Geometrical Structure Factor

★ allows us to take into account the effect of basis on diffraction intensity
(2 or more pt.)

Key Point : adding a basis to a Bravais lattice cannot add additional $\vec{K}$ vectors to the reciprocal lattice

– it can however remove $\vec{K}$ vectors from the reciprocal lattice compared to what there are in the reciprocal lattice with only single pt. basis

Example

1. Consider a S.C. lattice of side spacing a

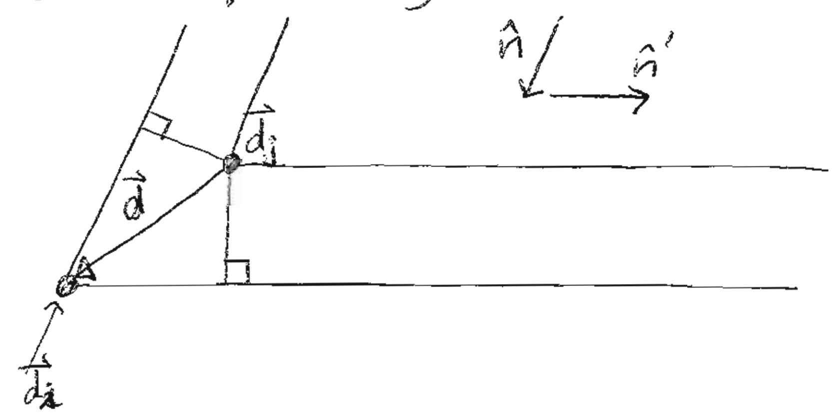
$\Rightarrow$ reciprocal lattice (also SC) having nearest neighbor distance $= \frac{2\pi}{a}$

2. Now add a body-center point.
$\Rightarrow$ (2 pt. - basis)
$\Rightarrow$ reciprocal fcc lattice of conventional cube edge $= \frac{4\pi}{a}$
$\Rightarrow$ e.g. $\frac{1}{2}$ the reciprocal lattice points are removed, (such as $\left(\frac{2\pi}{a}, 0\, 0\right)$)

To calculate the geometrical structure factor, begin with a consideration of path length difference for scattering from 2 arbitrary points in <u>real</u> space $\vec{d}_i$ and $\vec{d}_j$

($\vec{d}_i$ and $\vec{d}_j$ will be position vectors of basis points)

reconsider Von-Laue geometry



$$\Delta \text{ path length} = \vec{d} \cdot \hat{n} - \vec{d} \cdot \hat{n}'$$

$$\cancel{\Delta_1 = \vec{d}_1 \cdot (\hat{n} - \hat{n}')}$$

$$\cancel{\Delta_2 = \vec{d}_2 \cdot (\hat{n} - \hat{n}')}$$

$$\Delta = \vec{d} \cdot (\hat{n} - \hat{n}')$$

$$\vec{d} = \vec{d}_i - \vec{d}_j$$

$$\Rightarrow \Delta = (\vec{d}_i - \vec{d}_j) \cdot (\hat{n} - \hat{n}') \qquad \cancel{\Delta} = a\lambda$$

a = real number

mult. by $\frac{2\pi}{\lambda}$ to get Δphase

$$2\pi a = \left(\frac{2\pi}{\lambda}\right)\Delta = (\vec{d}_i - \vec{d}_j) \cdot (\vec{h} - \vec{h}')$$

$$\vec{h} = \frac{2\pi}{\lambda}\hat{n}$$

$$= (\vec{d}_i - \vec{d}_j) \cdot \vec{K}$$

$(\vec{d}_i - \vec{d}_j) \cdot \vec{K}$ = a phase difference

$\Rightarrow$ $d_i \cdot \vec{K}$ = the phase of scatter i

$\Rightarrow$ ~~the~~ spatially varying amplitude from scatter i

$$A_i \propto e^{i\vec{d}_i \cdot \vec{K}}$$

Total amplitude will be a sum of $e^{i\vec{d}_i \cdot \vec{K}}$ over i.

