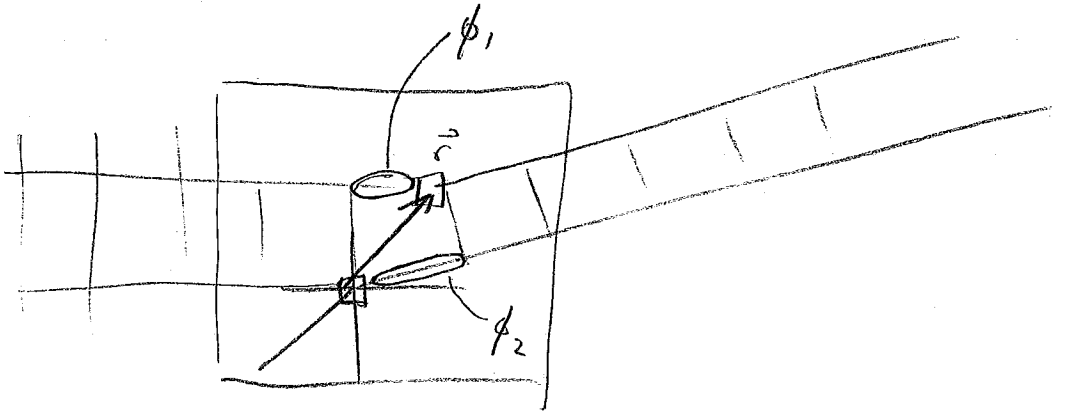
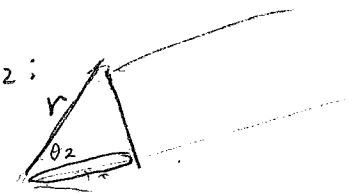
Better explanation of the $(\vec{k}-\vec{k}')\cdot\vec{r}$ factor



phase measured relative to origin

phase shift relative to reference = $\phi_2 - \phi_1$

Focusing on ϕ_2:



$\Delta PL_2 = r\cos\theta_2$

phase from that $\Delta PL = (k)(\Delta PL)$

$\phi_2 = \frac{2\pi}{\lambda} r\cos\theta_2$

$= \vec{k}'\cdot\vec{r}$ since θ_2 = ∠ between $\vec{r}$ and $\vec{k}'$ and magn. of $\vec{k}' = \frac{2\pi}{\lambda}$

Same thing for ϕ_1:

ϕ_1 will be $= \vec{k}\cdot\vec{r}$ since the relevant angle there will be the angle between $\vec{r}$ and $\vec{k}$

Net phase shift, $\phi_2 - \phi_1$:

$$\boxed{\Delta\phi = (\vec{k}'-\vec{k})\cdot\vec{r}}$$

skip "Brillouin Zone" for now, jump to

Fourier Analysis in the Basis

Back to $F = \int_{\text{volume of crystal}} n(\vec{r})\, e^{-i(\vec{s}k \cdot \vec{r})}\, dV$

Note: all cells contribute same amount if $\vec{s}k$ must $= \vec{G}$ for it to be non-zero

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

Note 3) Assume $n(\vec{r})$ only nonzero close to each nucleus

write $\vec{r} = \vec{r}_j + \vec{\rho}$

$\vec{r}_j$: vector pointing to j^{th} nucleus

$\vec{\rho}$: vector pointing to electron charge density surrounding nucleus (horrible symbol! not density!)

then $F = N \sum_j \int n(\vec{\rho})\, e^{-i\vec{G}\cdot(\vec{r}_j + \vec{\rho})}\, dV_\rho$ ← integrate over x unit cell volume

$= N \sum_j e^{-i\vec{G}\cdot\vec{r}_j} \underbrace{\int n(\vec{\rho})\, e^{-i\vec{G}\cdot\vec{\rho}}\, dV_\rho}$

f_j "atomic form factor" of j^{th} atom

also an atomic property!

$$\frac{F}{N} = \boxed{S_{\vec{G}} = \sum_j e^{-i\vec{G}\cdot\vec{r}_j} \cdot f_j}$$

"structure factor"

$$S_{\vec{G}} = \sum_j f_j e^{-i\vec{G}\cdot\vec{r}_j}$$

with $f_j = \int_{\text{all space}} n_j(\vec{r}) e^{-i\vec{G}\cdot\vec{r}}$ — only dependent on atom j. No info about structure!

Now $\vec{G}\cdot\vec{r} = (h_1\vec{b}_1 + h_2\vec{b}_2 + h_3\vec{b}_3)\cdot(x\vec{a}_1 + y\vec{a}_2 + z\vec{a}_3)$

remember $\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{ij}$

$= 2\pi(h_1 x + h_2 y + h_3 z)$

Note that $\vec{G} \neq 0$ is necessary but not sufficient condition for a spot. Second condition $S_{\vec{G}} \neq 0$

bcc structure — bcc lattice, all atoms identical

conventional (cubic) unit cell

2 atoms per lattice

(0,0,0)

and $(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})$ (a =

Use hkl for $v_1 v_2 v_3$?

$$S_{\vec{G}} = f \sum_{\text{basis}} e^{-i(\vec{G}\cdot\vec{r}_j)}$$

$$= f\left(1 + e^{-i2\pi\left(v_1\frac{1}{2} + v_2\frac{1}{2} + v_3\frac{1}{2}\right)}\right)$$

$$= \begin{cases} 0 & \text{if } v_1 + v_2 + v_3 = \text{odd} \\ 2f & \text{if } v_1 + v_2 + v_3 = \text{even} \end{cases}$$

Diffraction lines (200)(110)(222) etc ✓

(100)(300)(111) etc ✗

why no (100)? → Fig 6.9 p 91

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fcc structure conventional cell

fcc lattice, all atoms same
1 atom/primitive cell

(000)
(0 1/2 1/2)
(1/2 0 1/2)
(1/2 1/2 0)

$$S_G = f \sum_j e^{-i\vec{G}\cdot\vec{r}_j} \qquad \vec{G} = \nu_1\vec{b}_1 + \nu_2\vec{b}_2 + \nu_3\vec{b}_3$$

$$= f\left(1 + e^{-i2\pi\left(\frac{\nu_2}{2}+\frac{\nu_3}{2}\right)} + e^{-i2\pi\left(\frac{\nu_1}{2}+\frac{\nu_2}{2}\right)} + e^{-i2\pi\left(\frac{\nu_1}{2}+\frac{\nu_3}{2}\right)}\right)$$

ν_1	ν_2	ν_3	S
		0	$4f$
		1	$f(1+-1-1+1)=0$
		0	
		1	
		0	
		1	
		0	
		1	$4f$

0 = even
1 = odd

only diffracts spots that are all even or all odd !

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Atomic form factor (cont'd)

$$f_j = \int_{\text{all space}} n_j(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, dV \qquad dV = r^2 \sin\theta\, dr\, d\theta\, d\phi$$

align $\vec{G}$ with z axis
assume spherical symmetry for n_j

$$= 2\pi \int_0^\infty n_j(r)\, dr \int_0^\pi \sin\theta\, d\theta\, e^{-iGr\cos\theta} \times \left(\frac{+iGr}{+iGr}\right)$$

then $\int e^u\, du$

$$\frac{e^{-iGr\cos\theta}}{+iGr}\Big|_{\theta=0}^{\pi} = \frac{e^{iGr} - e^{-iGr}}{iGr}$$

$$= \frac{1}{Gr}\, 2\sin Gr$$

$$= 4\pi \int_0^\infty n_j(r)\, r^2\, \frac{\sin Gr}{Gr}\, dr$$

+4π0 in book! pg 42