

# Primitive lattice, unit cell, Bravais lattice, Space group

unit cell: repeating unit in a crystal

↳ want to tile all of space (fill it all, no voids)

\* can use vectors to define unit cell

Simple Example:

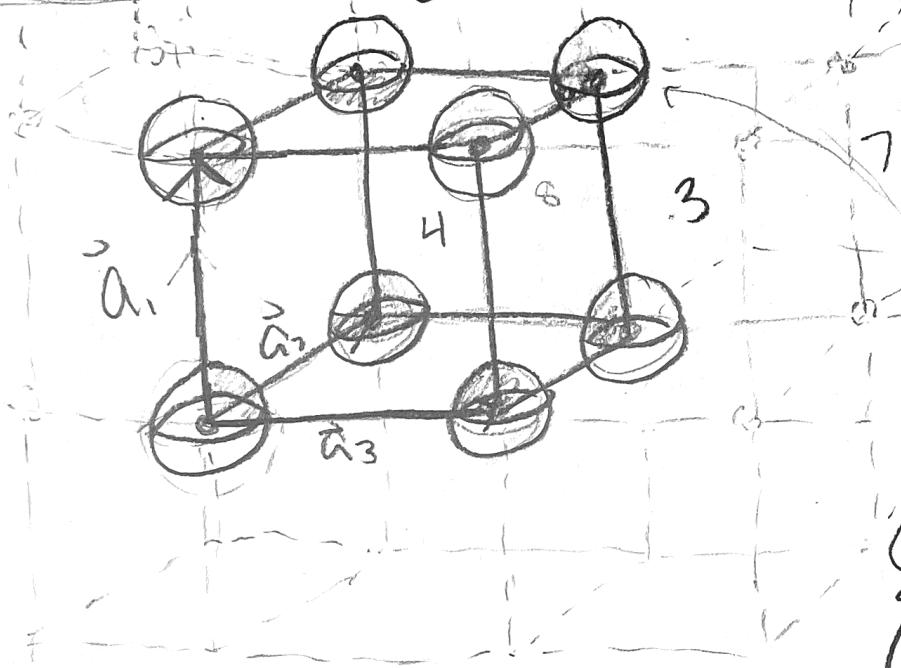
- can get to every atom w/ lattice vectors
- the origin can be moved, keeps it identical

•  $\vec{a}_1$  and  $\vec{a}_2$  are called lattice vectors

↳ my "stamp", no voids in structure, stamp all space



3D unit cell:



# of particles in unit cell = 1

$$\text{Packaging fraction} = \frac{\text{Volume}}{\text{Cell}} \cdot \frac{\# \text{ atoms}}{\text{cell}}$$

\* unit cell used to stamp & make entire crystal lattice

\* Note:

↳ How many atoms does this atom share unit cells w/?

{ 4 in one place  
4 in another place  
{  $\frac{1}{8}$  of atom in unit cell ↑

Another way to think about it is that there's only one atom per basis vector

↳ you stamp w/ basis vectors around 1 atom per basis vector comb'd

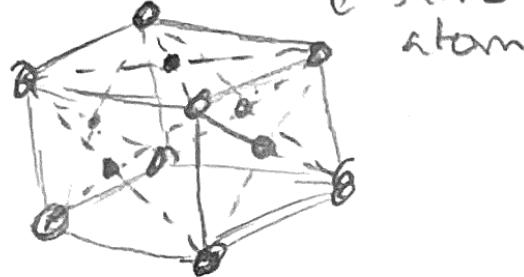
Reiterate definition:

Lattice: How to repeat

Basis: What to repeat

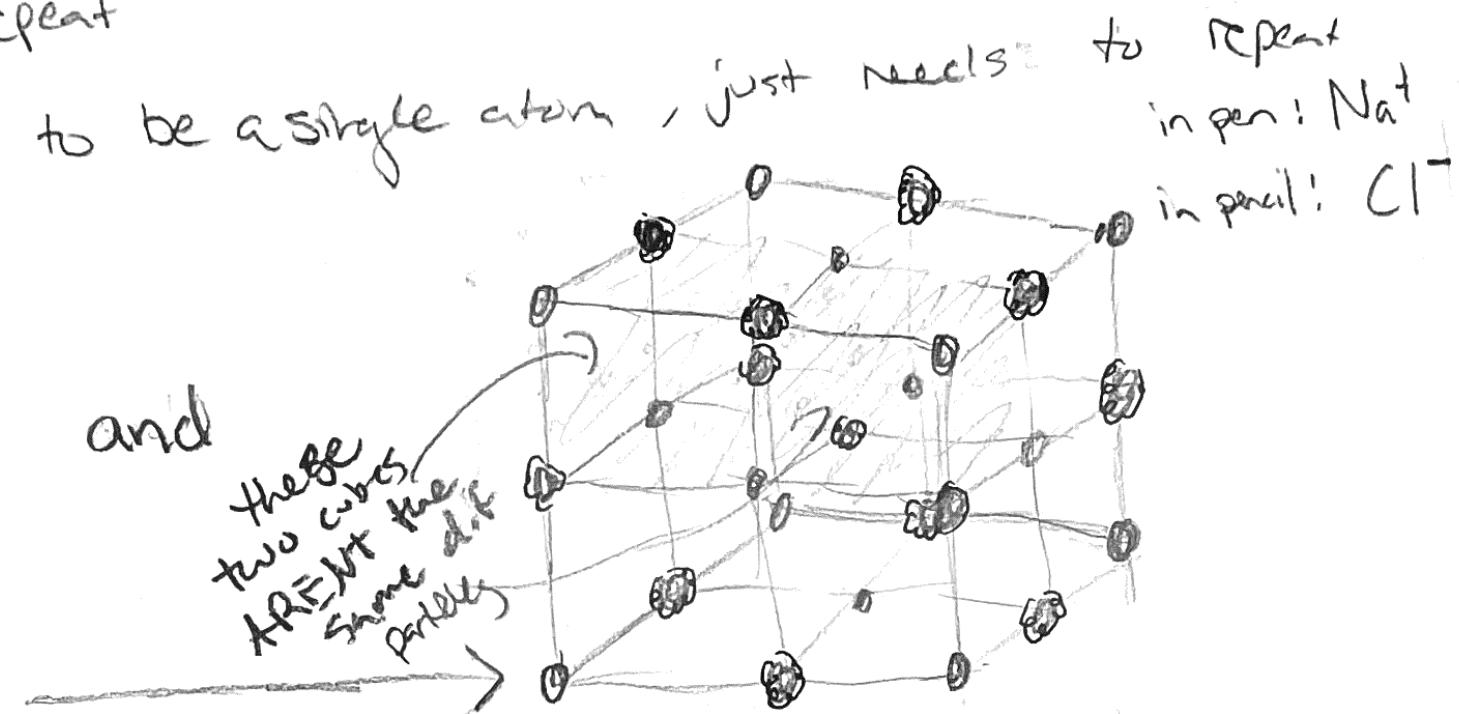
\*Basis doesn't have to be a single atom, just needs to repeat

Consider



and

these two works  
because they  
have diff  
sites



you think oh!

that is simple  
case

But that doesn't work, so it's really a  
face centered cell, that you can stamp the lattice w/

# Bravais Lattices

\* primitive cell: very smallest component of a lattice which when stacked together makes the lattice

↳ another def w/out lattice operations: smallest component of a lattice that can be repeated to reproduce whole structure AND containing only one lattice point

\* no one unique choice of primitive cell, just needs that minimum area/volume.

\* smallest possible volume: 1) only one lattice point 2) minimum number of atoms in basis?

