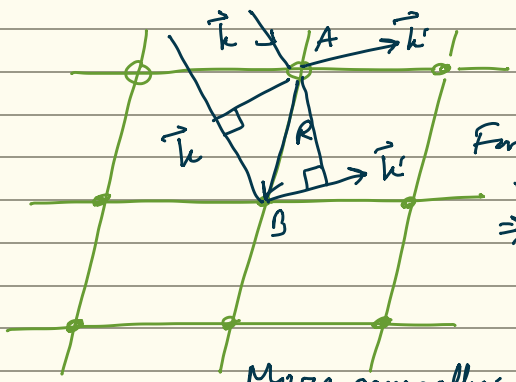
A more general way to understand Laue condition for lattice and lattice with basis

Diffraction from crystal (lattice + basis)



First let us consider lattice pts only. Recall, phase difference between rays scattered from lattice pts A and B : $e^{i(\vec{k}-\vec{k'})\cdot\vec{R}}$

For bright spot along $\vec{k'}$ scattering from all lattice pts must not cancel out to zero.

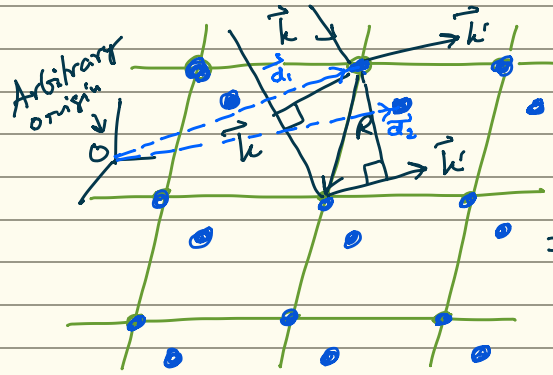
$\Rightarrow$ Net phase difference $\neq 0$ $\Rightarrow \sum_{\vec{R}}^{BVK} e^{i(\vec{k}-\vec{k'})\cdot\vec{R}} \neq 0$

Recall that $\vec{G}\cdot\vec{R} = n2\pi$

More generally, as derived in S.1 : $\lim_{N\to\infty} \sum_{e}^{R_N} e^{i\vec{k}\cdot\vec{R}} = N\,\delta_{\vec{k}\vec{G}}$ ($N \to$ # of UC in BVK)

$\Rightarrow (\vec{k}-\vec{k'}) = \vec{G}$: Von Laue condition.

Now add basis to lattice : Consider n basis atoms per lattice.



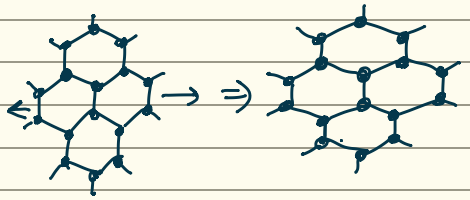
W.r.t an arbitrarily chosen basis atom set as $j=1$

$$\sum_{R}^{BVK}\sum_{j}^{n} e^{i(\vec{k}-\vec{k'})\cdot\{\vec{R}+(\vec{d}_j-\vec{d}_1)\}} \neq 0 \rightarrow \text{for bright spot along } \vec{k'}$$

$$= \sum_{R}^{BVK}\left[\underbrace{e^{i(\vec{k}-\vec{k'})\cdot\vec{R}}}_{j=1} + \sum_{j=2}^{n} e^{i(\vec{k}-\vec{k'})\cdot(\vec{R}+\vec{r}_j)}\right] \neq 0, \quad \vec{r}_j = \vec{d}_j - \vec{d}_1, \; j = 2\dots n$$

$$\Rightarrow \left(\underbrace{\sum_{R} e^{i(\vec{k}-\vec{k'})\cdot\vec{R}}}_{\vec{k}-\vec{k'}=\vec{G} \text{ for the sum to be non zero}}\right)\left(1+\sum_{j=2}^{n} e^{i(\vec{k}-\vec{k'})\cdot\vec{r}_j}\right) \neq 0$$

