STEFANO
CURTAROLO

LATTICE THINGS

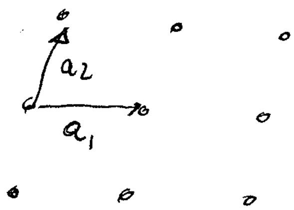
- DIRECT
- RECIPROCAL

NEED AM BOOK!

LATTICE

chap 4,7 A/M read

PERIODICITY



a) BRAVAIS LATTICE
infinite array of discrete points, exact images translated with a BRAVAIS LATICE

b) $\bar{R} = n_1 \bar{a}_1 + n_2 \bar{a}_2 + n_3 \bar{a}_3$

primitive vectors

PRIMITIVE UNIT CELL $\Downarrow$ CONTAINS 1 POINT

Linear combinations of $\bar{a}_1, \bar{a}_2, \bar{a}_3 \Rightarrow$ other primitive vectors

CUBIC , a

BCC $=$ $a_1 = a\hat{x}$ $\quad \bar{a}_2 = a\hat{y}$ $\quad \bar{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$

$\bar{a}_1 = \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z})$ $\quad \bar{a}_2 = \frac{a}{2}(\hat{x}-\hat{y}+\hat{z})$ $\quad \bar{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z})$

FCC $\quad a_1 = \frac{a}{2}(\hat{y}+\hat{z})$ $\quad a_2 = \frac{a}{2}(\hat{x}+\hat{z})$ $\quad a_3 = \frac{a}{2}(\hat{x}+\hat{y})$

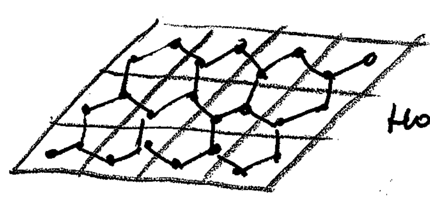
COORDINATION NUMBER # nearest neighbours

CUB $= 6$
BCC $= 8$
FCC $= 12$

PRIMITIVE & CONVENTIONAL

WIGNER & SEITZ — CONNECT TO NEIGHBOURS
— DRAW $\perp$ PLANE IN MEDIAN POINT

CRYSTAL WITH BASIS:



HONEYCOMB

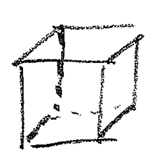
BCC CUBIC +
$0, \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$

FCC
$0 \quad \frac{a}{2}(\hat{x}+\hat{y}) \quad \frac{a}{2}(\hat{y}+\hat{z}) \quad \frac{a}{2}(\hat{z}+\hat{x})$

DIAMOND

HEXAGONAL c $\quad c = \sqrt{\frac{8}{3}}a = 1.63\,a$

DIRECTIONS
[1 0 0]

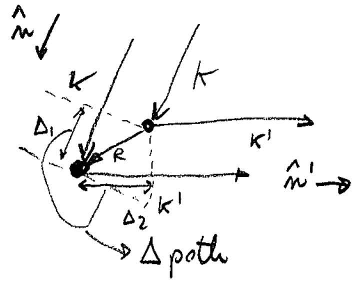


L 1

RECIPROCAL. chap 5, 6

VON LAUE construction

DIFFRACTION



K = incident wave

K' = diffracted

do they interfere CONSTRUCTIVELY?

if Δ path ~ m λ

Δ_1 = projection R over K ⇒ $\frac{\bar{R}\cdot\bar{K}}{|K|}$ R

Δ_2 = projection R over K' ⇒ $-\frac{\bar{R}\cdot\bar{K}'}{|K'|}$ =

because it is in the opposite direction

$$\Delta = \frac{\bar{R}\cdot(K-K')}{|K|} = m\lambda \quad \text{but} \quad K = \frac{2\pi}{\lambda}$$

$$\Rightarrow \boxed{\bar{R}\cdot(\bar{K}-\bar{K}') = 2\pi m}$$

$$\bar{R}\cdot\Delta\bar{K} = 2\pi m \Rightarrow \boxed{e^{i\bar{R}\cdot\Delta\bar{K}} = 1}$$

if $\bar{R} = n_1\bar{a}_1 + n_2\bar{a}_2 + n_3\bar{a}_3$

$$\Rightarrow \bar{K}\in\{\bar{G}\} = \underbrace{k_1}_{\text{integers}}\bar{b}_1 + k_2\bar{b}_2 + k_3\bar{b}_3 \quad \text{RECIPROCAL}$$

$$\boxed{b_i = 2\pi\frac{a_j\times a_k}{a_1\cdot(a_2\times a_3)}}$$

— $\bar{b}_i\cdot\bar{a}_j = \delta_{ij}$

$a_1\cdot(a_2\times a_3) = \det\begin{bmatrix} \vec{a}_1 \\ a_2 \\ a_3 \end{bmatrix}$ = Volume PRIMITIVE CELL

— $\bar{K}\cdot\bar{R} = 2\pi(\underbrace{k_1n_1 + k_2n_2 + k_3n_3}_{\text{integer}})$ ⇒

$v_R = \bar{a}_1\cdot(\bar{a}_2\times\bar{a}_3)$

$v_K = \frac{(2\pi)^3}{v_R}$

Reciprocal [Reciprocal] = Identity!

