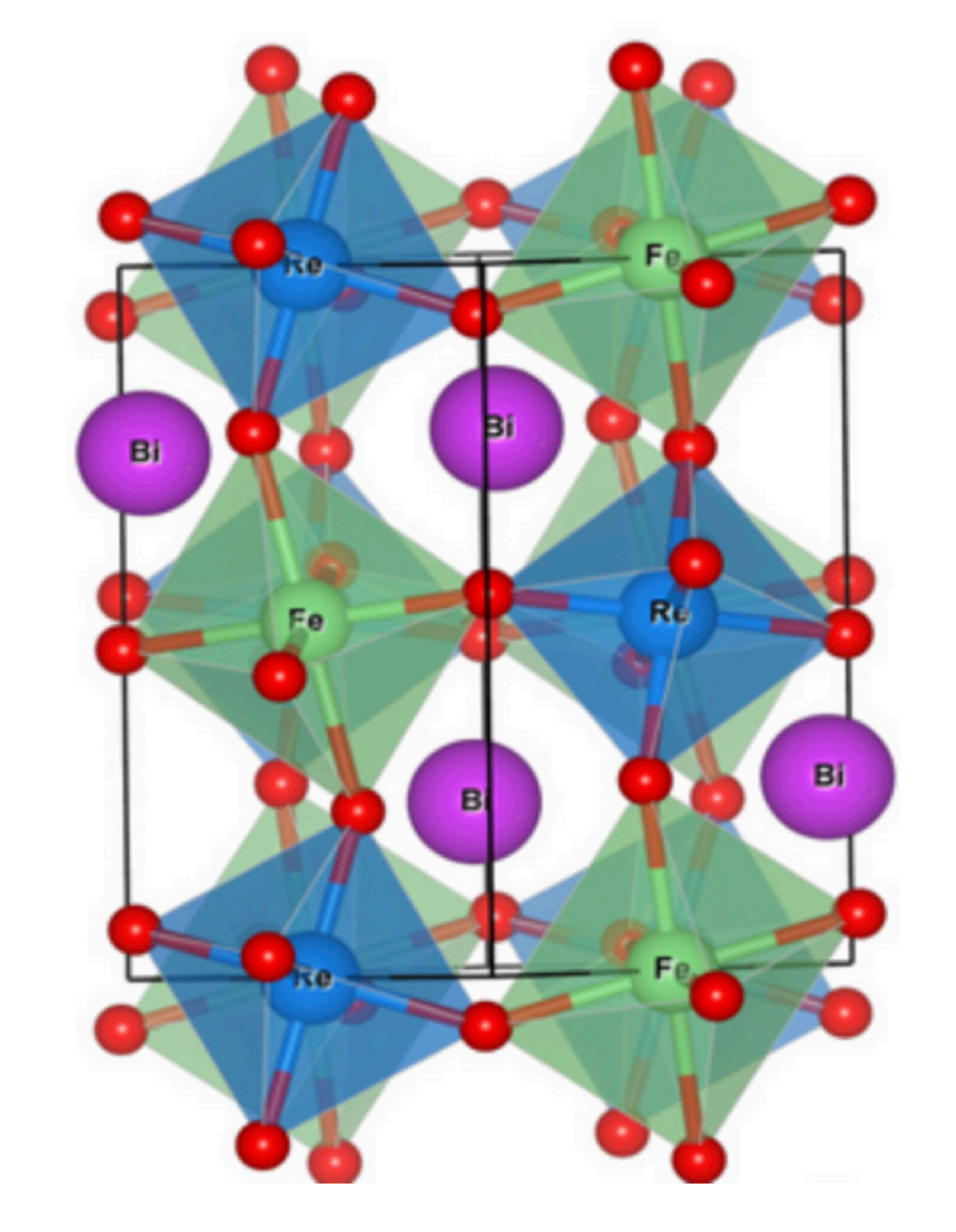

Structure of Solids - Reciprocal Lattice

Lecture 3

CHM 637
Chemistry & Physics of Materials

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Lecture Plan

- Introduction to the reciprocal lattice
- Fourier analysis in lattices

Interplanar distances and Miller indices

System	Interplanar spacing, d_{hkl}	Unit cell volume
Cubic	$1/d^2_{hkl} = [h^2 + k^2 + l^2]/a^2$	a^3
Tetragonal	$1/d^2_{hkl} = [(h^2 + k^2)/a^2] + [l^2/c^2]$	a^2c
Orthorhombic	$1/d^2_{hkl} = [h^2/a^2] + [k^2/b^2] + [l^2/c^2)]$	abc
Monoclinic	$1/d^2_{hkl} = [h^2/a^2 \sin^2 \beta] + [k^2/b^2] + [l^2/c^2 \sin^2 \beta] - [(2hl\cos \beta)/(ac \sin^2 \beta)]$	$abc \sin \beta$
Triclinic*	$1/d^2_{hkl} = [1/V^2] \{[S_{11}h^2] + [S_{22}k^2] + [S_{33}l^2] + [2S_{12}hk] + [2S_{23}kl] + [2S_{13}hl]\}$	$abc \sqrt{}(1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma)$
