PS #3 Solutions.

1. a) A & M 5.1 a) & b)

$$\bar{R} = n_1 \bar{a}_1 + n_2 \bar{a}_2 + n_3 \bar{a}_3$$

$$\bar{K} = m_1 \bar{b}_1 + m_2 \bar{b}_2 + m_3 \bar{b}_3$$

5.1 a) $b_i \cdot a_j = 2\pi \delta_{ij}$

$$b_1 \cdot (b_2 \times b_3) = \frac{(2\pi)^3}{a_1 \cdot (a_2 \times a_3)} \longrightarrow = \Omega.$$

$$b_1 = \frac{2\pi}{\Omega} (a_2 \times a_3)$$

$$= \frac{2\pi}{\Omega} (a_2 \times a_3) \cdot (b_2 \times b_3)$$

$$= \frac{2\pi}{\Omega} \Big[\underbrace{(a_2 \cdot b_2)}_{2\pi} \underbrace{(a_3 \cdot b_3)}_{2\pi} - \cancel{(a_3 \cdot b_2)}^{0} \cancel{(a_2 \cdot b_3)}^{0} \Big]$$

$$= \frac{(2\pi)^3}{\Omega}.$$

1. b) define: $a_1 = \frac{2\pi}{\Omega_b}(b_2 \times b_3)$

etc... where $\Omega_b = b_1 \cdot (b_2 \times b_3)$

$\frac{2\pi}{\Omega_b}(b_2 \times b_3)$

$\Rightarrow b_3 = \frac{2\pi}{\Omega_a}(a_1 \times a_2)$

$= \frac{2\pi}{\Omega_b}\frac{2\pi}{\Omega_a}\, b_2 \times (a_1 \times a_2)$

$= \frac{4\pi^2}{\Omega_b \Omega_a}\left[a_1(\underbrace{b_2 \cdot a_2}_{2\pi}) - \cancel{a_2(b_2 \cdot a_1)}^{0} \right]$

$= \frac{8\pi^3}{\Omega_b \Omega_a}\, a_1$

by defn $\Omega_b \Omega_a = 8\pi^3$

$= a_1$

b) FCC $\Rightarrow$ BCC

show reverse.

BCC lattice vectors.

$$a_1 = \frac{a}{2}(\hat{y}+\hat{z}-\hat{x})$$

$$a_2 = \frac{a}{2}(\hat{z}+\hat{x}-\hat{y})$$

$$a_3 = \frac{a}{2}(\hat{x}+\hat{y}-\hat{z}).$$

$$\Omega = a_1 \cdot (a_2 \times a_3) = \frac{a^3}{2}$$

$$b_1 = \frac{2\pi}{\Omega}(a_2 \times a_3)$$

$$= \frac{2\pi}{\Omega}\frac{a^2}{4}\underbrace{(\hat{z}+\hat{x}-\hat{y})\times(\hat{x}+\hat{y}-\hat{z})}$$

$$\Rightarrow 0\hat{x} + 2\hat{y} + 2\hat{z}$$

$$= \frac{4\pi}{a^3}\frac{a^2}{4}\cdot 2\,(\hat{y}+\hat{z})$$

$$= \frac{4\pi}{a}\cdot\frac{1}{2}(\hat{y}+\hat{z})$$

s.m. $b_2 = \frac{4\pi}{a}\cdot\frac{1}{2}(\hat{z}+\hat{x})$

$b_3 = \frac{4\pi}{a}\cdot\frac{1}{2}(\hat{x}+\hat{y})$

FCC w/ side $= \frac{4\pi}{a}$.

c) $a_1 = a\hat{x}$
$a_2 = a\hat{y}$
$a_3 = a\hat{z}.$

$$a_1 \cdot (a_2 \times a_3) = a^3$$

$$b_1 = \frac{2\pi}{a^3} a^2 \hat{x} = \frac{2\pi}{a}\hat{x}$$

$$b_2 = \frac{2\pi}{a}\hat{y} \qquad b_3 = \frac{2\pi}{a}\hat{z}.$$

$$c_1 = \frac{2\pi}{\Omega_b}(b_2 \times b_3)$$

$$\Omega_b = b_1 \cdot (b_2 \times b_3) = \frac{8\pi^3}{a^3}$$

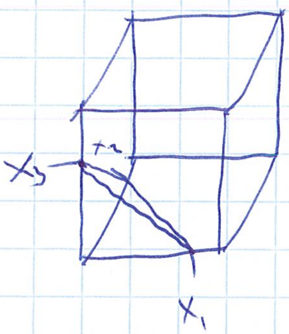
$$c_1 = \frac{2\pi a^3}{8\pi^3}\left(\frac{2\pi}{a}\right)^2 \hat{x} = a\hat{x} = a_1$$