↳ [# of lattice points def] → if a lattice point is shared by m adjacent unit cells around that lattice point, then the point is counted as  $\frac{1}{m}$

## Origin of Bravais Lattice Concept

\* any lattice can be defined by length of its two primitive translation vectors and the angle between them.

↳ infinite number of possible lattices one can describe this way (N.)

[Categorize lattices based on symmetry] or [impose cond. on length of prim trans vectors & angle]

\* These symmetries are categorized into different types \*

↳ point groups (mirror symmetries, inversion symmetries, rotation symmetries)

↳ translational symmetries

2D \* rotational invariance over  $2\pi$  and  $\pi$  (1 and 2-fold symmetry) & all 2D lattices  
 ↳ called oblique lattices { 1 oblique + three 4 = 5 Bravais lattices in 2D }

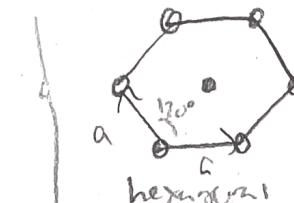
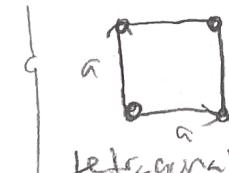
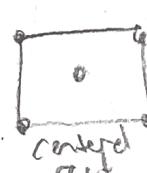
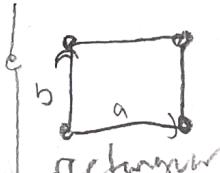
4 types of restrictions on lengths/angles of prim trans vectors → square, hexagonal, rectangular, centered rectangular

## 3D 14 Bravais lattices

1. waste basket category: triclinic, then monoclinic, orthorhombic, tetragonal, cubic, trigonal, hexagonal

pictures on the back

## 2D Cells



$$\text{area} = |a \times b|$$

Lattice System      Primitive      Base-Centred      Body-centred      Face-Centred

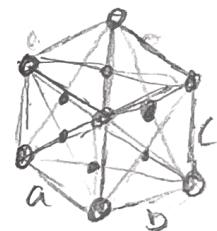
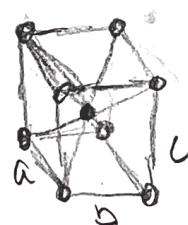
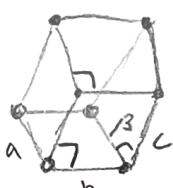
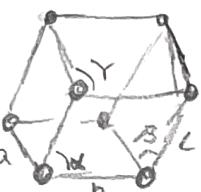
Triclinic

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

Monoclinic

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

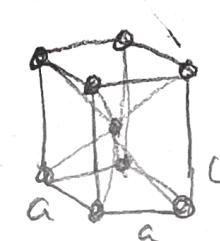
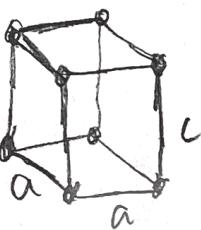
Orthorhombic



Tetragonal

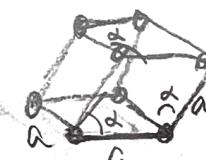
$$a = b$$

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



Hexagonal

Rhombohedral  
 $\alpha = \beta = \gamma$   
 $a = b = c$



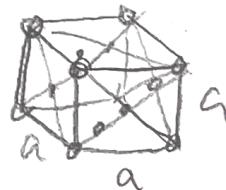
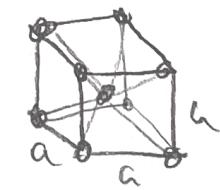
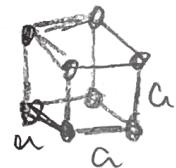
Hexagonal  
 $a = b$   
 $\alpha = \beta = 90^\circ$   
 $\gamma = 120^\circ$



Cubic

$$a = b = c$$

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



# Brillouin Zone Construction

- Brillouin Zone: is any primitive cell of the reciprocal lattice

\* physical waves in crystals are unchanged if their wave vector is shifted by a reciprocal lattice vector  $\vec{k} \rightarrow \vec{k} + \vec{G}$