Hexagonal	$1/d^2_{hkl} = [4/3] [(h^2 + hk + k^2)/a^2] + [k^2/b^2] + [l^2/c^2)]$	$[\sqrt{}(3)/2] [a^2c] \approx 0.866\, a^2c$
Rhombohedral	$1/d^2_{hkl} = \{[(h^2 + k^2 + l^2 \sin^2 \alpha) + 2(hk + kl + hl) (\cos^2 \alpha - \cos \alpha]/[a^2(1 - 3 \cos^2 \alpha + 2\cos^3 \alpha)]\}$	$a^3 \sqrt{}(1 - 3 \cos^2\alpha + 2 \cos^3 \alpha)$

*$S_{11} = b^2c^2 \sin^2 \alpha$; $S_{22} = a^2c^2 \sin^2\beta$; $S_{33} = a^2b^2 \sin^2 \gamma$; $S_{12} = abc^2(\cos \alpha \cos \beta - \cos \gamma)$; $S_{23} = a^2bc(\cos \beta \cos \gamma - \cos \alpha)$; $S_{13} = ab^2c(\cos \gamma \cos \alpha - \cos \beta)$; $V =$ unit cell volume.

Reciprocal lattice

$(n_1, n_2, n_3) \longrightarrow$ Direct lattice $\quad n_i \in \mathbb{Z}$

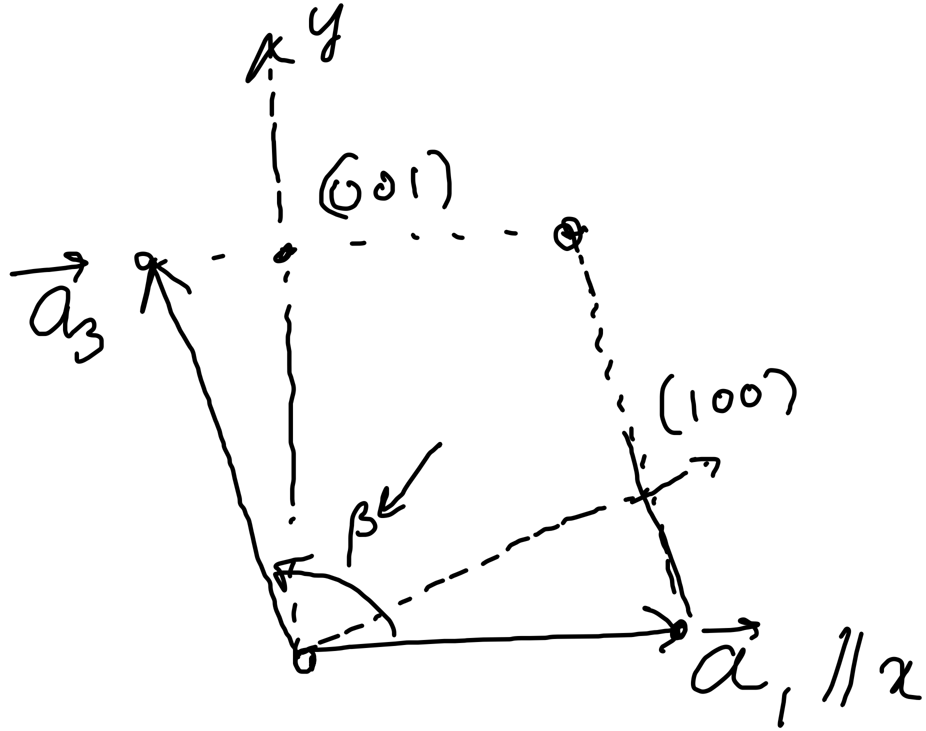
$(h, k, l) \longrightarrow$ Reciprocal lattice

