5.1 $\quad \vec b_i \cdot \vec a_j = 2\pi\delta_{ij}$

$$\vec b_1 = \frac{2\pi(\vec a_2\times\vec a_3)}{\vec a_1\cdot(\vec a_2\times\vec a_3)}$$

$$\vec b_1\cdot(\vec b_2\times\vec b_3) = \frac{2\pi}{\vec a_1\cdot(\vec a_2\times\vec a_3)}\,(\vec a_2\times\vec a_3)\cdot(\vec b_2\times\vec b_3)$$

from the vector relation: $(\vec A\times\vec B)\cdot(\vec C\times\vec D) = (\vec A\cdot\vec C)(\vec B\cdot\vec D) - (\vec A\cdot\vec D)(\vec B\cdot\vec C)$

$$\Rightarrow (\vec a_2\times\vec a_3)\cdot(\vec b_2\times\vec b_3) = (\vec a_2\cdot\vec b_2)(\vec a_3\cdot\vec b_3) - (\vec a_2\cdot\vec b_3)(\vec a_3\cdot\vec b_2) = (2\pi)^2 - 0 \Rightarrow$$

$$\Rightarrow \boxed{\vec b_1\cdot(\vec b_2\times\vec b_3) = (2\pi)^3/\vec a_1\cdot(\vec a_2\times\vec a_3)}$$

(b) show that $\quad 2\pi\dfrac{\vec b_2\times\vec b_3}{\vec b_1\cdot(\vec b_2\times\vec b_3)} = \vec a_1$, etc.

$$\vec b_2\times\vec b_3 = \frac{2\pi(\vec a_3\times\vec a_1)\times\vec b_3}{\vec a_1\cdot(\vec a_2\times\vec a_3)}$$

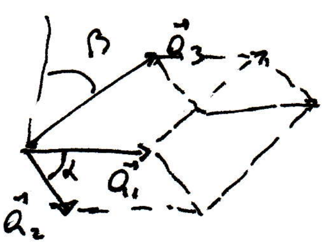
using $\vec A\times(\vec B\times\vec C) = (\vec A\cdot\vec C)\vec B - (\vec A\cdot\vec B)\vec C \Rightarrow$

$$(\vec a_3\times\vec a_1)\times\vec b_3 = -\vec b_3\times(\vec a_3\times\vec a_1) = -(\vec b_3\cdot\vec a_1)\vec a_3 + (\vec b_3\cdot\vec a_3)\vec a_1 = 2\pi\vec a_1 \Rightarrow \boxed{\vec b_2\times\vec b_3 = \frac{2\pi}{\vec a_1\cdot(\vec a_2\times\vec a_3)}\cdot 2\pi\vec a_1}$$

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

etc

(c)



area of base parallelogram is $a_1 a_2 \sin\alpha$

area of parallelepiped = area of base parallelogram × height

height $= a_3\cos\beta$. $\vec a_1\times\vec a_2$ is ⊥ to plane of $a_1, a_2 \Rightarrow$ // height,

and $|\vec a_1\times\vec a_2| = a_1 a_2\sin\theta$, so

$$(\vec a_1\times\vec a_2)\cdot\vec a_3 = a_1 a_2\sin\theta\cdot a_3\cdot\cos\beta = V$$

by cyclic permutation $= \vec a_1\cdot(\vec a_2\times\vec a_3)$

For powder method: $K = 2k \sin \frac{1}{2}\phi$

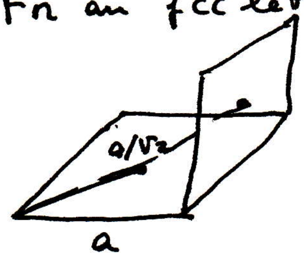
From the data given, we have for $K/2k$

A	B	C
0.360	0.249	0.365
0.416	0.350	0.596
0.588	0.429	0.701
0.690	0.497	0.843

so for the ratio of reciprocal lattice vector lengths K_j/K_1, $j = 2,3,4$

A	B	C
1.155	1.41	1.63
1.63	1.72	1.92
1.92	2	2.31

For an fcc lattice



nn distance: $\frac{a}{\sqrt{2}}$

nnn distance: a

3rd nn ": $\sqrt{\frac{3}{2}}\,a$

4th nn ": $\sqrt{2}\,a$

1.41   1.72   2

So B is an fcc reciprocal lattice $\Rightarrow$ $\boxed{\text{direct lattice is BCC for B}}$

