Geometric Structure factor

$$S_G = \sum_{j=1}^{s} e^{-i\vec{G}\cdot\vec{r}_j} \underbrace{\iiint n_j(\vec{\rho}_j)\, e^{-i\vec{G}\cdot\vec{\rho}_j}\, dV}_{f_j}$$

s-atom basis

f_j for 1 atom in basis

atomic form factor

$$S_{\vec{G}} = \sum_{j=1}^{s} f_j\, e^{-i\vec{G}\cdot\vec{r}_j}$$

$$\vec{r}_j = x_j\,\vec{a}_1 + y_j\,\vec{a}_2 + z_j\,\vec{a}_3$$

fractions < 1

$$\vec{G} = p_1\vec{b}_1 + p_2\vec{b}_2 + p_3\vec{b}_3$$

integers

$$S_{\vec{G}} = \sum_{j=1}^{s} f_j\, e^{-2\pi i\,(p_1 x_j + p_2 y_j + p_3 z_j)}$$

$S_{\vec{G}}$ can be complex, $F_{\vec{G}}$ can be complex

Intensity of scattered radiation $\propto F_{\vec{G}}^{*} F_{\vec{G}} = |F_{\vec{G}}|^2$

e.g. simple cubic

$$S_{\vec{G}} = f_1 e^{-2\pi i (P_1 0 + P_2 0 + P_3 0)} = f_1 e^0 = f_1$$

Should get scattering from <u>all</u> Miller planes

(100), (110), (111), (200), ... $(5,1,3)$ ..

$\downarrow d_1$ $\quad \downarrow d_2$ $\quad \downarrow d_3$

~~Simple~~ $2d \sin\theta = n\lambda$

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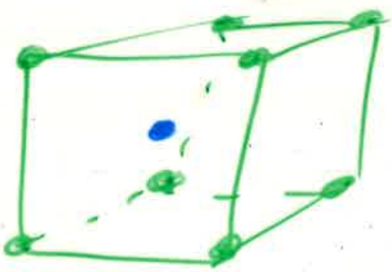
e.g. bcc body-centered cubic

Use conventional cubic cell (not primitive)



$s = 2$ atoms in the basis.

$(x_1, y_1, z_1) = (0, 0, 0)$

$(x_2, y_2, z_2) = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

same atoms at corners & in center $f_1 = f_2 = f$

$$S_{\vec{G}} = f\left[1 + e^{-2\pi i (\frac{1}{2}P_1 + \frac{1}{2}P_2 + \frac{1}{2}P_3)}\right]$$

$$e^0 = f\left[1 + e^{-\pi i (P_1 + P_2 + P_3)}\right]$$

$h \quad k \quad \ell$

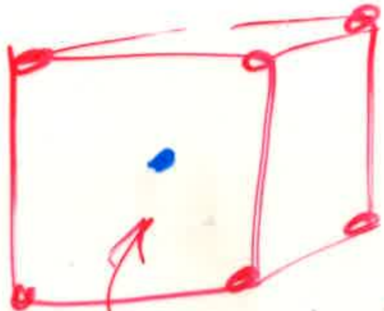
$S_{\vec{G}} = 0$ if $P_1 + P_2 + P_3$ is odd // $S_{\vec{G}} = 2f$ if sum is even

Bragg

⟹ No diffraction peaks at

(100) (300) (111) (221) ----

Why?



scattering from this plane (2,0,0)

is interfering destructively with radiation from this plane (100)

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fcc - face-centered cubic

Use conventional cubic (non-primitive) cell

basis : 4 atoms

$$(x_1, y_1, z_1) = (0,0,0)$$
$$(x_2\, y_2\, z_2) = (\tfrac{1}{2}, \tfrac{1}{2}, 0) \leftarrow$$
$$(x_3\, y_3\, z_3) = (\tfrac{1}{2}, 0, \tfrac{1}{2}) \leftarrow$$
$$(x_4\, y_4\, z_4) = (0, \tfrac{1}{2}, \tfrac{1}{2}) \leftarrow$$

$$f_1 = f_2 = f_3 = f_4 = f$$

$$S_{\vec{G}} = f\left[1 + e^{-\pi i (p_1+p_2)} + e^{-\pi i (p_1+p_3)} + e^{-\pi i (p_2+p_3)}\right]$$

$$= \begin{cases} \emptyset, & \text{1 even \& 2 odd, or 1 odd 2 even} \\ 4f, & \text{all even, or all odd} \end{cases}$$