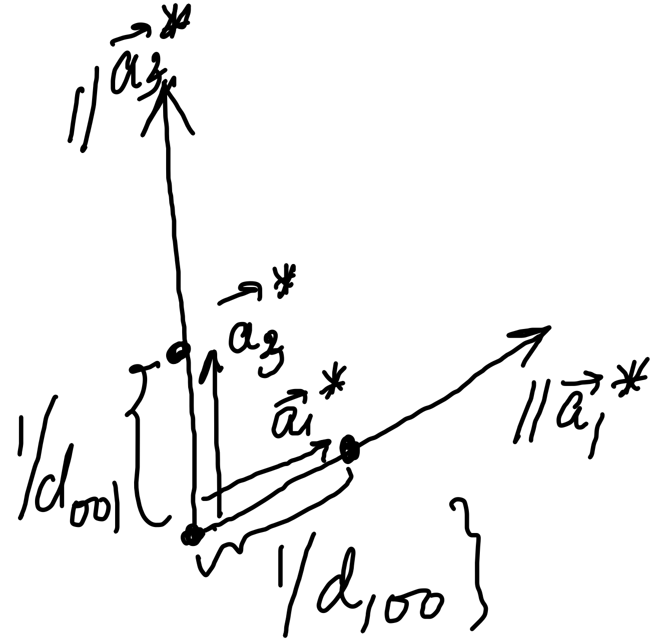
$\vec{a}_1, \vec{a}_2, \vec{a}_3 \longrightarrow$ lattice axes of the Direct lattice

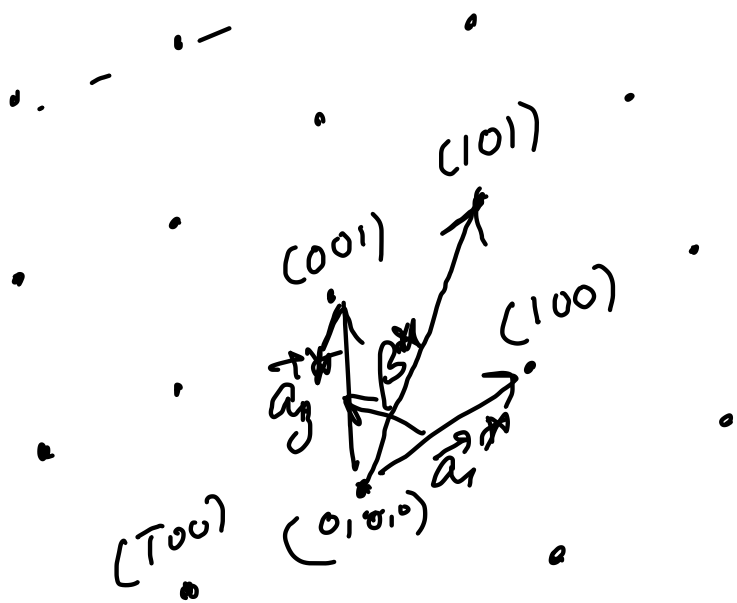
$\vec{a}_1^{\,*}, \vec{a}_2^{\,*}, \vec{a}_3^{\,*} \longrightarrow$ primitive reciprocal lattice vectors