$$c_2 = a\hat{y} = a_2$$

$$c_3 = a\hat{z} = a_3$$

Problem #2

a) $K = hb_1 + kb_2 + lb_3$



$\bar{x}_1 = x_1 \bar{a}_1$
$\bar{x}_2 = x_2 \bar{a}_2$
$\bar{x}_3 = x_3 \bar{a}_3$

$x_1 = \frac{1}{h}$

$x_2 = 1/k$

$x_3 = 1/l.$

$\therefore$ vectors $\bar{r}_1 = \bar{x}_1 - \bar{x}_2$ lie in plane.
$\bar{r}_2 = \bar{x}_2 - \bar{x}_3$

$$\bar{r}_1 = \frac{\bar{a}_1}{h} - \frac{\bar{a}_2}{k} \;;\; \bar{r}_2 = \frac{\bar{a}_2}{k} - \frac{\bar{a}_3}{l}$$

$$\bar{K} \cdot \bar{r}_1 = 2\pi \frac{h}{h} - 2\pi \frac{k}{k} + 0 = 0.$$

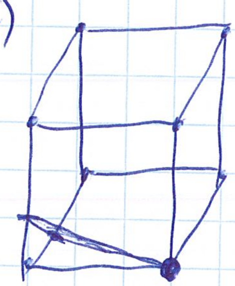
$$\bar{K} \cdot \bar{r}_2 = 0 + 2\pi \frac{k}{k} - 2\pi \frac{l}{l} = 0.$$

$\bar{K}$ is $\perp$ to $\bar{r}_1$ & $\bar{r}_2$ which lie in plane

$\therefore$ $\bar{K}$ is $\perp$ to plane.

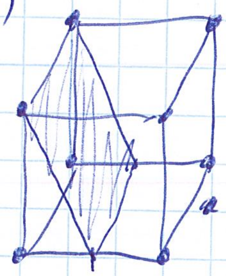
2 b)

i)



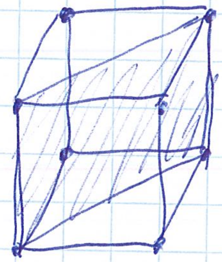
$(1\,3\,3)$

ii)



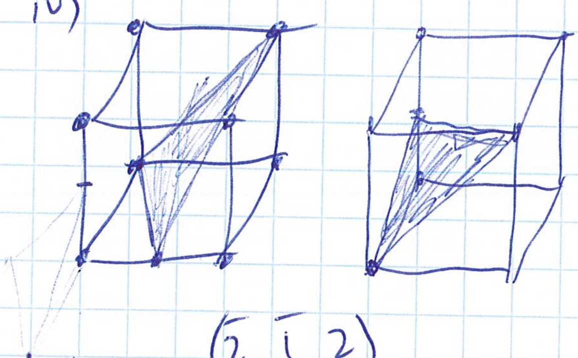
$(2\,0\,1)$

iii)



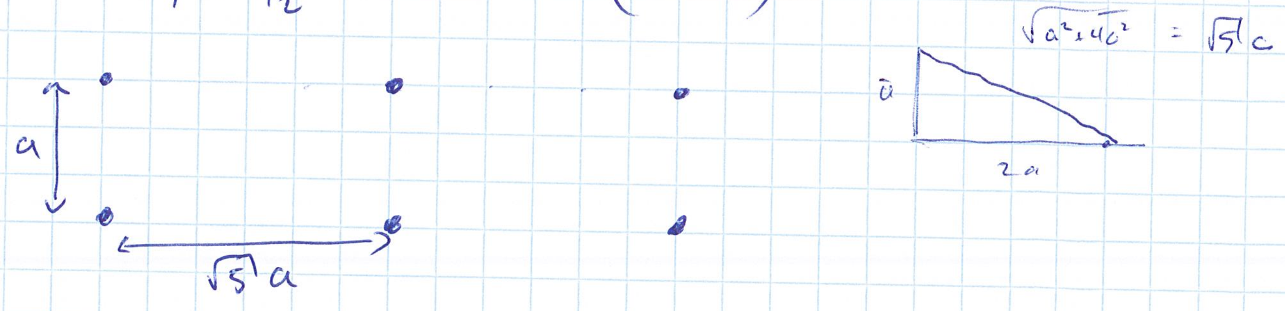
$(\bar{1}\,1\,0)$

iv)

