}^* = 0$   $\vec{a} \cdot \vec{b}^* = 0$ ,  $\vec{b} \cdot \vec{b}^* = 2\pi$ ,  $\vec{c} \cdot \vec{c}^* = 0$   $\vec{a} \cdot \vec{c}^* = 0$ ,  $\vec{b} \cdot \vec{c}^* = 0$ ,  $\vec{c} \cdot \vec{c}^* = 2\pi$ .  $\vec{a}' = g\pi \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot \vec{b} \times \vec{c}}, \quad \vec{b}'' = g\pi \frac{\vec{c} \times \vec{a}}{\vec{a} \cdot \vec{b} \times \vec{c}}, \quad \vec{c}'' = g\pi \frac{\vec{a} \times \vec{b}}{\vec{a} \cdot \vec{b} \times \vec{c}}$ reciprocal lattice vector 3x = hax+ kbx+ lcx properly (i) reciprocal lattice is normal to lattice plane of direct crystal lattice-7x. (3,-32) = (hax+ kbx+ lex). (2,-2) = 0. Similarly 7x. (7,-73) =0. in direct lattice is reciprocal of reciprocal lattice. se = self-reciprocal. bee >> fee reciprocal of each other. Definition of R.L.  $\vec{T} = u_1\vec{a} + u_2\vec{b} + u_3\vec{e}$  direct lattice vector of say k constitutes a plane wave eik. I which may not have the periodicity of Bravais lattice but R has that periodicity.  $e^{i\vec{k}\cdot(\vec{\tau}+\vec{\tau})}=e^{i\vec{k}\cdot\vec{r}}$  or  $e^{i\vec{k}\cdot\vec{\tau}}=1$ R = K, a\* + K2 b\* + K3 c\* = : k. + = 2x(K, n, + K2u2 + K3u3) If eik. = 1, then k. + must be 2x x integer => Kukzik, integers

So from  $\vec{k}$  only  $\vec{k}$  which is linear combination of  $\vec{a}^*, \vec{b}^*, \vec{c}^*$  with integral wefficient makes  $\vec{k}$  a reciprocal lattice vector.

Reciprocal of reciprocal lattice

As by construction, reciprocal lattice is a Brawais lattice, reciprocal gives back the direct lattice.

$$b^{**} = 2\pi \frac{\vec{c}^* \times \vec{a}^*}{\vec{a}^* \cdot \vec{b}^* \times \vec{c}^*}$$
,  $\vec{c}^{**} = 2\pi \frac{\vec{a}^* \times \vec{b}^*}{\vec{a}^* \cdot \vec{b}^* \times \vec{c}^*}$  as three vectors generated by primitive vectors  $\vec{a}^*$ ,  $\vec{b}^*$ ,  $\vec{c}^*$ . Check first,  $\vec{a}^* \cdot \vec{b}^* \times \vec{c}^* = \frac{(2\pi)^3}{\vec{a} \cdot \vec{b} \times \vec{c}}$  I then show that  $\vec{a}^* = \vec{a}$ .

$$\therefore \vec{a}^* = 2\pi \frac{b\hat{j} \times c\hat{k}}{a\hat{i} \cdot (b\hat{j} \times c\hat{k})} = 2\pi \frac{be}{abe} \hat{i} = \frac{2\pi}{a} \hat{i}$$

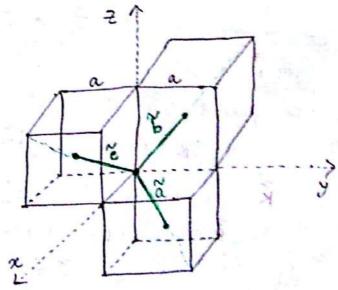
$$\vec{b}^* = 2\pi \frac{c\hat{k} \times a\hat{i}}{a\hat{i} \cdot (b\hat{j} \times c\hat{k})} = \frac{2\pi}{b}\hat{j} = \frac{2\pi}{a}\hat{j} \quad (a=b=c)$$

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

lattier constant = 27/a.

Reciprocal of bee lattice

$$\frac{1}{2} = \frac{a_{2}(\hat{i} + \hat{j} - \hat{k})}{2} = \frac{a_{2}(\hat{i} + \hat{j} + \hat{k})}{2} = \frac{a_{2}(\hat{i} + \hat{j} + \hat{k})}{2} = \frac{a_{2}(\hat{i} - \hat{j} + \hat{k})}{2}.$$



volume of primitive cell = 
$$\vec{\alpha} \cdot \vec{k} \times \vec{c} = \vec{a}/2$$
.