$$\Rightarrow \text{Total Amplitude} \propto \sum_i e^{i\vec{K}\cdot\vec{d}_i}$$

$$\Rightarrow \boxed{S_K = \sum_{i=1}^{n} e^{i\vec{K}\cdot\vec{d}_i}}$$

geometrical structure factor

Consider a bcc as a SC + basis

bcc = SC + 2-atom basis

SC: $\vec{a}_1 = a\hat{x}$ $\vec{a}_2 = a\hat{y}$, $\vec{a}_3 = a\hat{z}$

2-atom basis: $\vec{d}_1 = 0$, $\vec{d}_2 = \frac{a}{2}(\hat{x} + \hat{y} + \hat{z})$

reciprocal of SC: = SC with side $\frac{2\pi}{a}$

$\vec{b}_1 = \frac{2\pi}{a}\hat{x}$, $\vec{b}_2 = \frac{2\pi}{a}\hat{y}$, $\vec{b}_3 = \frac{2\pi}{a}\hat{z}$

$\Rightarrow$ general $\vec{K} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$

$$\vec{K} = \frac{2\pi}{a}\left(n_1\hat{x} + n_2\hat{y} + n_3\hat{z}\right)$$

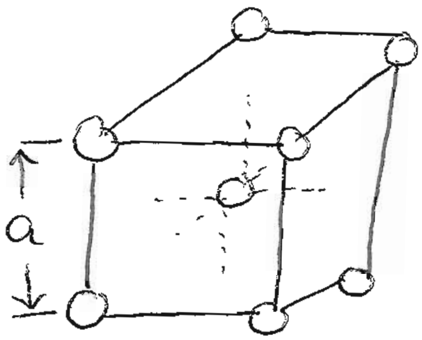
$$\Rightarrow \quad S_K = \sum_{i=1}^{2} e^{i\vec{K}\cdot\vec{d}_i}$$

$$\vec{K}\cdot\vec{d}_1 = 0$$
$$\vec{K}\cdot\vec{d}_2 = \pi(n_1 + n_2 + n_3)$$

$$\Rightarrow S_K = 1 + e^{i\pi(n_1+n_2+n_3)}$$

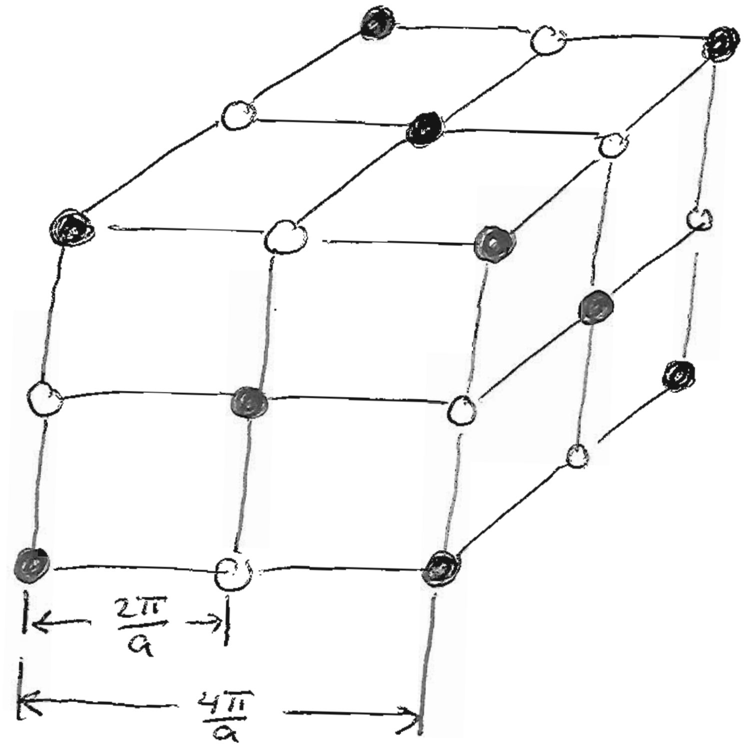
$$= \begin{cases} 0 & (n_1+n_2+n_3 = \text{odd}) \\ 2 & (n_1+n_2+n_3 = \text{even} \end{cases}$$

<u>bcc</u>



sc + 2-pt. basis

<u>all</u> the points are reciprocal lattice points of the SC lattice



Only the solid pts. ($\sum_i n_i = \text{even}$) have $S_K = 2$ $\Rightarrow$ <u>diffraction intensity = 4</u>

the empty circle pts ($\sum_i n_i = \text{odd}$) have $S_K = 0$ $\Rightarrow$ <u>diffraction intensity = 0</u>