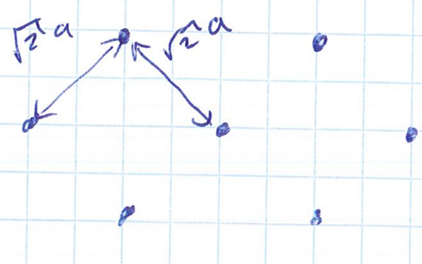


$(2\,\bar{1}\,2)$

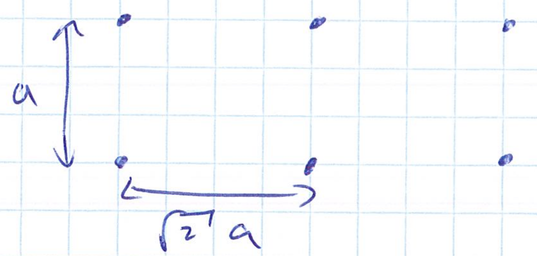
c) i) $\frac{1}{1} : \frac{1}{1/2} : -$ => $(1\,2\,0)$



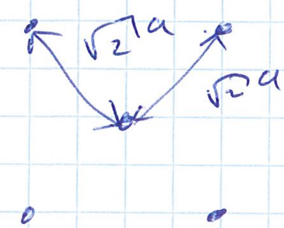
ii) $\frac{1}{1} : \frac{1}{1} : \frac{1}{1}$ => $(1\,1\,1)$



iii) $\frac{1}{\infty} : \frac{1}{-1} : \frac{1}{1} \Rightarrow (0\,\bar{1}\,1)$

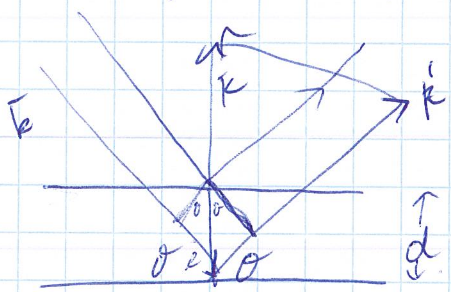


iv) $(\bar{1}\,\bar{1}\,1)$



Problem 3

Show: $\bar{K} = k - k'$ $\iff$ $2d\sin\theta = m\lambda$.



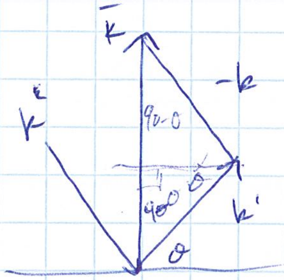
$$\sin\theta = \frac{\ell}{d} \qquad \ell = d\sin\theta.$$

$$\Delta\ell = 2\ell = 2d\sin\theta.$$

$$\therefore \quad 2d\sin\theta = m\lambda \qquad m = \text{integer}.$$

$$\bar{K} = k - k'$$

note $|\bar{K}| = \frac{2\pi}{d} m$, m integer.



$$\cancel{\alpha + 180 - 2\theta = 180}$$
$$\alpha = 2\theta.$$

$$\frac{\frac{|\bar{K}|}{2}}{|k'|} = \sin\theta.$$

$$\frac{|\bar{K}|}{2} = |k|\sin\theta \qquad |k| = \frac{2\pi}{\lambda}.$$

$$\frac{2\pi}{d} m = 2\,\frac{2\pi}{\lambda}\sin\theta$$

$$\therefore \quad 2d\sin\theta = m\lambda$$

Problem 4

A&M 6.1 a & 6.