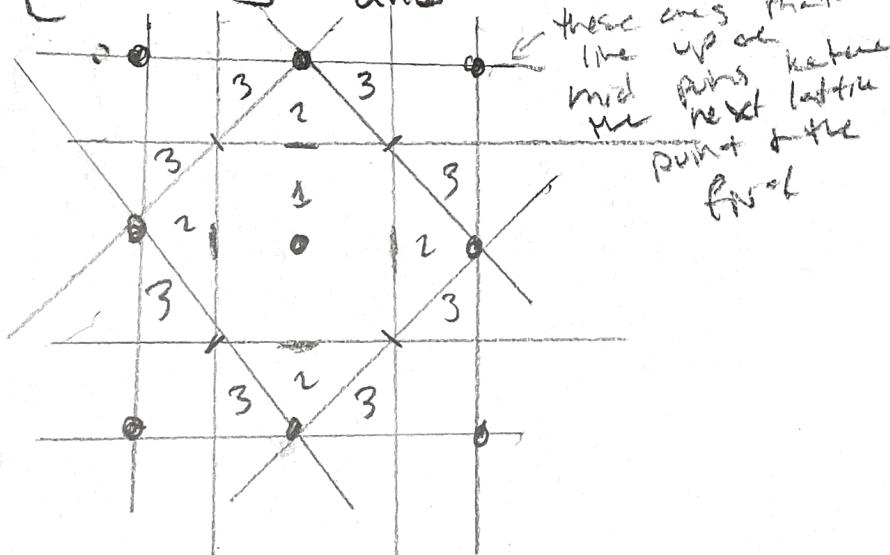
↳ Brillouin zone is defined to include each different crystal momentum once (one lattice point)

→ X-rays have different rules involving their wave length

[Can make any primitive unit cell a Brillouin zone, but for now, construct one analogously to Wigner-Seitz cell for direct lattice]

Definition! Start w/  $\vec{G} = 0$ , all  $\vec{k}$ -points that are closest to 0 define the first Brillouin zone, second & so on

↳ [construct the zones] → Draw perpendicular bisector between the point 0 and each of the reciprocal lattice vectors



these ones that  
lie up on  
mid paths between  
the next lattice  
point & the  
first

\* Each zone has the  
same area, or volume

# Miller Indices

\* notation for describing lattice planes (or reciprocal lattice vectors)

1) choose vectors  $\vec{a}_i$  for unit cell in direct space (primitive or non)

2) construct  $\vec{b}_j$  vectors (satisfy  $\vec{a}_i \cdot \vec{b}_j = 2\pi S_{ij}$ )

↳ write  $(h k l) \rightarrow \vec{b}_{(hkl)} = h \vec{b}_1 + k \vec{b}_2 + l \vec{b}_3$

## [Note]

\* if  $\vec{a}$  make primitive lattice then  $\vec{b}$  will be

the primitive lattice vectors for reciprocal lattice

↳  $(hkl)$  represent a reciprocal lattice vector

↳ to represent a family of lattice planes, take shortest  
reciprocal lattice vector,  $h, k, l$  have no common  
divisors

↳ (if they share divisors, then they aren't the shortest  
reciprocal lattice vector, then it doubles meaning  
some planes don't hit lattice points)

\* if conventional cell for  $\vec{a}$  then  $\vec{b}$  will not  
be primitive reciprocal lattice vectors,

↳ THEN not all integer sets of miller indices  
will be reciprocal lattice vectors

## Selection Rules for Miller Indices

$$d_{(hkl)} = \frac{2\pi}{|G|} = \frac{2\pi}{G \cdot G} = \frac{2\pi}{\sqrt{h^2 b_1^2 + k^2 b_2^2 + l^2 b_3^2}}$$

assuming forms an orthogonal basis

↳ the magnitude of  $\vec{b}$  for orthogonal basis reduces to  $|\vec{b}| = \frac{2\pi}{|a_i|}$