 $\vec{a} \times = 3\pi \frac{\vec{k} \times \vec{c}}{\vec{k} \cdot \vec{k} \times \vec{c}} = \frac{2\pi}{\alpha} (\hat{i} + \hat{j})$ ,

 $\vec{b} \times = 3\pi \frac{\vec{k} \times \vec{c}}{\vec{k} \cdot \vec{k} \times \vec{c}} = \frac{2\pi}{\alpha} (\hat{i} + \hat{k})$ .

 $\vec{c} \times = 3\pi \frac{\vec{k} \times \vec{c}}{\vec{k} \cdot \vec{k} \times \vec{c}} = \frac{2\pi}{\alpha} (\hat{i} + \hat{k})$ .

Reciprocal of fee lattice  $\vec{a} = \frac{2\pi}{\alpha} (\hat{i} + \hat{k})$ .

 $\vec{c} = \frac{2\pi}{\alpha} (\hat{i} + \hat{k})$ .

volume of primitive cell =  $\vec{a} \cdot \vec{b} \times \vec{c} = \frac{3}{4}$ .

and  $\vec{a} \times = \frac{2\pi}{\alpha} (\hat{i} + \hat{j} - \hat{k})$ ,  $\vec{b} \times = \frac{2\pi}{\alpha} (-\hat{i} + \hat{j} + \hat{k})$ ,  $\vec{c} \times = \frac{2\pi}{\alpha} (\hat{i} + \hat{j} + \hat{k})$ .

Reciprocal bee lattice vectors = primitive fee lattice vectors.

Reciprocal fee lattice vectors = primitive bee lattice vectors.

Crystal diffraction

Why use X-ray for crystollagraphy?

Atomic spacing (say for Nacl) is 2.8 Å. When X-ray is produced by accelerating electrons through a potential difference V, eV = hr? = he are not as a second of the control of

Maximum intensity from reflected beam (waves) from two different atomic planes (deavage planes) with path difference equal to integral multiple of 2 x-ray.

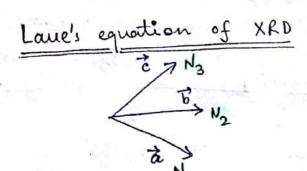
Cleavage planes/ Bragg planes I

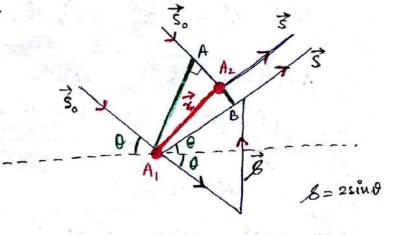
Path difference between ray
[AB,BC] L [DE, EF] is KE + EL

= dsind + dsind = 2 deind. So for constructive interference,

$$2d sin \theta = h \lambda$$
,  $n = 1, 2, 3, \dots \Rightarrow Bragg's law.$ 

A, O = Known, d = unknown.





Assumptions: (a) The primary X-ray beam travels within the crystal at the speed of light. (b) Each scattered wavelet travels through the crystal without getting rescattered.

Say N, number of points along direction à N2 number of points along direction à N3 number of points along direction à Total N = N, N2 N3 points in the crystal lattice.

Path difference between two x-roys is  $d = \vec{r}_n \cdot \vec{s} - \vec{r}_n \cdot \vec{s}_0 = \vec{r}_n \cdot \vec{s}$ : Phase difference is  $\frac{2\pi}{2}d = \frac{2\pi}{2}\vec{r}_n \cdot \vec{s} = k\vec{r}_n \cdot \vec{s}$ 

remember:  $\vec{s}$ ,  $\vec{s}$ , unit vector,  $|\vec{s}| = 8 = a \sin \theta$ ,  $\vec{r}_n = n th lattice$ point from origin =  $\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{e}$ .