$K = 2k \sin \phi/2$

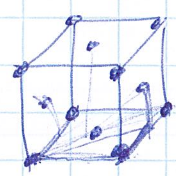
Is $\frac{|K|}{|K_0|} = \frac{\sin \phi/2}{\sin \phi_0/2}$

A	B	C
42.2	28.8	42.8
49.2	41.0	73.2
72.0	50.8	89.0
87.3	59.6	115.0

A	B	C
1	1	1
1.156	1.408	1.634
1.633	1.725	1.921
1.917	1.998	2.311

$\sqrt{\frac{5}{4} + \frac{1}{4}} = \sqrt{\frac{6}{4}}$

Need 4 smallest $\bar{K}$ vectors.



$\sqrt{a^2 + \frac{1}{4}a^2}$

$\frac{\sqrt{5}}{2} a$

for BCC → recip. is FCC.

Nearest Neighbors $(0,0,0)$ $\underset{1}{(\tfrac{1}{2},\tfrac{1}{2},0)}$, $\underset{2}{(1,0,0)}$, $\underset{3}{(1\,1\,0)}$, $\underset{4}{(1,\tfrac{1}{2},\tfrac{1}{2})}$

$|K_1| \propto \frac{1}{\sqrt{2}}$ $\qquad \sqrt{2} \approx 1.41$ $\qquad \sqrt{\frac{2}{4} + 1} = \sqrt{\frac{6}{4}} = \frac{\sqrt{6}}{2}$

$|K_2| \propto 1$ $\qquad 2$

$|K_3| \propto \sqrt{2}$

$|K_4| \propto \frac{\sqrt{6}}{2}$ $\qquad \frac{\sqrt{2}\sqrt{6}}{2} = \frac{\sqrt{12}}{2} = \sqrt{3} \approx 1.73$

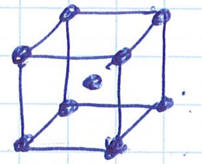
then $\frac{K_2}{K_1} = 1.41$

$\frac{K_3}{K_1} = 1.73$

$K_4/K_1 = 2$

Sample B is BCC.

FCC $\Rightarrow$ BCC recip.



$(000) \to (\tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}) \to (1\ 00)$
$\to (1\ 1\ 0) \to (\tfrac{3}{2}\ \tfrac{1}{2}\ \tfrac{1}{2})$

$K_1 \to \frac{\sqrt{3}}{2}$ $\quad 2/\sqrt{3} = 1.15$

$K_2 \to 1$ $\quad 2\sqrt{2}/\sqrt{3} \Rightarrow 1.63$

$K_3 \to \sqrt{2}$ $\quad \frac{2\sqrt{11}}{2\sqrt{3}} \Rightarrow 1.91.$

$K_4 \to \sqrt{11}/2$

$\left(\frac{9}{4} + \frac{1}{4} + \frac{1}{4}\right)^{1/2} = \sqrt{\frac{11}{4}} = \frac{\sqrt{11}}{2}.$

Sample A.

$\therefore$ A $\Rightarrow$ FCC

B $\Rightarrow$ BCC

C $\Rightarrow$ diamond.

b) $K = 2k \sin \varphi/2$

For cubic cell a FCC recip. BCC side $4\pi/a$.

$\Rightarrow$ or $a_* = \frac{4\pi}{b}$.

take (100) $\cancel{K\ d = 2\pi/|K|}$

$|K|$ = side of cell $= 4\pi/a$.

Sample A 100 is 2nd peak. $\varphi = 49.2$.

$\therefore K = 2 \cdot \frac{2\pi}{1.5\text{Å}} \sin \frac{49.2}{2}$

$a = \frac{4\pi}{|K|} = \frac{2 \cdot 1.5\text{Å}}{2 \cdot \sin 49.2/2} = 3.60\ \text{Å}$

5. a) $f_j(k) = \int \rho_j(\bar{r})\, e^{ik\cdot r}\, d r$

take $\rho(\bar{r}) = Z\,\delta(r)$ $\quad \int \rho\, dr = Z$.