$|\vec{a}_1^{\,*}| = 1/d_{100} \qquad |\vec{a}_3^{\,*}| = 1/d_{001}$

$|\vec{a}_2^{\,*}| = 1/d_{010}$

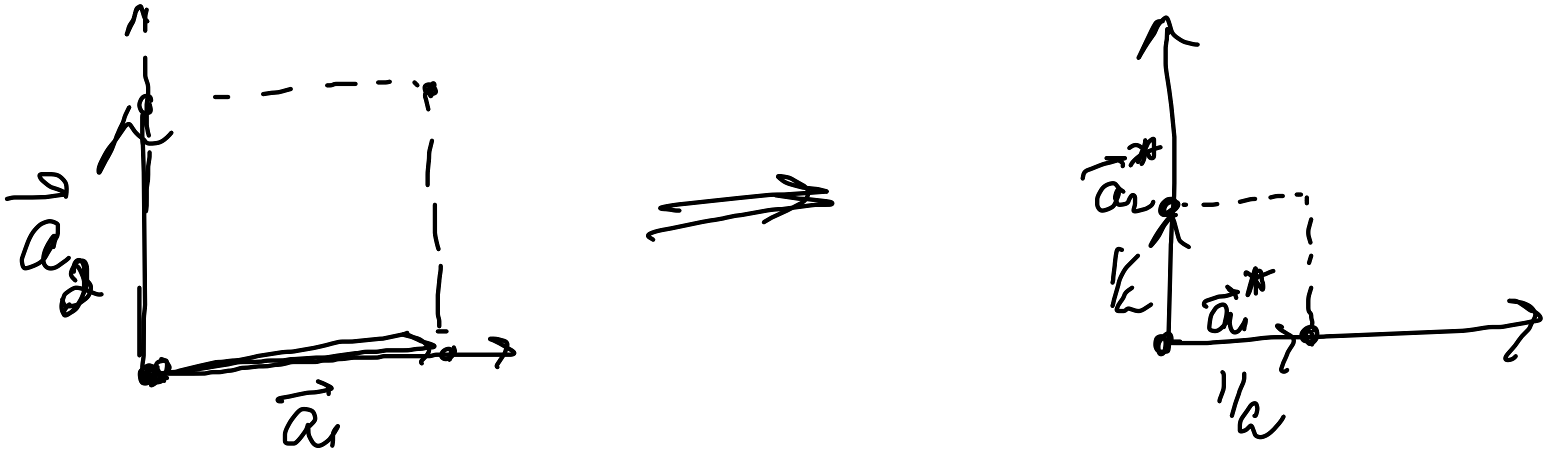


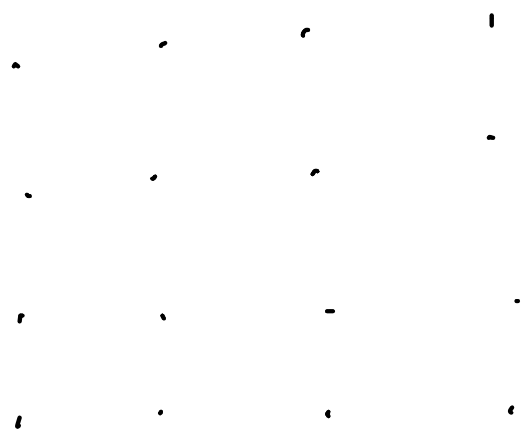




Reciprocal lattice

$1/d_{hkl}$


$\vec{a}_2$
$\vec{a}_1$
$\vec{a}_2^*$
$1/a$
$\vec{a}_1^*$
$1/a$



Fourier Series on a lattice

$$V(x \pm \underset{\wedge}{m} a) = V(x) \qquad m \in \mathbb{Z}$$

1-d periodic fn.

$$V(x) = \sum_{n=-\infty}^{\infty} e^{in\frac{2\pi x}{a}} V_n \rightarrow \text{F.S.}$$

where $V_n = \frac{1}{a}\int_0^a dx\, V(x)\, e^{-i\frac{2\pi n}{a}x}$

Fourier components

$$\frac{1}{a}\int_0^a e^{i\frac{2\pi(m-n)x}{a}} dx = \delta_{m,n}$$

For 3-dimensions, $\vec{a}_1, \vec{a}_2, \vec{a}_3 \rightarrow$ primitive lattice vectors

$$V(\vec{r} + \vec{R}) = V(\vec{r})$$

lattice vector $\leftarrow \vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$

$n_1, n_2, n_3 \in \mathbb{Z}$

$$\boxed{V(\vec{r}) = \sum_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} V_{\vec{G}}}$$