R1 | WIGNER SEITZ OF RECIPROCAL is BRILLOUIN ZONE

MILLER INDICES (h, k, l)

Plane with Miller indices (h, k, l) is $\perp$ to Reciprocal vector

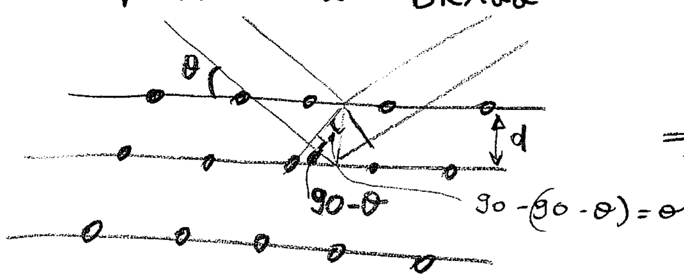
$$\left(h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3\right)$$

but where.

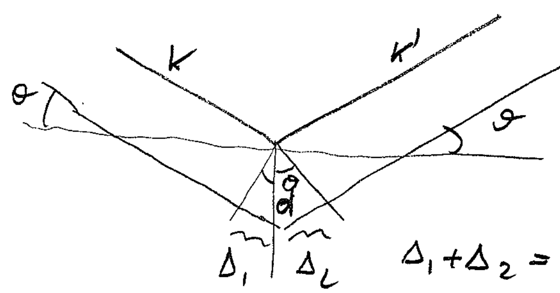
Miller: set of INTEGERS with NO COMMON FACTOR (?) inversely proportional to intercepts of crystal plane along crystal axes. $(h; k, l) = \frac{1}{x_1} : \frac{1}{x_2} : \frac{1}{x_3}$

EXAMPLES BOOK AM 93.

LAUE construction equivalent to BRAGG



$\Rightarrow$



$\Delta_1 + \Delta_2 = m\lambda$

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

in CUBIC depends on orientation

$$\boxed{d = \frac{a}{\sqrt{h^2+k^2+l^2}}}$$

in general

$$\boxed{\frac{(2\pi)^2}{d_{hkl}^2} = |\bar{g}|^2}$$

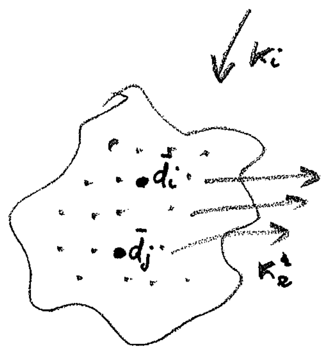
vector of reciprocal lattice

R12

STRUCTURE FACTOR
FOR CRYSTAL WITH n-basis

BRAGG peak is present when Δk is in reciprocal ~~group~~ lattice.

for a solid $e^{i(k'-k)\bar{R}} = 1$ $\forall \bar{R} \in$ BRAVAIS



$k_2^{\prime} - k_i = \bar{K}$ $\bar{d}_i - \bar{d}_j$ distance

$\bar{K}(\bar{d}_i - d_j)$ path difference $\Big\}$ total phase is $e^{i\bar{K}(d_i - d_j)}$ $\Rightarrow$

$\Rightarrow$ each point carries a phase

point$(i) \Rightarrow e^{i\bar{K}\cdot\bar{d}_i}$ phase

$\Rightarrow$ SUM OF ALL ~~PHASES will~~ decide Amplitude diffraction

basis

$$\boxed{S_{\bar{K}} = \sum_i^n e^{i\bar{K}\cdot\bar{d}_i}}$$

geometrical structure factor

$$I_K \propto |S_K|^2$$

$\Rightarrow$

BCC $\Rightarrow$ Reciprocal $[BCC] = FCC$ $\Rightarrow$ too pain to analize (we want cubic)

$BCC = CUBIC + 2\text{-base} \left[0, \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})\right]$

Reciprocal $[CUB] = CUB$ $b = \frac{2\pi}{a}$ $\bar{K} = (h\hat{x} + k\hat{y} + l\hat{z})\left(\frac{2\pi}{a}\right)$

$$S_K = \left[1 + e^{i\bar{K}\cdot\frac{1}{2}a(\hat{x}+\hat{y}+\hat{z})}\right] = \begin{cases} 2 & h+k+l = \text{even} \\ 0 & h+k+l = \text{odd} \end{cases}$$

get S Factor FOR FCC, MONO DIA HEX

DIFF FROM A POLYATOMIC CRYSTAL

$$S_K = \sum_i^n f_i(\bar{K}) e^{i\bar{K}\cdot\bar{d}}$$

then

depends on density of electrons of atom i

R3