[Rewriting]  $\rightarrow \frac{1}{|d|^2} = \frac{h^2}{a_1^2} + \frac{k^2}{a_2^2} + \frac{l^2}{a_3^2}$  [for cubic case]  $\rightarrow d_{(hkl)} = \sqrt{h^2 + k^2 + l^2}$

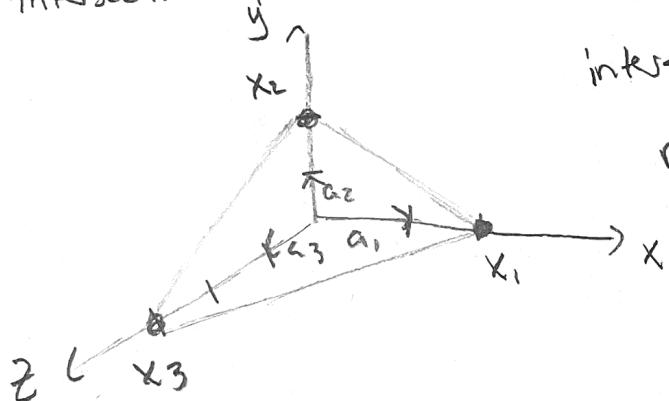
[Shortcut for figuring out geometry of lattice planes] → look at intersection of plane w/ 3 coordinate axes (in units of lattice constants)

intersection points  $x_1, x_2, x_3 \rightarrow \frac{1}{x_1} = h, \frac{1}{x_2} = k, \frac{1}{x_3} = l$

intersects at  $x=2, y=2, z=3$  (units of  $a$ )

reciprocals:  $\frac{1}{2}, \frac{1}{2}, \frac{1}{3}$

↳ smallest number to mult all by & for it not to be a frac  $\rightarrow 6 \text{ so } (3, 3, 2)$



[Assuming orthogonal axes]  $\rightarrow \frac{1}{d^2} = \frac{3^2}{a_1^2} + \frac{3^2}{a_2^2} + \frac{2^2}{a_3^2}$

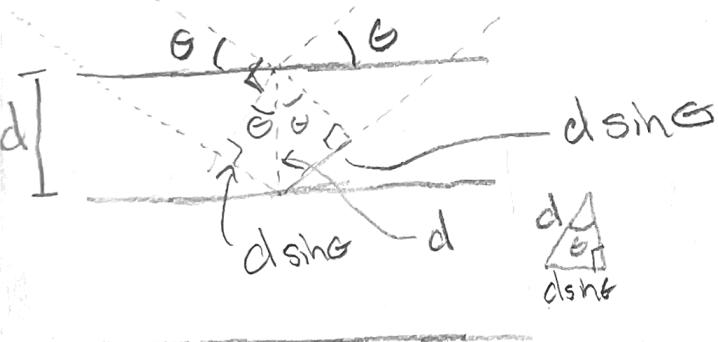
# Solid State Physics

## Chapter 2

Bragg eq derivation

$\theta$ : angle of incidence  
 $\theta_i = \theta_{\text{reflected}}$

\* Path length difference between the two is separated by 2d sinθ



if that distance is λ or a wave length, the two will meet up in add., thus for constructive interference

the ones we see :

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

\* Bragg gives nice statement for constructive interference,

↳ We want more, deeper analysis to determine scattering intensity from atoms (special dist. of electric field of atom)

### Fourier Analysis

integer multiple of basis vectors keeps you on an atom (crystal stays same)

$$\vec{T} = u_1 \vec{a}_1 + u_2 \vec{a}_2 + u_3 \vec{a}_3 \quad (\vec{a}_1, \vec{a}_2, \vec{a}_3 \text{ are crystal axes})$$

$n(\vec{r})$  = electron number density and thus  $n(\vec{r} + \vec{T}) = n(\vec{r})$

