Recall, $\vec{G}_{m_1 m_2 m_3} \cdot \vec{R}_{l_1 l_2 l_3} = m 2\pi$

$$\vec{G}_{m_1 m_2 m_3} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3$$

$$\vec{R}_{l_1 l_2 l_3} = l_1 \vec{a}_1 + l_2 \vec{a}_2 + l_3 \vec{a}_3$$

$\{\vec{R}_{l_1 l_2 l_3}\} \longrightarrow$ Bravais Lattice (BL)

$\{\vec{G}_{m_1 m_2 m_3}\} \longrightarrow$ Reciprocal Lattice (RL)

BL : $l(\vec{r}) = \lim_{N\to\infty} \sum_{\vec{R}}^{N} \delta(\vec{r} - \vec{R})$ ; $N = N_1 N_2 N_3 \to$ Bulk cell

$$FT(BL)(\vec{k}) \to \int_{-\infty}^{+\infty} d^3r \, e^{i\vec{k}\cdot\vec{r}} l(\vec{r}) = \lim_{N\to\infty} \sum_{R}^{N} \int_{-\infty}^{+\infty} d^3r \, e^{i\vec{k}\cdot\vec{r}} \delta(\vec{r} - \vec{R})$$

$$= \lim_{N\to\infty} \sum_{R} e^{i\vec{k}\cdot\vec{R}} = \lim_{\{N\}\to\infty} \sum_{l_1 l_2 l_3} e^{i\vec{k}_{n_1 n_2 n_3}\cdot\vec{R}_{l_1 l_2 l_3}}$$

$$= \lim_{\{N\}\to\infty} \sum_{l_1 l_2 l_3}^{N_1 N_2 N_3} e^{i\left(\frac{n_1}{N_1}\vec{b}_1 + \frac{n_2}{N_2}\vec{b}_2 + \frac{n_3}{N_3}\vec{b}_3\right)\cdot\left(l_1\vec{a}_1 + l_2\vec{a}_2 + l_3\vec{a}_3\right)}$$

$$= \lim_{\cdots} \sum e^{i2\pi\left(\frac{n_1 l_1}{N_1} + \frac{n_2 l_2}{N_2} + \frac{n_3 l_3}{N_3}\right)} \quad \because \vec{a}_i\cdot\vec{b}_j = 2\pi\delta_{ij}$$

$= N$ if $n_1 = m_1 N_1$, $n_2 = m_2 N_2$, $n_3 = m_3 N_3$

ie $\vec{k}_{n_1 n_2 n_3} = \vec{G}_{m_1 m_2 m_3} \Rightarrow \vec{k} \in \{\vec{G}\}$

If $\vec{k} \neq \vec{G}$: $n_j$ not integer multiple of $N_j$

$$\therefore n_j = n_j' + m_j N_j, \quad 1 \leq n_j' < N_j$$

$$\therefore \lim_{N_j\to\infty} \sum_{R_j}^{N_j} e^{i k_j R_j} = \lim_{N_j\to\infty} \sum_{l_j}^{N_j} e^{i2\pi n_j' l_j/N_j}$$

$$= \lim_{N_j\to\infty} \frac{N_j}{2\pi} \sum_{l_j}^{N_j} e^{i2\pi n_j' l_j/N_j}\left(\frac{2\pi}{N_j}\right)$$

$$= \lim_{N_j\to\infty} \frac{N_j}{2\pi} \int^{2\pi} e^{i n_j' \theta}\, \underbrace{d\theta}$$

$$= \lim_{N_j \to \infty} \frac{N_j}{2\pi} \frac{1}{n_j'} \sin n_j' 2\pi$$

$$= \lim_{N_j \to \infty} N_j \left( \frac{\sin n_j' 2\pi}{n_j' 2\pi} \right) \to \begin{cases} 1 & \text{as } n_j' \to 0 \\ 0 & \text{if } n_j' \neq 0 \end{cases}$$

$$\boxed{\therefore \lim_{N \to \infty} \sum_{\vec{R}}^{R_N} e^{i\vec{k}\cdot\vec{R}} = N \delta_{\vec{k}\vec{G}} \quad \Rightarrow \lim_{N \to \infty} \sum_{\vec{R}} e^{i\vec{G}\cdot\vec{R}} = N}$$

$$\therefore FT(BL)(\vec{k}) = N \text{ if } \vec{k} \in \{\vec{G}\}$$
$$= 0 \text{ else.}$$

$$\Rightarrow FT_{\vec{k}}(BL) = N\delta(\vec{k} - \vec{G})$$

$$\Rightarrow \boxed{FT(BL) \to RL}$$

we will see $FT(bcc\ BL) = fcc\ RL$
$FT(fcc\ BL) = bcc\ RL$
more such exists

## FT of cell periodic charge density

$$FT\left[\varphi(\vec{r})\right](\vec{k}) = \int d^3r \, e^{i\vec{k}\cdot\vec{r}} \varphi(\vec{r})$$

$$= \sum_{R}^{\infty} \int_{\text{cell}} d^3r \, e^{i\vec{k}\cdot(\vec{r}+\vec{R})} \varphi(\vec{r}+\vec{R})$$

$$= \sum_{R}^{\infty} e^{i\vec{k}\cdot\vec{R}} \underbrace{\int_{\text{cell}} d^3r \, e^{i\vec{k}\cdot\vec{r}} \varphi(\vec{r})}$$

$$= N \delta_{\vec{k}\vec{G}} \times S(\vec{k})$$

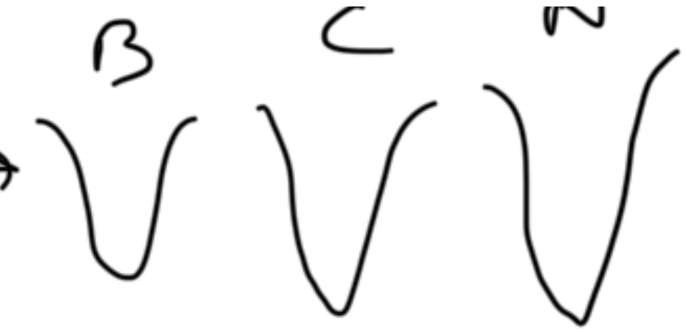
$S(\vec{k})$ ↓ structure factor.

$\therefore$ $FT[\varphi(r)](\vec{k})$ would peak at $\vec{k} = \vec{G}$ and peak height will be $S(\vec{G})$

Structure factor reveals the structure of the unit cell.

$$\sum \, e^{i\vec{G}_n\cdot\vec{r}}$$

Suppose $\psi(r) = \sum_n C_n \, e$




$\therefore \; S(\vec{G}_n) \propto C_n$ ,

$C_n$ follows $V_n$ and $V_n \propto Z_n$

$\downarrow$ # of proton in nuclear of n th atom.

$\therefore \; \dfrac{2\pi}{|\vec{G}_n|}$ give periodicity of the n th atom.