Lecture 10

Reciprocal Lattice & Brillouin Zone.
R.L. BZ

in 1D $R_n = na$ $n = 1, 2, 3, \ldots$

def: Given a direct lattice point R, a point G is a point in the reciprocal lattice if and only if:

$$e^{i\bar{G}\cdot\bar{R}} = 1$$

To construct the reciprocal lattice we write down

$$R = n_1 a_1 + n_2 \bar{a}_2 + n_3 a_3$$

a_1, a_2, a_3 are primitive lattice vector

Two points to claim:

1.) the reciprocal lattice as defined by $e^{iG\cdot R} = 1$ is also a lattice but in the reciprocal space

2) The primitive reciprocal lattice vectors are connected to the direct ones as

$$\bar{a}_i \cdot \bar{b}_j = 2\pi\,\delta_{ij} \qquad \delta = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

To keep this relation we can construct

$$\bar{b}_1 = \frac{2\pi\ \bar{a}_2 \times \bar{a}_3}{a_1\cdot(\bar{a}_2 \times \bar{a}_3)} \longleftarrow \text{volume span by } \bar{a}_1, \bar{a}_2\ \bar{a}_3$$

$$\bar{b}_2 = \frac{2\pi\ \bar{a}_3 \times \bar{a}_1}{}$$

$$\bar{b}_3 = \frac{2\pi\ \bar{a}_1 \times a_3}{}$$

Lets check e.g.

$$\bar{a}_1\cdot\bar{b}_1 = \frac{2\pi\ \cancel{a_1\cdot(a_2\times a_3)}}{\cancel{a_1\cdot(a_2\times a_3)}} = 2\pi$$

$$\bar{a}_2\cdot\bar{b}_1 = \frac{2\pi\ \overbrace{a_2\cdot(a_2\times a_3)}^{=0}}{a_1\cdot(a\times a_3)} = 0$$

Lets prove that $b_1\ b_2\ b_3$ are also primitive

To prove this we write an arbitrary point in the reciprocal space as

$$\bar{G} = m_1 \bar{b}_1 + m_2 \bar{b}_2 + m_3 \bar{b}_3 .$$

and lets assume m_1, m_2, m_3

Lets form:

$$e^{i\bar{G}\cdot\bar{R}} = e^{i(m_1\bar{b}_1 + m_2\bar{b}_2 + m_3\bar{b}_3)\cdot(n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3)} = e^{2\pi i (n_1 m_1 + n_2 \cdot m_2 + n_3 \cdot m_3)}$$

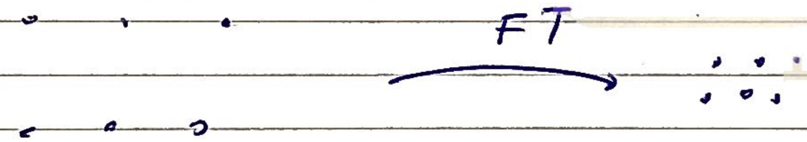
we know $n_1\ n_2\ n_3$ are integer

so to satisfy $e^{iGR} = 1$

$m_1\ m_2\ m_3$ must be integer as well.

RECIPROCAL LATTICE AS A FOURIER TRANSFORMATION

Direct lattice



Lets start with $R_n = a \cdot n$

we can introduce the density of lattice points

$$\rho(r) = \sum_n \delta(r - an)$$

$$F(\rho(r)) = \int dr\, e^{ikr} \rho(r) = \sum_n \int dr\, e^{ikr} \delta(r - an)$$

$$= \sum_n e^{ikan} = \frac{2\pi}{a} \sum_m \delta\left(k - \frac{2\pi m}{a}\right)$$

property of δ function

Poisson ressumation formula

Note $e^{ikan} = 1$ if $k = \frac{2\pi m}{a}$

and we get infinity in the $\sum$.

if $k \neq \frac{2\pi m}{a}$ the sum oscillates arround "0" and the total is zero.

in 3D

$$F(\rho(r)) = \underbrace{\sum_R e^{ik\cdot R}}_{\text{sum over point } R} = \frac{(2\pi)^D}{V} \sum_G \delta^D(k-G)$$

this is the sum over points $\bar{G}$

D is the dimensionality 1, 2, 3
and δ^D is the D dimentional ~~wav~~ function
e.g. $\delta(\bar{r}-\bar{r}_0) = \delta(x-x_0)\,\delta(y-y_0)$

Again if k is the point of the reciprocal lattice then $e^{ik\cdot R} = 1$ and the $\Sigma \to \infty$ otherwize 0.