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If y is the displacement of the scattered wave from origin at a distance R at time t with amplitude Ao, then Jo = Ao eint. : displacement from on is y = Ao e int oikin. 3 i. Total displacement due to the whole Bravais lattice is Y = Z Ao eint eixin. Z =  $\sum_{N_1=0}^{N_2-1} \sum_{N_2=0}^{N_2-1} \sum_{N_3=0}^{N_3-1} e^{i\kappa [(n_1\vec{a}+n_2\vec{b}+n_3\vec{c})\cdot\vec{B}]} \frac{A_0}{R} e^{i\omega t}$  $= \frac{\Lambda_0}{R} e^{i\omega t} \sum_{N_1=0}^{N_1-1} e^{i\kappa n_1 \vec{a} \cdot \vec{k}} \sum_{N_2=0}^{N_2-1} e^{i\kappa n_2 \vec{b} \cdot \vec{k}} \sum_{N_3=0}^{N_3-1} e^{i\kappa n_3 \vec{c} \cdot \vec{k}}$ Now \( \frac{1}{2} = \frac{1}{2} \tau \frac{1}{2} = \frac{1}{2} \tau \frac{1}{2} \tau \frac{1}{2} = \frac{1}{2} \tau \frac{1  $\frac{1-e^{iN_{1}(\vec{a}\cdot\vec{z})K}}{1-e^{iKn_{1}\vec{a}\cdot\vec{z}}} = \frac{1-e^{i(\vec{a}\cdot\vec{z})K}}{1-e^{i(\vec{a}\cdot\vec{z})K}}$   $\frac{1-e^{iN_{1}(\vec{a}\cdot\vec{z})K}}{N_{1}=0} = \frac{1-e^{iN_{1}(\vec{a}\cdot\vec{z})K}}{N_{1}(\vec{a}\cdot\vec{z})K}$   $= \frac{1-e^{iN_{1}(\vec{a}\cdot\vec{z})K}}{1-e^{iN_{1}(\vec{a}\cdot\vec{z})K}} = \frac{1-e^{iN_{1}(\vec{a}\cdot\vec{z})K}}{1-e^{iN_{1}(\vec{a}\cdot\vec{z})K}}$  $= \frac{1-e^{iN_1(\vec{a}\cdot\vec{x})K}}{1-e^{i(\vec{a}\cdot\vec{x})K}} \times \frac{1-e^{-iN_1(\vec{a}\cdot\vec{x})K}}{1-e^{-i(\vec{a}\cdot\vec{x})K}}$ = 1- cos {N, (a. &) k} + i sin {N, (a. &) k} x 1- cos{(a. \$)K} - isin\$(a. \$)K}. 1- 65 & N, (a. 3) K3 + isin & N, (a. 3) K3 1- cos & (a. 2) k} + isin & (a. 2) k} = (1- cos & N, (a. B) K})2+(sin & N, (a. B)K})2 (1- ws & (a. 8)K) 2+ (sin s(a. 8)K)2  $\frac{1-\cos\xi\,N_1(\vec{a}\cdot\vec{z})K^2_3}{1-\cos\xi\,(\vec{a}\cdot\vec{z})K^2_3} = \frac{\sin^2\xi\,N_1(\vec{a}\cdot\vec{z})K^2_3}{\sin^2\xi\,(\vec{a}\cdot\vec{z})K^2_3} = \frac{\sin^2(N_1\Psi_1)}{\sin^2(\Psi_1)}$ sin (N, 41)

where  $\psi_1 = \frac{1}{2} \, \text{Ka.Z.}$ is Total intensity  $I = YY^* = \left(\frac{|A_0|}{R}\right)^2 \frac{\sin^2(N_1 \Psi_1)}{\sin^2(\Psi_1)} \frac{\sin^2(N_2 \Psi_2)}{\sin^2(\Psi_2)} \frac{\sin^2(N_3 \Psi_3)}{\sin^2(\Psi_3)}$ 41 = 1 Ka. 3 = 1 Klall slosd = 1 2 a 2 sind wid = 2 xa sind wid Similarly 42 = 1 Kb. = 276 sind cosps, 43 = 1 K c. 8 = 2xc sind ws 8 [Notice the analogy of I with [h, K, 1] plane with anglis d, T, B] In  $\lim_{\Psi_1 \to h\pi}$ ,  $\frac{\sin^2(N_1 \Psi_1)}{\sin^2 \Psi_1}$  is maximum =  $N_1^2$ Similarly  $\lim_{\gamma \to KX} \frac{\sin^2(N_2 \psi_2)}{\sin^2(\gamma)} = N_2^2$ ,  $\lim_{\gamma \to LX} \frac{\sin^2(N_3 \psi_3)}{\sin^2(\gamma)} = N_3^2$ Then  $I_{\text{max}} = \left(\frac{|A_0|}{R}\right)^2 N_1^2 N_2^2 N_3^2 = \frac{|A_0|^2}{\rho^2} N^2$ 2a sino cosd = ha.  $2\pi b \sin \theta \cos \beta = k\pi$ ,  $2b \sin \theta \cos \beta = k\lambda$ 20 sino cost = 22 exceindoso = ex, " Laure equations! Bragg's law from Laure equations from Laue equation, direction cosiner of \$ are  $cosd = \frac{h\lambda}{2a sin\theta}$ ,  $cos \beta = \frac{k\lambda}{2b sin\theta}$ 

But also see that if (h,K,L) is a miller plane with equation  $\frac{\alpha}{a/h} + \frac{y}{b/k} + \frac{z}{e/e} = 1 \quad \text{then} \quad \frac{a}{h} \cos \alpha = \frac{b}{k} \cos \beta = \frac{c}{k} \cos \beta = d.$