$\vec{g}_1, \vec{g}_2, \vec{g}_3 \rightarrow$ primitive reciprocal lattice vectors

$$\vec{G} = j_1 \vec{g}_1 + j_2 \vec{g}_2 + j_3 \vec{g}_3$$ → general reciprocal lattice vectors

$$j_1, j_2, j_3 \in \mathbb{Z}$$

$$\vec{g}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{[\vec{a}_1 \vec{a}_2 \vec{a}_3]}$$

$L^2 / L^3 \sim 1/L$

$[\vec{a}_1 \vec{a}_2 \vec{a}_3] \rightarrow \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$ $\equiv$ Vol. of ~~un~~ unit cell $= V$

$$\vec{g}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{[\vec{a}_1 \vec{a}_2 \vec{a}_3]}$$

$$\vec{g}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{[\vec{a}_1 \vec{a}_2 \vec{a}_3]}$$

$$V(\vec{r}) = \sum_{j_1} \sum_{j_2} \sum_{j_3} V_{j_1 j_2 j_3} \, e^{i \vec{r} \cdot (j_1 \vec{g}_1 + j_2 \vec{g}_2 + j_3 \vec{g}_3)}$$

$$= \sum_{\vec{G}} V_{\vec{G}} \, e^{i \underbrace{\vec{G} \cdot \vec{r}}}$$

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

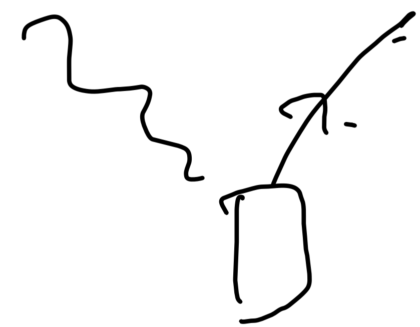
$$\vec{g}_i \cdot \vec{a}_j = 2\pi\,\delta_{i,j} \qquad \vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

$$V(\vec{r}+\vec{R}) = \sum_{\vec{G}} V_{\vec{G}}\, e^{i\vec{G}\cdot(n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3)} \times e^{i\vec{G}\cdot\vec{r}}$$

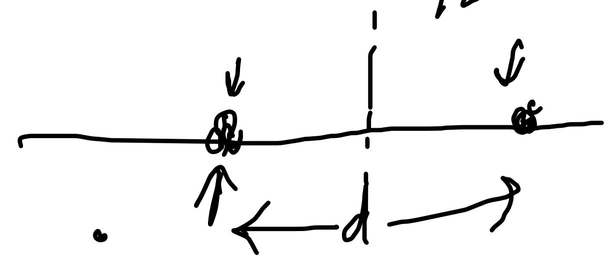
$$= \sum_{\vec{G}} V_{\vec{G}}\, e^{i\underline{(j_1 n_1 + j_2 n_2 + j_3 n_3)}2\pi} \times e^{i\vec{G}\cdot\vec{r}}$$

$$= \sum_{\vec{G}} V_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}} = V(\vec{r})$$

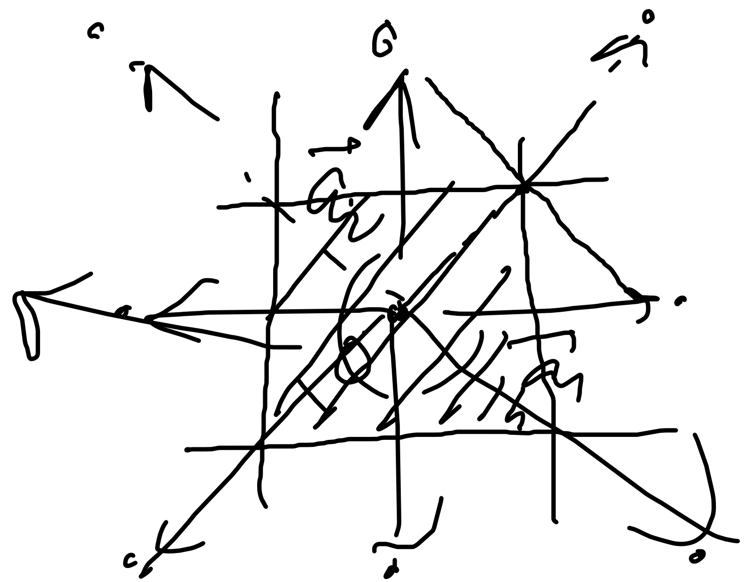
$\vec{g}_1, \vec{g}_2, \vec{g}_3$



Wigner-Seitz cell



Vol. of WS $= V$



$\{\vec{r}\}$.

