project: SF-1

The Structure Factor

The scattering amplitude for x-rays off a crystal $\sim |F|^2$ where

$$F_{\vec{\Delta k}} = \int dV\, n(\vec{r})\, e^{-i\vec{\Delta k}\cdot\vec{r}}$$

ρ charge density

We have argued $\vec{\Delta k}$ is ~~big~~ big only if it matches a reciprocal lattice vector $\vec{\Delta k} = \vec{G}$, the von Laue condition

$$F_{\vec{G}} = \int dV\, n(r)\, e^{-i\vec{G}\cdot\vec{r}}$$

N identical cells

$$= N \int_{cell} dV\, n(r)\, e^{-i\vec{G}\cdot\vec{r}}$$

$$\equiv N S_G$$

If there are S atoms in the cell, at positions r_j

$$n(r) = \sum_{j=1}^{S} n_j(r - r_j)$$

$$S_G = \sum_j \int dV\, n_j(r - r_j)\, e^{-iG\cdot r} \qquad r = \rho + r_j \quad \rho = r - r_j$$

$$= \sum_j \left[\int dV\, n_j(\rho)\, e^{-iG\cdot\rho}\right] e^{-i\vec{G}\cdot\vec{r}_j}$$

$$\equiv f_j$$

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

$$G = v_1 \vec{b}_1 + v_2 \vec{b}_2 + v_3 \vec{b}_3$$

$$\vec{r}_j \cdot \vec{G} = 2\pi(v_1 x_j + v_2 y_j + v_3 z_j)$$

project: SF-2

redundant labeling since $v_1 v_2 v_3$ specify G?

$$S_G(v_1 v_2 v_3) = \sum_j f_j e^{-i2\pi(v_1 x_j + v_2 y_j + v_3 z_j)}$$

$$I \sim |S_G|^2$$

Intensity of xray scattering

$\boxed{\text{Example 1}}$ bcc : 2 atoms/cell

$x_1 = 0 \quad x_2 = 1/2$

$y_1 = 0 \quad y_2 = 1/2$

$z_1 = 0 \quad z_2 = 1/2$

$$S(v_1 v_2 v_3) = \underbrace{f}_{\text{Identical atoms}}\left(1 + e^{-i\pi(v_1+v_2+v_3)}\right) = \begin{cases} 0 & v_1+v_2+v_3 = \text{odd} \\ 2f & v_1+v_2+v_3 = \text{even} \end{cases}$$

So, eg., x ray scattering of Na, which is bcc

does not have peaks at (100), (300), (111),.. ← $v_1+v_2+v_3$ odd

but has peaks at (200) (110) (222) ← $v_1+v_2+v_3$ even

$\boxed{\text{Example 2}}$ fcc

x	0	1/2	0	1/2
y	0	1/2	1/2	0
z	0	0	1/2	1/2

$$S(v_1 v_2 v_3) = f\left[1 + e^{-i\pi(v_1+v_2)} + e^{-i\pi(v_1+v_3)} + e^{-i\pi(v_2+v_3)}\right]$$

S vanishes if one or two of $v_1 v_2 v_3$ odd

$S = 4f$ if all three $v_1 v_2 v_3$ odd or all three even

~~KCl, KBr are fcc~~

DIVOGA

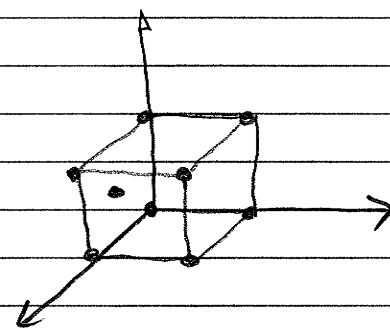
project:
SF-3 fcc

KCl $\quad K^+ \; Cl^-$ ← same # electron

$$\Rightarrow f(K^+) \approx f(Cl^-)$$

so fcc looks like sc of $a/2$

sc has all $v_1 v_2 v_3$ with peaks, but have $a/2$ so v_1 v_2 v_3 need ~~to be even to compensate~~ for $1/2$ in $a/2$.



KCl has peaks at (200) (220) (222) (400) (420)

KBr is also fcc but $f(K^+) \neq f(Br)$ so really ~~looks like fcc~~ follows fcc calculation of page SF-2

Condition is $v_1 v_2 v_3$ all even **or** $v_1 v_2 v_3$ all odd

(111) (200) (220) (311) (222) (400) (331) (420)

"extra peaks" not in KCl

See Figure 17 of Kittel