day 6 pg 41

fcc structure conventional cell

fcc lattice, all atoms same
1 atom/primitive cell

(000)
(0 ½ ½)
(½ 0 ½)
(½ ½ 0)

$$S_G = f \sum e^{-i\vec{G}\cdot\vec{r}_j} \qquad \vec{G} = v_1\vec{b}_1 + v_2\vec{b}_2 + v_3\vec{b}_3$$

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

v_1	v_2	v_3	S
		0	$4f$
		1	$f(1+-1-1+1)=0$
		0	
		1	
		0	
		1	$4f$

0 = even
1 = odd

only diffracts spots that are all even or all odd !

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day 7 pg

Atomic form factor (revisited)

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

align $\vec{G}$ with $\hat{z}$
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 $\int e^u\, du$

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

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

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

4πρ in bank! pg 42

Atomic form factor cont.

if $n_j(r)$ only $\neq 0$ around $r=0$
(all electrons at origin)

then $\frac{\sin Gr}{Gr} = \sin c(Gr) = 1$

$$f_j = \int 4\pi r^2 n_j(r)\, dr$$

↳ electron density

= # electrons in j^{th} atom

= Z (atomic number)

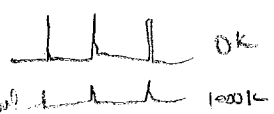
Also when $G = 0$ (forward), $f_j = Z$

Note: we assumed electrons didn't rearrange when we put atoms in crystal. (I said "look up f_j in table")

In practice, electrons do rearrange

... but the "free atom" values of f_j continue to work pretty well.

Temperature (Appendix A)



} total diffracted intensity stays same

background increases because lattice energy randomly $\vec{r}_j = \vec{r}_j^{\,0} + \vec{u}_j$ ↑ vibrational displacement

Averaging over thermal vibrations

$$\langle S_G^2 \rangle = \sum_j f_j^2 \langle e^{-i\vec{G}\cdot\vec{r}_j} e^{+i\vec{G}\cdot\vec{r}_j} \rangle$$

↳ $1 - i\langle \vec{G}\cdot\vec{u} \rangle - \frac{1}{2}\langle (\vec{G}\cdot\vec{u})^2 \rangle + \cdots$

↳ $= 0$

↳ $-\frac{1}{2} G^2 \langle u^2 \rangle \langle \cos^2 \rangle$

↳ $= \frac{1}{3}$ assuming isotropic

$$= \sum_j \text{regular}\left(1 - \tfrac{1}{6} G^2 \langle u^2 \rangle\right)$$

$$= \left(\sum_j \text{regular}\right) \times \underbrace{e^{-\frac{1}{6} G^2 \langle u^2 \rangle}}_{\text{Debye Waller factor}}$$

Brillouin Zones

(I think I follow the BZ construction & diffraction.

skip it, do the BZ section at end of chapter)

What are the reciprocal lattices?

For sc

$$b_1 = \left(\frac{2\pi}{a}, 0, 0\right)$$
$$b_2 = \left(0, \frac{2\pi}{a}, 0\right)$$
$$b_3 = \left(0, 0, \frac{2\pi}{a}\right)$$

} already derived

Recip Lattice = simple cubic!

new lattice const = $\frac{2\pi}{a}$

For bcc have to use primitive lattice vectors

$$a_1 = \tfrac{1}{2}a(-1,1,1)$$
$$a_2 = \tfrac{1}{2}a(1,-1,1)$$
$$a_3 = \tfrac{1}{2}a(1,1,-1)$$

} $b_i = 2\pi \dfrac{a_j \times a_k}{\text{volume}}$

Volume $= a_1 \cdot (a_2 \times a_3)$

(easier way) $= \dfrac{\text{conventional volume}}{2} = \dfrac{a^3}{2}$

$$b_1 = \frac{2\pi}{a}(0,1,1)$$
$$b_2 = \frac{2\pi}{a}(1,0,1)$$
$$b_3 = \frac{2\pi}{a}(1,1,0)$$

} primitive vectors of fcc!

conventional cell length: $\frac{1}{2}b_0 = \frac{2\pi}{a}$, $b_0 = \frac{4\pi}{a}$ ↓ length of conventional cell of recip. lattice

WS cell in recip. space = "1st Brillouin Zone"

Volume $= \frac{1}{4}\left(\frac{4\pi}{a}\right)^3$

4 fcc has 4 atoms in conv. cell.

For fcc $a_1 = \frac{1}{2}a(0,1,1)$

$a_2 = \frac{1}{2}a(1,0,1)$

$a_3 = \frac{1}{2}a(1,1,0)$

one guess as to recip. lattice? Yep, bcc

conventional cell Length $= 4\pi/a$

$b_1 = \frac{1}{2}\left(\frac{4\pi}{a}\right)(-1,1,1)$

$b_2 = \frac{1}{2}\left(\frac{4\pi}{a}\right)(1,-1,1)$

$b_3 = \frac{1}{2}\left(\frac{4\pi}{a}\right)(1,1,-1)$