$$\boxed{\int_{WS} e^{i(\vec{G}-\vec{G}')\cdot\vec{r}}\, d^3r = V_{WS}\, \delta_{\vec{G},\vec{G}'}}$$

$$\delta_{j_1,j_1'}\,\delta_{j_2 j_2'}\,\delta_{j_3 j_3'}$$

$$V_{\vec{G}} = \frac{1}{V_{WS}} \int_{WS} V(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, d^3r$$

$$V_{WS} = \left|\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)\right| = V$$

$$\vec{G} = j_1 \vec{g}_1 + j_2 \vec{g}_2 + j_3 \vec{g}_3$$

$$\vec{G} = (j_1, j_2, j_3)$$

→ common divisor $\Rightarrow$ reducible

→ no common divisor $\Rightarrow$ irreducible.

$(2, 4, 6) \rightarrow$ reducible

$(1, 2, 3) \rightarrow$ irreducible

Consider the set of all (direct) pts. $\vec{r}$, such that for a given $\vec{G} = (j_1, j_2, j_3)$ irreducible

we have $\boxed{\vec{G} \cdot \vec{r} = 2\pi}$

$$\Rightarrow \hat{G} \cdot \vec{r} = \frac{2\pi}{|\vec{G}|} = \frac{2\pi}{G}$$

$\vec{r} \cdot \hat{n} = d \longrightarrow$ eqn of a plane

$\Rightarrow \vec{r}$ lie on a plane whose normal is $\hat{G}$ & its distance from the origin is $2\pi/G$

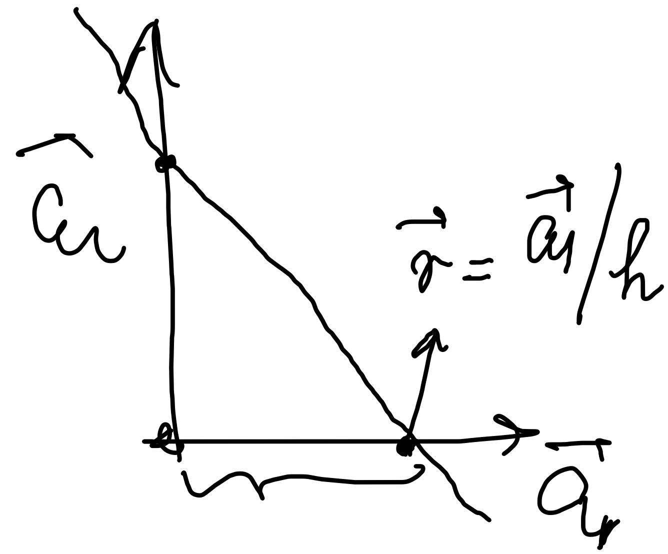
$$\vec{G} \cdot \vec{r} = 2\pi m$$

$m \in \mathbb{Z}$
$m > 0$

$$\hat{G} \cdot \vec{r} = \frac{2\pi}{G} m$$

A family of planes normal to $\hat{G}$ and separated by $2\pi/G = d$

$$\vec{G}\cdot\vec{r} = 2\pi$$



$$\vec{G}\cdot(\vec{a}_1/h) = 2\pi$$

$$\vec{G} = j_1\vec{g}_1 + j_2\vec{g}_2 + j_3\vec{g}_3$$

$$\vec{G}\cdot(\vec{a}_1/h) = 2\pi j_1/h = 2\pi$$

$$\Rightarrow j_1/h = 1 \text{ or } j_1 = h$$

if $\vec{r} = \vec{a}_2/k$ then $j_2 = k$

$j_3 = l$ $\quad (j_1, j_2, j_3) \longleftrightarrow (h, k, l)$