So we get the reciprocal lattice ∞ peaks

FT of any periodic function

e.g. $\bar{a}_1 = a\bar{x}$ $\quad a_2 = a\bar{y}$ $\quad a_3 = a\bar{z}$

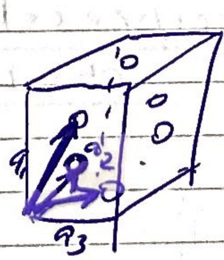
1) cubic lattice $\rightarrow$ $\bar{b}_1 = \frac{2\pi}{a}\bar{x}$

$\bar{b}_2 = \frac{2\pi}{a}\bar{y}$

$\bar{b}_3 = \frac{2\pi}{a}\bar{z}$

2) fcc with a conventional u.c

$$\begin{cases} a_1 = \frac{a}{2}(\bar{y}+\bar{z}) \\ a_2 = \frac{a}{2}(\bar{z}+\bar{x}) \\ a_3 = \frac{a}{2}(\bar{x}+\bar{y}) \end{cases}$$



$b_1 = \frac{4\pi}{a}\frac{1}{2}(y+z-x)$ $\quad b_2 = \frac{4\pi}{a}\frac{1}{2}(z+x-y)$

$b_3 = \frac{4\pi}{a}\frac{1}{2}(x+y-z)$

this is bcc!
with a side length of $\frac{4\pi}{a}$

FT of any periodic function

Lets have $\rho(\bar{r})$ which is periodic

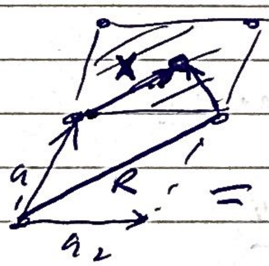
$\rho(\bar{r}+\bar{R}) = \rho(\bar{r})$ then

$$F[\rho(r)] = \int dr\, e^{ik\bar{r}} \rho(\bar{r}) =$$

$$= \sum_R \int_{\text{unit-cell}} d\bar{x}\, e^{i(x+R)} \rho(x+R) = \sum_R e^{ik\cdot R} \int_{U.C} dx\, e^{ikx} \rho(x) =$$

x - is any vector within the unit cell.

ρ is invariant unto $x \to x+R$



$$= (2\pi)^D \sum_G \delta^D(k-G) \cdot S(k)$$

Where $\boxed{S(k) = \int_{U.C} dx\, e^{ikx} \rho(x)}$

THE STRUCTURE FACTOR

=> SUPER IMPORTANT FOR ANY SCATTERING.

Reciprocal Lattice as FAMILIES OF LATTICE PLANES.

def. A lattice plane is a plane containing at least 3-non collinear point's of a lattice

def. A family of lattice planes is an infinite set of equally separated (parallel) lattice planes which taken all together contain ALL points of the lattice.

(see power point with examples).

Claim: 1) The families of lattice planes $\Longleftrightarrow$ are in 1-to-1 correspondance with the possible directions of reciprocal lattice vectors to which they are normal.

2). Spacing between these planes is

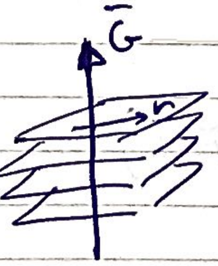
$$d = \frac{2\pi}{|\bar{G}_{min}|}$$

where $|\vec{G}|$ is min length of the reciprocal vector.

Consider a set of planes defined by points $\bar{r}$ such that

$$\bar{G}\cdot\bar{r} = 2\pi m$$

this describes an infinite set of parallel planes normal to G



but not each plane goes through the lattice points $\bar{r}$

the spacing is $d = \frac{2\pi}{G}$. To prove 2 adjacent planes must be $G(r_2 - r_1) = 2\pi(m+1-m) = 2\pi$

Thus the spacing is $\frac{2\pi}{G}$.

Clearly many different G will define parallel sets of planes
as G goes up the number of planes will go up. So whatever value of
we select there will be a plane which includes all lattice points.