[This periodicity leads itself]  $\rightarrow n(x) = n_0 + \sum_{p \geq 0} [C_p \cos(\frac{2\pi p}{a} x) + S_p \sin(\frac{2\pi p}{a} x)]$   
 [well to Fourier analysis]

{ensures  $n(x)$  has period a}  
 {or spacing of atoms}  
 $n(x+a) = n(x)$

\*  $\frac{2\pi p}{a}$  = point in reciprocal lattice  
 or Fourier space of crystal

Reciprocal lattice points tell us allowed terms in Fourier series

$$n(x) = \sum_p n_p e^{i \frac{2\pi p}{a} x}$$

lumped constant

$$\text{require } n^*_{-p} = n_p$$

$\frac{1}{a}$  (reciprocal!)

$$(\vec{G} \cdot \vec{r})_x = \frac{2\pi p}{a} x$$

3D

$$n(\vec{r}) = \sum_{\vec{G}} n_G e^{i\vec{G} \cdot \vec{r}}$$

find a set of vectors  $\vec{G}$  such that  
 $n(\vec{r})$  is invariant under all  
crystal transformations  $\vec{T}$

(getting Fourier coefficients)

$$n_0 = \frac{1}{a} \int_0^a dx n(x) e^{-i\frac{2\pi}{a} x} \quad \text{or} \quad n_0 = \frac{1}{V_i} \int_{\text{cell}} dV n(\vec{r}) e^{-i\vec{G} \cdot \vec{r}}$$

[Second Tool, Reciprocal lattice Vectors]

↳ find vectors  $\vec{G}$

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

$a_1, a_2, a_3$  = primitive vectors of crystal lattice

$b_1, b_2, b_3$ : primitive vectors of reciprocal crystal lattice

and  $\boxed{\vec{G} = v_1 \vec{b}_1 + v_2 \vec{b}_2 + v_3 \vec{b}_3}$ . reciprocal lattice vector

$$n(\vec{r} + \vec{T}) = \underset{\text{Fourier}}{\underset{\text{expanded}}{\sum}} n_G e^{i\vec{G} \cdot \vec{r}} e^{i\vec{G} \cdot \vec{T}}$$

and scalar

$$e^{i\vec{G} \cdot \vec{T}} = e^{i(v_1 b_1 + v_2 b_2 + v_3 b_3) \cdot (a_1 a_1 + a_2 a_2 + a_3 a_3)} = e^{i(2\pi(v_1 u_1 + v_2 u_2 + v_3 u_3))}$$

$$e^{2\pi i} = 1$$

↳  $\boxed{\text{We proved that the } \vec{b} \text{ vectors keep the inversion we needed}}$   $\rightarrow n(\vec{r} + \vec{T}) = \sum n_G e^{i\vec{G} \cdot \vec{r}} e^{i\vec{G} \cdot \vec{T}} = \sum n_G e^{i\vec{G} \cdot \vec{r}} = n(\vec{r})$

## Additional Clarifying notes

$$\vec{k} = \vec{G} = V_1 \vec{b}_1 + V_2 \vec{b}_2 + V_3 \vec{b}_3 , \quad \vec{T} = U_1 \vec{a}_1 + U_2 \vec{a}_2 + U_3 \vec{a}_3$$

We saw:  $(\vec{G} \cdot \vec{G})^{\frac{1}{2}} = \text{needed to equal 1, condition} = 1$

$$\hookrightarrow \text{so } \vec{G} \cdot \vec{T} = 2\pi m$$

$$\text{Generally: } \vec{G} \cdot \vec{T} = V_1 U_1 \vec{a}_1 \cdot \vec{b}_3 + V_1 U_2 \vec{a}_2 \cdot \vec{b}_3 + V_1 U_3 \vec{a}_3 \cdot \vec{b}_3 \\ + V_2 U_1 \vec{a}_1 \cdot \vec{b}_2 + V_2 U_2 \vec{a}_2 \cdot \vec{b}_2 + V_2 U_3 \vec{a}_3 \cdot \vec{b}_2 \\ + V_3 U_1 \vec{a}_1 \cdot \vec{b}_1 + V_3 U_2 \vec{a}_2 \cdot \vec{b}_1 + V_3 U_3 \vec{a}_3 \cdot \vec{b}_1$$