For a bcc lattice:

nn distance $= \sqrt{3}/2\,a$

nnn $= a$

3rd nn $= \sqrt{2}\,a$

4th nn $= \sqrt{\frac{11}{4}}\,a$

1.155   1.63   1.91

Reciprocal of fcc is BCC $\Rightarrow$ $\boxed{\text{direct lattice is FCC for A}}$

Diamond lattice is fcc with some diffraction rings missing due to structure factor of basis

$$S_K = 1 + e^{i\frac{\pi}{2}(n_1+n_2+n_3)}$$

gives 0 for $n_1+n_2+n_3$ = twice an odd number. e.g. (1, 1, 0)

so 1.55 is missing, 1.63 is there, etc.

so $\boxed{\text{direct lattice is diamond for C}}$

(b) $K = 2k \sin \frac{1}{2}\phi$. $k = \frac{2\pi}{\lambda}$, $\lambda = 1.5\text{Å}$

B: $\frac{K}{2k} = 0.249$ for $K = \frac{4\pi}{a} \cdot \frac{1}{\sqrt{2}}$ $\Rightarrow$

$$\frac{4\pi}{a} \cdot \frac{1}{\sqrt{2}} = \frac{4\pi}{\lambda} \times 0.249 \Rightarrow \boxed{a = \frac{\lambda}{\sqrt{2} \times 0.249} = 4.26\text{Å}} \boxed{\text{for B}}$$

A: $K = \frac{4\pi}{a} \frac{\sqrt{3}}{2}$ for $\frac{K}{2k} = 0.360$ $\Rightarrow$

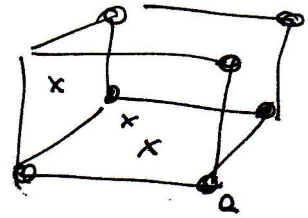
$$\frac{4\pi}{a} \frac{\sqrt{3}}{2} = \frac{4\pi}{\lambda} \times 0.360 \Rightarrow \boxed{a = \frac{\sqrt{3}\,\lambda}{2 \times 0.360} = 3.61\text{Å}} \boxed{\text{for A}}$$

C: $\frac{K_C}{K_A} = \frac{0.365}{0.360} \Rightarrow a_C = a_A \cdot \frac{0.360}{0.365} \Rightarrow \boxed{a = 3.56\text{Å for C}}$

(c) Missing rings would be there $\Rightarrow$ same as A properly scaled

$\boxed{42.8^\circ,\ 49.9^\circ,\ 73.4^\circ,\ 89.0^\circ}$

6.2



$$S_K = \sum_j e^{i\vec{K}\cdot\vec{d}_j}$$

$\vec{d}_1 = 0$, $\vec{d}_2 = \frac{a}{2}(\hat{x}+\hat{y})$, $\vec{d}_3 = \frac{a}{2}(\hat{y}+\hat{z})$, $\vec{d}_4 = \frac{a}{2}(\hat{z}+\hat{x})$

$$S_K = 1 + e^{i\vec{K}\cdot\frac{a}{2}(\hat{x}+\hat{y})} + e^{i\vec{K}\cdot\frac{a}{2}(\hat{y}+\hat{z})} + e^{i\vec{K}\cdot\frac{a}{2}(\hat{z}+\hat{x})}$$

for sc lattice, $\vec{K} = \frac{2\pi}{a}(m_1\hat{x} + m_2\hat{y} + m_3\hat{z}) \Rightarrow$

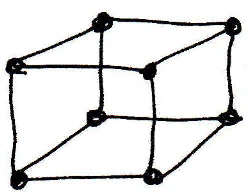
$$\Rightarrow S_K = 1 + e^{i\pi(m_1+m_2)} + e^{i\pi(m_2+m_3)} + e^{i\pi(m_3+m_1)}$$

if m_1 is odd, m_2 & m_3 even $\Rightarrow$ $S_K = 1-1+1-1=0$

if m_1 and m_2 are ~~eve~~ odd, m_3 even, $S_K = 1+1-1-1=0$

if m_1, m_2, m_3 are all odd or all even $\Rightarrow$ $S_K = 1+1+1+1=4$

So S_K is nonzero for m_1, m_2, m_3 all even or all odd.