Note that this looks like stretched graphene



$$\Rightarrow \underbrace{\left(\sum_{R} e^{i\vec{G}\cdot\vec{R}}\right)}_{f_L}\underbrace{\left(1+\sum_{j=2}^{n} e^{i\vec{G}\cdot\vec{r}_j}\right)}_{f_b} \neq 0$$

f_b Geometrical Str. factor of basis (Ashcroft)

Note that f_L is already non zero with $\vec{k}-\vec{k'}=\vec{G}$. Additionally f_b has to be $\neq 0$

$\therefore f_{crystal} = f_L \times f_b$

Note that $f_b \neq 0$ would further select of subset of $\{G\}$ which makes $f_L \neq 0$

Recall structure factor defined in S.1 : $S(k) = \int_{cell} d^3r\, e^{i\vec{k}\cdot\vec{r}}\,\rho(\vec{r})$

If $\rho(\vec{r})$ within cell is approximated as $\sum_{j}^{n}\delta(\vec{r}-\vec{d}_j)$ then $S(G) = \sum_{j}^{n} e^{i\vec{G}\cdot\vec{d}_j}$

$$\therefore f_b = 1+\sum_{j=2}^{n} e^{i\vec{G}\cdot\vec{r}_{j1}} = e^{i\vec{G}\cdot(\vec{d}_1-\vec{d}_1)} + \sum_{j=2}^{n} e^{i\vec{G}\cdot(\vec{d}_j-\vec{d}_1)} = \sum_{j=1}^{n} e^{i\vec{G}\cdot\vec{d}_j} = S(G) \Rightarrow f_b = S(G)$$

with atoms as delta fn:

BCC → Cubic with two basis:

$d_1 = (0,0,0)$; $d_2 = (a/2, a/2, a/2)$

$\therefore$ Geom. Str. fact. $= 1 + e^{i(\hat{x}h\frac{2\pi}{a} + \hat{y}k\frac{2\pi}{a} + \hat{z}l\frac{2\pi}{a})(\hat{x}\frac{a}{2} + \hat{y}\frac{a}{2} + \hat{z}\frac{a}{2})}$

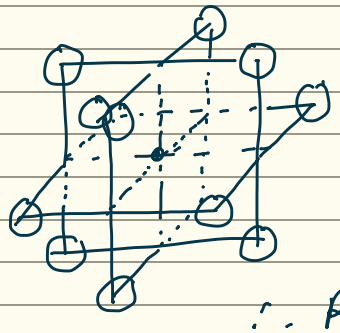
$= 1 + e^{(h+k+l)2\pi}$

$= 0$ if $(h+k+l)$ is odd

$\Rightarrow$ bright spots for shortest $\sqrt{h^2+k^2+l^2}$:

(1 1 0)	(0 1 1)	(1 0 1)
(1 −1 0)	(0 1 −1)	(1 0 −1)
(−1 1 0)	(0 −1 1)	(−1 0 1)
(−1 −1 0)	(0 −1 −1)	(−1 0 −1)

} fcc direction around origin.



As argued above, these must be the allowed directions of $\vec{G}$ vectors for a bcc real lattice.

$\therefore$ Reciprocal lattice of bcc constitutes an fcc lattice.

Similarly " " " fcc " " bcc "

The latter is more tedious to show since fcc in a cubic unit cell implies a basis of four atoms:

$d_1 = (0,0,0)$, $d_2 = (\frac{a}{2}\frac{a}{2}0)$, $d_3 = (0\frac{a}{2}\frac{a}{2})$, $d_4 = (\frac{a}{2}0\frac{a}{2})$ (try!)

For polyatomic basis (→ atoms of different types) the unit amplitude:

$$f_1(h) + \sum_{j=2}^{n} f_j(h)\, e^{\vec{G}\cdot(\vec{d}_j - \vec{d}_1)}$$

where $f(h)$ is the atomic form factor

$$f_j(h) = -\frac{1}{e}\int_{\text{cell}} d^3r\; e^{i\vec{h}\cdot\vec{r}}\rho_j(\vec{r})$$

$$= \frac{-1}{e} S_j(h)$$ → contribution to structure factor from the jth atom in the basis.