$$= (V_1 \ V_2 \ V_3) \begin{bmatrix} \vec{b}_3 \cdot \vec{a}_3 & \vec{b}_2 \cdot \vec{a}_3 & \vec{b}_1 \cdot \vec{a}_3 \\ \vec{b}_2 \cdot \vec{a}_2 & \vec{b}_1 \cdot \vec{a}_2 & \vec{b}_3 \cdot \vec{a}_2 \\ \vec{b}_1 \cdot \vec{a}_1 & \vec{b}_3 \cdot \vec{a}_1 & \vec{b}_2 \cdot \vec{a}_1 \end{bmatrix} \begin{pmatrix} U_1 \\ U_2 \\ U_3 \end{pmatrix} = 2\pi m$$

defining dot product      "changing basis to reciprocal lattice basis"

\* can choose  $b$  basis to be for  $\vec{G}$ , let's pick easiest one orthogonal to  $a$   
think quantum, can make basis of vector anything, choose simplest one.

$$\hookrightarrow \boxed{\vec{b}_1 \cdot \vec{a}_j = 2\pi S_{ij}} \quad \text{use this to construct } b \text{ basis}$$

$$\hookrightarrow \text{a result} \rightarrow (V_1 \ V_2 \ V_3) \begin{bmatrix} 2\pi & 0 & 0 \\ 0 & 2\pi & 0 \\ 0 & 0 & 2\pi \end{bmatrix} \begin{pmatrix} U_1 \\ U_2 \\ U_3 \end{pmatrix} = 2\pi m \rightarrow U_1 V_1 + U_2 V_2 + U_3 V_3 = m$$

use the condition] choose  $b_1 \cdot a_j = 0$  conditions

$$\hookrightarrow \vec{b}_1 \cdot \vec{a}_2 = \vec{b}_1 \cdot \vec{a}_3 = 0 \rightarrow \vec{b}_1 = C \cdot \vec{a}_2 \times \vec{a}_3 \quad \left( \begin{array}{l} b_1 \text{ is a vector perpendicular} \\ \text{to } a_2 \text{ and } a_3, \text{ w/ a} \\ \text{scalar} \end{array} \right)$$

because of these defining dot products

$$\rightarrow \vec{a}_1 \cdot \vec{b}_1 = C \cdot \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = 2\pi \rightarrow a_1 \cdot b_1 = 2\pi$$

so  $C = \frac{2\pi}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \rightarrow$  volume of parallelepiped spanned by 3 primitive translation vectors, of the original bravais lattice

By similar manner;

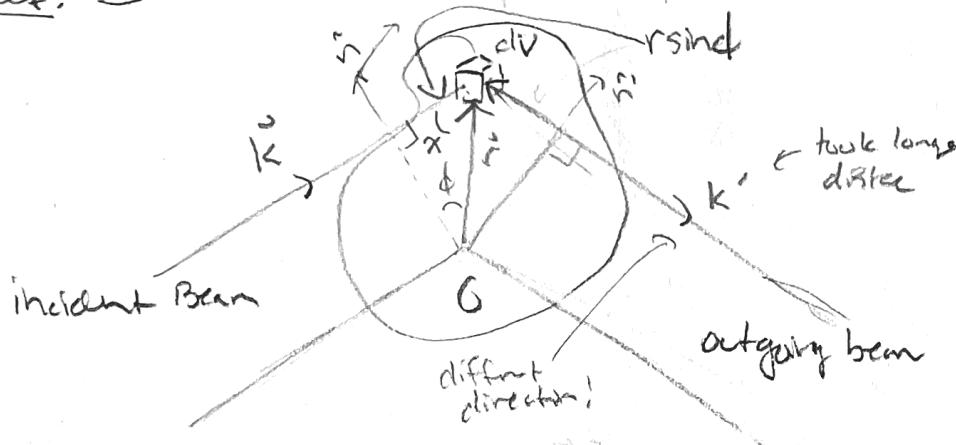
$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{V}, \quad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{V}, \quad \vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{V}$$

just like  
matrix  
multiplication  
.....