For m_1, m_2, m_3 all even: $m_1 = 2n_1$, $m_2 = 2n_2$, $m_3 = 2n_3 \Rightarrow$

$\Rightarrow \vec{K} = \frac{4\pi}{a}(n_1\hat{x} + n_2\hat{y} + n_3\hat{z})$ is a sc lattice of side $\frac{4\pi}{a}$

For m_1, m_2, m_3 all odd, $m_1 = 2n_1+1$, $m_2 = 2n_2+1$, $m_3 = 2n_3+1 \Rightarrow$

$$\Rightarrow \vec{K} = \frac{2\pi}{a}\left((n_1+\tfrac{1}{2})\hat{x} + (n_2+\tfrac{1}{2})\hat{y} + (n_3+\tfrac{1}{2})\hat{z}\right)$$

these are the center points of the cube in the bcc lattice.

8.2 $$g_n(\varepsilon) = \int_{S_n(\varepsilon)} \frac{dS}{4\pi^3} \frac{1}{|\vec{\nabla}_k \varepsilon(\vec{k})|}$$

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m} \Rightarrow \vec{\nabla}_k \varepsilon_k = \frac{\hbar^2 \vec{k}}{m} \Rightarrow g_n(\varepsilon) = \frac{m}{\hbar^2} \frac{1}{4\pi^3} \int \frac{dS}{k}$$

The surface is a sphere of radius $k_F \Rightarrow$

$$\int \frac{dS}{k} = \int \frac{dS}{k_F} = \frac{S}{k_F} = 4\pi k_F \Rightarrow g_n(\varepsilon) = \frac{m}{\hbar^2} \frac{1}{4\pi^3} \cdot 4\pi k_F$$

$$\Rightarrow g_n(\varepsilon) = \frac{m k_F}{\hbar^2 \pi^2}$$

(b) $$\varepsilon_n(\vec{k}) = \varepsilon_0 + \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right)$$

$$g_n(\varepsilon) = \int \frac{d^3k}{4\pi^3} \delta(\varepsilon - \varepsilon_n(k))$$

change variables to $k_x'^2 = \frac{\hbar^2 k_x^2}{2m_x}$, etc $\Rightarrow$

$$g_n(\varepsilon) = \frac{(m_x m_y m_z)^{1/2}}{4\pi^3} \frac{2^{3/2}}{\hbar^3} \int d^3k' \, \delta(\varepsilon - \varepsilon_0 - k^2)$$

$$= C \cdot \int dk \, k^2 \delta(\varepsilon - \varepsilon_0 - k^2) = C' \int dx \sqrt{x} \, \delta(\varepsilon - \varepsilon_0 - x)$$

$$k^2 = x \Rightarrow k^2 dk \propto \sqrt{x} \, dx$$

$$\Rightarrow g_n(\varepsilon) \propto \sqrt{\varepsilon - \varepsilon_0}$$

(b) If $g_n(\varepsilon) = C\sqrt{\varepsilon - \varepsilon_0}$ it is just like free electrons, except integrals start at ε_0 instead of 0, i.e.

$$n = \int_{\varepsilon_0}^{\varepsilon_F} d\varepsilon \, g_n(\varepsilon)$$, since $g(\varepsilon_F) = \frac{3n}{2\varepsilon_F}$ for free electrons

$$\Rightarrow g_n(\varepsilon) = \frac{3}{2} \frac{n}{\varepsilon_F - \varepsilon_0}$$ here.