$\therefore f_j(k) = Z \underbrace{\int \delta(r) \cdot e^{ik\cdot r}\, dr}_{\text{FT of } \delta(r) = 1.}$

$\therefore F_j(k) = Z$ constant #
= total # of e^-'s.

b) take $\rho(\bar{r}) = \rho(r)$

wt $\bar{k}\cdot\bar{r} = kr\cos\theta$

$$f_j(k) = \iiint \rho(r)\, e^{ikr\cos\theta}\, d^3r$$

d^3r in spherical coords $= r^2\, dr\, d\varphi\, \underbrace{d(\cos\theta)}_{= \sin\theta\, d\theta.}$

$$f = \int_0^\infty\int_{-1}^{1} \rho(r)\, r^2\, e^{ikr\cos\theta}\, d(\cos\theta)\, dr \int_0^{2\pi} d\varphi$$

$$= 2\pi \int \rho(r) r^2 \left[\frac{1}{ikr}\left(e^{ikr\cos\theta}\Big|_{-1}^{1} \right)\right] dr$$

$$= 2\pi \int \rho(r) r^2 \frac{1}{ikr} \underbrace{\left[e^{ikr} - e^{-ikr} \right]}_{= 2i\sin kr.} dr$$

$$= 4\pi \int \rho(r) r^2 \frac{\sin kr}{kr}\, dr$$

Problem 6

Cl $d = (\frac{1}{2},0,0), (0,\frac{1}{2},0), (0,0,\frac{1}{2}), (\frac{1}{2},\frac{1}{2},\frac{1}{2})$

Na $d = 0, (\frac{1}{2},\frac{1}{2},0), (\frac{1}{2},0,\frac{1}{2}), (0,\frac{1}{2},\frac{1}{2})$

$$\bar{K} = \cancel{\frac{2\pi}{a}}\, h\bar{b}_1 + k\bar{b}_2 + l\bar{b}_3$$

$$d = x_1\bar{a}_1 + x_2\bar{a}_2 + x_3\bar{a}_3$$

$$a_i b_j = 2\pi\, \delta_{ij} \cancel{(i=j)}$$

$$\bar{K}\cdot\bar{d} = (hx_1 + kx_2 + lx_3)2\pi$$

$$S_{\bar{K}} = \sum_j f_j e^{i\bar{K}\cdot\bar{d}_i}$$

$$= f_{K^+}\left[1 + e^{2\pi i(h+k)} + e^{i\pi(k+l)} + e^{i\pi(l+h)}\right]$$

$$+ f_{Cl^-}\left[e^{i\pi h} + e^{i\pi k} + e^{i\pi l} + e^{i\pi(h+k+l)}\right]$$

$$= f_{K^+}\left[1 + (-1)^{(h+k)} + (-1)^{(k+l)} + (-1)^{(l+h)}\right]$$

$$+ f_{Cl^-}\left[(-1)^h + (-1)^k + (-1)^l + (-1)^{(h+k+l)}\right]$$

$h+k+l \to$ even $\Rightarrow$ 2 odd 1 even $= 0$

or all even. $\Rightarrow 4(f_K + f_{Cl})$

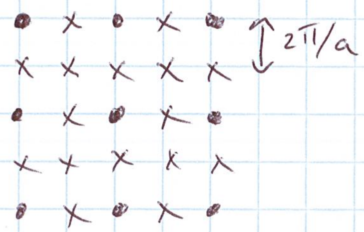
$h+k+l \Rightarrow$ odd $\rightarrow$ 2 even, 1 odd $\Rightarrow 0$

$\rightarrow$ all odd $\Rightarrow 4(f_K - f_{Cl})$

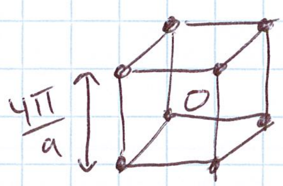
$$\Rightarrow \quad S_K = \begin{cases} 4(f_K + f_{Cl}) & \Rightarrow h,k,l \text{ even} \\ 4(f_K - f_{Cl}) & \Rightarrow h,k,l \text{ odd} \\ 0 & \Rightarrow \text{mixed} \end{cases}$$

Recip.

$l = 0$ even



$l = 1$ odd



$\bullet \rightarrow |4(f_K + f_{Cl})|^2$

$o \rightarrow |4(f_K - f_{Cl})|^2$

if $f_K = f_{Cl} \Rightarrow$ simple cubic w/ side $\frac{4\pi}{a}$.

$\Rightarrow$ orig lattice $\Rightarrow$ simple cube w/ side $= \frac{2\pi}{4\pi/a} = \frac{a}{2}$