# Diffraction Conditions

$\tilde{G} = \{\tilde{b}_1, \tilde{b}_2, \tilde{b}_3\}$  determines possible X-ray reflections

Proof:  $\rightarrow$



difference in path length

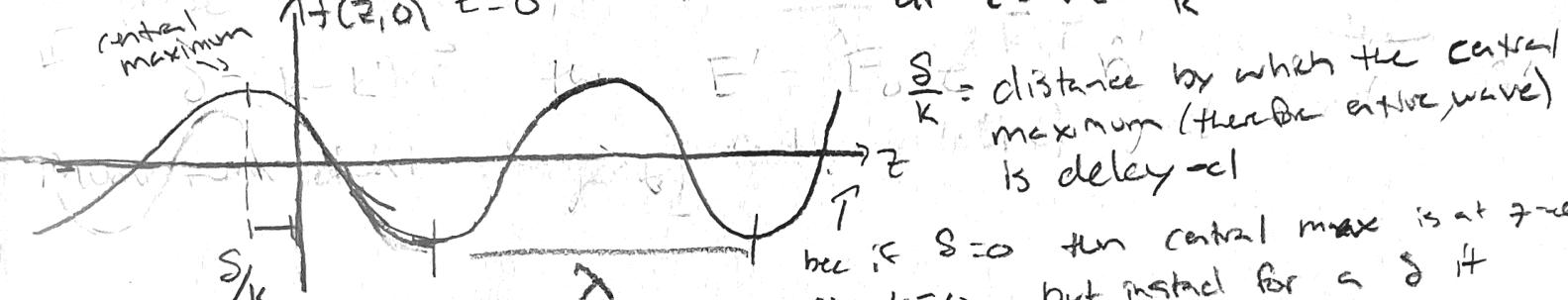
$$= 2\pi r \sin \theta$$

leads to a diff in phase

$$\frac{2\pi r \sin \theta}{\lambda} \quad \frac{2\pi}{\lambda} = K$$

Consider the function  $f(z, t) = A \cos(k(z - vt) + S)$  that satisfies the wave eq

$$\nabla f(z, 0) \quad t=0$$



bec if  $S=0$  then central max is at  $z=0$  at  $t=0$ , but instead for  $\approx S$  it is shifted

Generalizing to 3D,  $S = k \cdot \vec{r}$

Our phase is  $S = \vec{k} \cdot \vec{r} = \frac{1}{2} 2\pi r \sin \theta$  or  $\cos(\frac{3\pi}{2} - \theta) = \sin \theta$

$$\hookrightarrow \vec{k} \cdot \vec{r} = kr \cos(\alpha) = kr(\frac{\pi}{2} - \phi) = kr \sin \phi \quad \text{or}$$

↑ sign of  $\vec{k}$  & its angle between, otherwise  $\pi + \text{that}$  but that  $\pi$  adds up to  $\cos$

$$\hookrightarrow \vec{k} \cdot \vec{r} = \frac{2\pi r}{\lambda} \sin \theta$$

or total diff in phase angle

$$S_{\text{tot}} = S_{\text{inc}} + S_{\text{ref}} = \vec{k} \cdot \vec{r} + S_{\text{rec}} = \vec{k} \cdot \vec{r} - \vec{k}' \cdot \vec{r}$$

$\vec{k} \cdot \vec{r} - \vec{k}' \cdot \vec{r}$  = distance the central maximum is displaced here, ahead in this case of  $\phi$