<u>Net Result</u>: equivalent to fcc = Recip (bcc) with lattice const. = $\frac{4\pi}{a}$

$$\overset{\uparrow}{0} \quad 1 \quad \overset{\downarrow}{\cancel{2}} \quad 3 \quad \overset{\uparrow}{4} \quad 5 \quad \overset{\downarrow}{\cancel{6}} \quad 7 \quad \overset{\uparrow}{8}$$

Diamond

Real lattice = fcc + basis

fcc: $\vec{a}_1 = \frac{a}{2}(\hat{y} + \hat{z}) \quad \vec{a}_2 = \frac{a}{2}(\hat{z} + \hat{x}) \quad a_3 = \frac{a}{2}(\hat{x} + \hat{y})$

basis: $\vec{d}_1 = 0 \qquad \vec{d}_2 = \frac{a}{4}(\hat{x} + \hat{y} + \hat{z})$

Reciprocal of fcc = bcc

$$\vec{b}_1 = \frac{4\pi}{a}\frac{1}{2}(\hat{y} + \hat{z} - \hat{x}) ; \quad \vec{b}_2 = \frac{4\pi}{a}\frac{1}{2}(\hat{z} + \hat{x} - \hat{y})$$

$$\vec{b}_3 = \frac{4\pi}{a}\frac{1}{2}(\hat{x} + \hat{y} - \hat{z})$$

$$\vec{K} = \sum n_i \vec{b}_i$$

$$S_K = \sum e^{i\vec{K}\cdot\vec{d}_i}$$

$$\vec{K}\cdot\vec{d}_1 = 0$$

$$\vec{K}\cdot\vec{d}_2 = \left(\frac{2\pi}{a}\right)\left(\frac{a}{4}\right) n_1 + \cdots$$

$$\vec{K}\cdot\vec{d}_2 = \frac{\pi}{2} n_1 + \frac{\pi}{2} n_2 + \frac{\pi}{2} n_3$$

$$\Rightarrow \boxed{S_K = 1 + e^{i\frac{\pi}{2}(n_1 + n_2 + n_3)}}$$

Diamond case

$$\vec{K} = \sum n_i \vec{b}_i = \frac{4\pi}{a}\left(-\frac{n_1}{2} + \frac{n_2}{2} + \frac{n_3}{2}\right)\hat{x}$$

$$+ \frac{4\pi}{a}\left(\frac{n_1}{2} - \frac{n_2}{2} + \frac{n_3}{2}\right)\hat{y}$$

$$+ \frac{4\pi}{a}\left(\frac{n_1}{2} + \frac{n_2}{2} - \frac{n_3}{2}\right)\hat{z}$$

$$= \frac{4\pi}{a}\left(\frac{n_1}{2} + \frac{n_2}{2} + \frac{n_3}{2} - n_1\right)\hat{x}$$

$$+ \frac{4\pi}{a}\left(\frac{n_1}{2} + \frac{n_2}{2} + \frac{n_3}{2} - n_2\right)\hat{y}$$

$$+ \frac{4\pi}{a}\left(\frac{n_1}{2} + \frac{n_2}{2} + \frac{n_3}{2} - n_3\right)\hat{z}$$

$$\boxed{\vec{K} = \frac{4\pi}{a}(\nu_1)\hat{x} + \frac{4\pi}{a}(\nu_2)\hat{y} + \frac{4\pi}{a}(\nu_3)\hat{z}}$$

$$\nu_1 = \frac{n_1}{2} + \frac{n_2}{2} + \frac{n_3}{2} - n_1$$

$$\nu_2 = \frac{n_1}{2} + \frac{n_2}{2} + \frac{n_3}{2} - n_2$$

$$\nu_3 = \frac{n_1}{2} + \frac{n_2}{2} + \frac{n_3}{2} - n_3$$

$$\Rightarrow \boxed{\nu_i = \frac{1}{2}(n_1 + n_2 + n_3) - n_i} \quad \boxed{\sum_{i=1}^{3} \nu_i = \frac{1}{2}(n_1 + n_2 + n_3)}$$

Diamond

$$S_K = 1 + e^{i\frac{\pi}{2}(n_1+n_2+n_3)}$$ (106)

