day 6 pg 5

fcc structure conventional cell

fcc lattice, all atoms same
1 atom/primitive cell

(000)
$(0\frac{1}{2}\frac{1}{2})$
$(\frac{1}{2}0\frac{1}{2})$
$(\frac{1}{2}\frac{1}{2}0)$

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

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

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

0 = even
1 = odd

only diffraction spots that are all even or all odd !

day 7 pg 1

Atomic form factor revisited

$$dV = r^2 \sin\theta \, dr\, d\theta\, d\phi$$

$$f_j = \int_{\substack{\text{all}\\\text{space}}} n_j(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, dV$$

align z axis with G
assume spherical symmetry for n

$$= 2\pi \int_0^{\infty} n_j(r)\,dr \underbrace{\int_0^{\pi} \sin\theta\, d\theta\, e^{-iGr\cos\theta}}_{\left.\frac{e^{-iGr\cos\theta}}{+iGr}\right|_{\theta=0}^{\pi} = \frac{e^{iGr}-e^{-iGr}}{iGr}} \quad \times\left(\frac{+iGr}{+iGr}\right)$$

then $\int e^u du$

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

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

typo in book!
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Atomic form factor cont.

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

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

$$f_j = \int 4\pi r^2 \, \underbrace{n_j(r)}_{\text{electron density}} \, dr$$

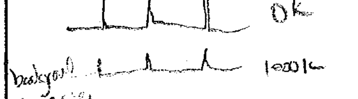
$=$ # electrons in j^{th} atom
$= Z$ (atomic number)

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 changing randomly

$\vec{r} = \vec{r}_j + \vec{u}$
vibrating "shake"

Average over thermal vibrations

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

$e^{-i\vec{G}\cdot\vec{u}} \to 1 - i\underbrace{\langle \vec{G}\cdot\vec{u} \rangle}_{=0} - \frac{1}{2}\langle (\vec{G}\cdot\vec{u})^2 \rangle + \dots$

$\langle (\vec{G}\cdot\vec{u})^2 \rangle \to -\frac{1}{2} G^2 \langle u^2 \rangle \langle \cos^2\theta \rangle$, $\langle \cos^2\theta \rangle = \frac{1}{3}$ average over sphere

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

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

Brillouin Zones

(I didn't follow the BZ construction of 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 discussed

Recip lattice = simple cubic!

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

For bcc have to use primitive lattice vectors

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

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

$$\text{Volume} = a_1 \cdot (a_2 \times a_3)$$
$$(\text{easier way}) = \frac{\text{conventional volume}}{2} = \frac{a^3}{2}$$

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

$$\boxed{\text{WS cell in recip. space = "1}^{\text{st}}\text{ Brillouin Zone"}}$$

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

fcc has 4 atoms in conv. cell.

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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 = $4\pi/a$

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

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

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

TOPS.
35500