Lattice planes and Miller indices. (M.i)

To describe lattice planes introduce useful notation. = Miller indices

1. Choose edge vectors $\bar{a}_i$ (primitive or not)
2. Construct $\bar{b}_j$ such as $\bar{a}_i \cdot \bar{b}_j = 2\pi\delta_{ij}$
3. In terms of those vectors write down h, k, l or (hkl) with h, k, l of the reciprocal vector.

$$G_{h,k,l} = \bar{h} b_1 + \bar{k} b_2 + \bar{l} b_3$$

the M.i. can be negative
e.g. $(1\ {-1}\ 1) \stackrel{\text{def}}{=} (1\bar{1}1)$

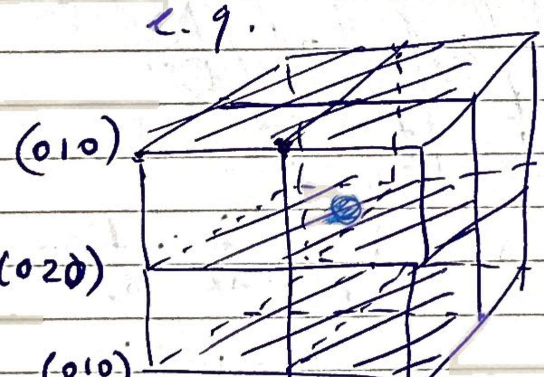
Since G defines a vector of reciprocal space to represent a family of lattice planes one needs to take the shortest reciprocal vector in the given direction =

so h, k, l should have no common divisors.

Otherwise h, k, l will represent the family of planes which is not a family of lattice planes (some lattice points are not on the plane)

Conversly, if we choose $\bar{a}_i$ the edge of the conventional unit cell then $\bar{b}_i$ will not be primitive reciprocal vectors

e.g.



(010) lattice planes.
which is fine and every lattice point in the plane

But for BCC we will miss one point by (010) planes
but will ~~hit~~ hit them with (020)

So the (020) is the true family of lattice points

~~The distance between planes:~~

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

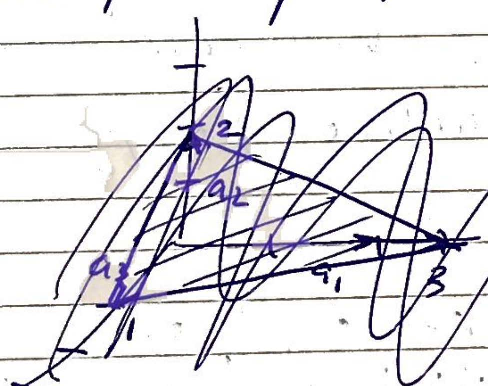
for orthogonal axis $|b_i| = 2\pi/|a_i|$ so

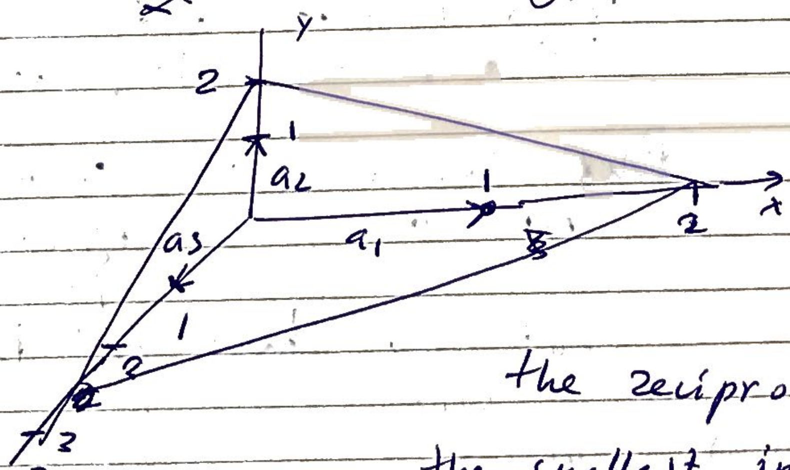
$$\frac{1}{|d_{hkl}|^2} = \frac{h^2}{a_1^2} + \frac{k^2}{a_2^2} + \frac{l^2}{a_3^2}$$

For cubic lattices:

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

Easy way to construct the planes:
LOOK AT THE INTERSECTION





$$\frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3} =$$

$$= h : k : l$$

intercepts at

$x = 2 \quad y = 2 \quad z = 3$

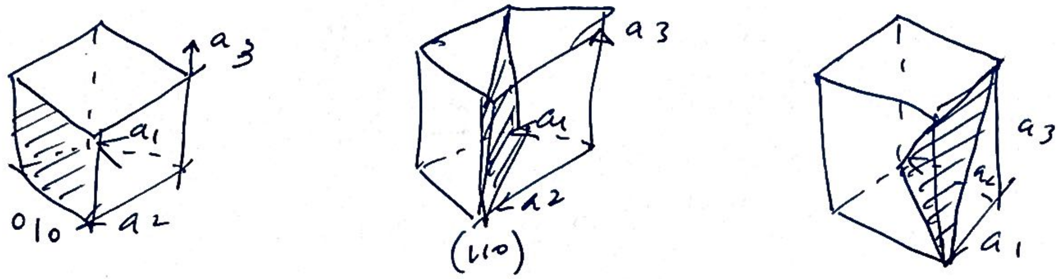
the reciprocals are $\frac{1}{2} \quad \frac{1}{2} \quad \frac{1}{3}$

the smallest integers havin those ratios 3 3 2

Thus the M.i of this lattic planes are (332)

The spacing $\frac{1}{|d_{332}|^2} = \frac{3^2}{a_1^2} + \frac{3^2}{a_2^2} + \frac{2^2}{a_3^2}$

L10



Ways to Specify directions:

(h, k, l) are Miller Indexes

- Thus the plane with intercepts 4, -2, 1 is called (4, -2, 1) plane
- The directions in the real space are given as [111]
- The collection of identical plane e.g. (010) (100) (001) = {100}

or {hkl} are (hkl) planes and all identical by symmetry

L 10

Brillouin Zone

Def. A BZ is any primitive u.c. of the reciprocal lattice (r.l.)

E.g.. a W.Z. primitive cell of the r.l. is the BZ.

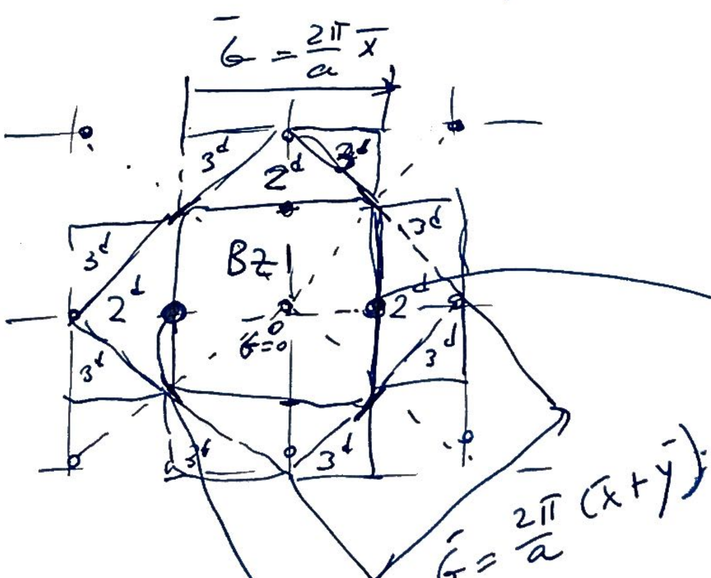
- Now because of the symmetry connections like

real fcc → reciprocal bcc

the BZ of fcc is fcc WZ cell.

To develop BZ:

Start with reciprocal lattice point $G=0$, create a W.Z. construction which will define the 1st BZ.



Note: - 1st BZ is Connected

- the higher order BZ are disconnected

→ The BZ boundary can be crossed by a vector from "0" to $+G$

$G = \frac{2\pi}{a}$

if we add to the point at the zone boundary $-\bar{G}$ it takes us to the other side of the BZ. Boundary

This means that BZ boundary pairs symmetric around o. occur in parallel.

L10

- Each BZ has exactly the same total <u>area</u> or volume in 3D.

- High symmetry points of the BZ are labeled as

$\Gamma\ (k=0)\ ,\ X = \left(\frac{2\pi}{a}\right)\bar{y}\ ,\ L\ ,\ K\ ,\ W\ ,\ M$