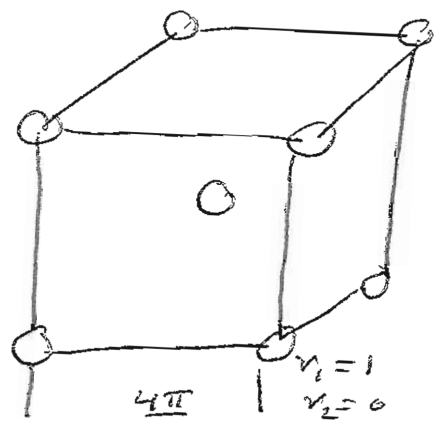
$$S_K = \begin{cases} 2 & n_1+n_2+n_3 \text{ twice an even number} \\ 1 \pm i & n_1+n_2+n_3 \text{ odd} \\ 0 & n_1+n_2+n_3 \text{ twice an odd number} \end{cases}$$

can write

$$\vec{K} = \frac{4\pi}{a}(\nu_1 \hat{x} + \nu_2 \hat{y} + \nu_3 \hat{z})$$

$$\nu_i = \frac{1}{2}(n_1+n_2+n_3) - n_i$$

$$\sum_{i=1}^{3} \nu_i = \frac{1}{2}(n_1+n_2+n_3)$$



For $n_1+n_2+n_3$ twice an odd number $\Rightarrow S = 0$

$\Rightarrow \nu_i = (\text{odd}) - n_i$ = integer − integer = integer

also $\Rightarrow \sum \nu_i = \text{odd} \Rightarrow S = 0$

e.g. $\nu_1 = 1 \quad \nu_2 = 0 \quad \nu_3 = 0$

$\Rightarrow \sum \nu_i = 1 \Rightarrow \sum n = 2$ = twice an odd

$\frac{1}{2}$ of the "corner" points with zero amplitude of diffraction

Diamond Cont

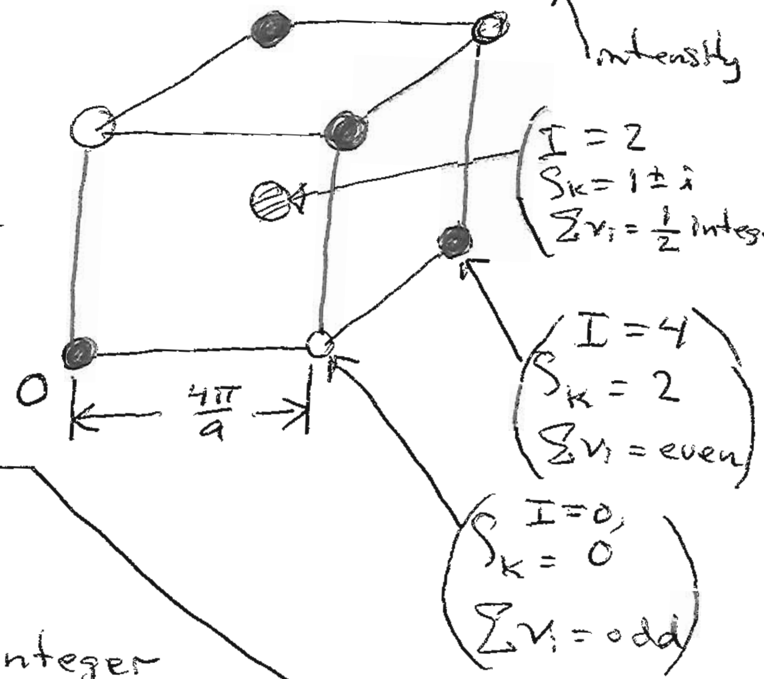
For $n_1 + n_2 + n_3$ twice an even number $\Rightarrow S_K = 2$

$\Rightarrow \quad \nu_i =$ even number $- n_i =$ integer

$\sum \nu_i =$ even number ; $S_K = 2 = \boxed{I = 4}$

intensity

↑ ½ of the corner pts with amplitude of diffraction maximum $(= 2 = S_K)$



Body-centered points

effectively $\nu_i = \frac{1}{2}$ integer

$\Rightarrow S_K = 1 \pm i$

$\Rightarrow$ Intensity $= |S_K|^2 = (1 \pm i)(1 \mp i) = 2$

$\boxed{I = 2}$ intensity

partial destructive interference

↑ all of the "body-centered" points