Points

731 Homework #6

Due October 18th, 2006

20	1. A&M, problem 6.1	a) 7 b) 7 c) 6
15	2. A&M, problem 6.2	a) 8 b) 7
25	3. A&M, problem 6.3	a) 5 b) 5 c) 5 d) 5 e) 5
15	4. A&M, problem 6.4	a) 7 b) 8
20	5. A&M, problem 6.5	a) 7 b) 7 c) 6

Total = 95

6.1

a) $K = 2k \sin(\varphi/2)$, ratio of $\sin(\varphi/2) = \dfrac{\sin(\varphi_i/2)}{\sin(\varphi_1/2)}$

	φ	$\varphi/2$	K ratio	K ratio
A)	42.2	21.1	0.35999	1
	49.2	24.6	0.4163	1.1564
	72	36	0.5878	1.6328
	87.3	43.65	0.69	1.1966
B)	28.8	14.4	0.24869	1
	41	20.5	0.35	1.407
	50.8	25.4	0.4289	1.7246
	59.6	29.8	0.49697	1.998
c)	42.8	21.4	0.36488	1
	73.2	36.6	0.59622	1.634
	89.0	44.5	0.701	1.9212
	115.0	57.5	0.834	2.311

Case A — fcc Structure

Case B — Bcc Structure

C — Diamond Structure.

B>

Case A.

$$K = \frac{2\pi}{\lambda} = 2\pi/1.5$$

the Smallest K $= K_{min} = \frac{4\pi}{a} \cdot \frac{\sqrt{3}}{2}$

$$K = 2k \sin\left(\frac{42.2}{2}\right)$$

$$\Rightarrow \frac{4\pi}{a} \cdot \frac{\sqrt{3}}{2} = 2 \cdot \frac{2\pi}{1.5} \sin(21.2) \Rightarrow \boxed{a = 3.6\ A^o}$$

Case B : bcc : $K_{min} = \frac{4\pi}{a} \cdot \frac{\sqrt{2}}{2} = 2 \cdot \frac{2\pi}{1.5} \sin(14.4)$

$$\rightarrow \boxed{a = 4.265\ A^o}$$

Case C $\boxed{a = 3.56\ A^o}$

C> 4 minimum k.

$\frac{4\pi}{a} \cdot \frac{\sqrt{3}}{2}$, $\frac{4\pi}{a}$, $\sqrt{2}\,\frac{4\pi}{a}$, $\sqrt{3}\,\frac{4\pi}{a}$; $a = 3.56$

use $K = 2k \sin(\phi/2)$; $\lambda = 1.5$.

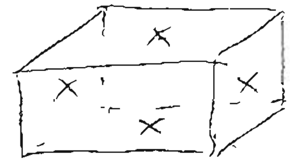
$\theta_1 = 42.8^o$

$\theta_2 = 49.84^o$

$\theta_3 = 73.15^o$

$\theta_4 = 93.73^o$

6.2.



a) $S_K = \sum_{i=1}^{n} e^{i\vec{K}\cdot d_i}$. $K = \frac{2\pi}{a}(n_1\hat{x} + n_2\hat{y} + n_3\hat{z})$

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

+ if n_1, n_2, n_3 are even $S_K = 4$
+ if one of them odd $S_K = 0$
  if two of them is odd $S_K = 0$
  if all are odd $S_K = 4$

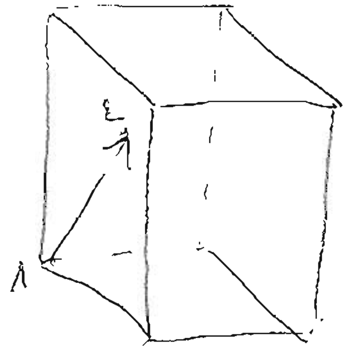
$S_K = \begin{cases} 0 \\ 4 \end{cases}$

b) if we Remove $S_K = 0$; we only have $S_K = 4$

cell of side $= 4\pi/a \Rightarrow$ BCC.

6.3 (4)

a)



$$\vec{d_1} = 0$$
$$\vec{d_2} = \frac{1}{3}\vec{a_1} + \frac{1}{3}\vec{a_2} + \frac{1}{2}\vec{a_3}$$
$$\vec{K} = n_1\vec{b_1} + n_2\vec{b_2} + n_3\vec{b_3}.$$

$$S_K = \sum_{j=}^{1} e^{i\vec{K}\vec{d_j}} = 1 + e^{i2\pi\left(\frac{n_1}{3} + \frac{n_2}{3} + n_3/2\right)}$$

$$=$$

$$S_K = \begin{cases} 1 + e^{i6\pi/3} & n_1 = n_2 = n_3 = 0 \\ 1 + e^{i2\pi/3} & n_1 = 1 \quad n_2 = n_3 = 0 \text{ or } n_1 = n_3 = 0, n_2 = \\ 1 + e^{i4\pi/3} & n_1 = n_2 = 1 \quad n_3 = 0 \\ 1 + e^{i3\pi/3} & n_1 = n_2 = 0,\ n_3 = 1 \end{cases}$$

$$S_K = \begin{cases} 1 + e^{i\,5/3\,\pi} & n_1 = 1,\ n_2 = 0,\ n_3 = 1 \text{ or } n_1 = 1,\ n_2 = n_3 = 1 \\ 1 + e^{i\pi/3} & n_1 = n_2 = n_3 = 1 \end{cases}$$

$$\Rightarrow \quad S_K = 1 + e^{i\pi n/3}, \quad n = 1, 2, 3 \ldots 6$$

3(b) $K = 0$, $n_3 = 0$

$$S_K = \begin{cases} 1 + e^{i\,0\pi/3} \neq 0 & n_1 = n_2 = n_3 = 0 \\ 1 + e^{i\,2\pi/3} \neq 0 & n_1 = 1, n_2 = n_3 = 0 \text{ or } n_1 = 0, n_2 = 1, n_3 = 0 \\ 1 + e^{i\,4\pi/3} \neq 0 & n_1 = n_2 = 1, n_3 = 0 \end{cases}$$

$\Rightarrow$ all reciprocal lattice points have nonvanishing structure factor in the plane perpendicular to the c axis containing $\vec{K} = 0$

(3c) if $n_3 =$ odd, and n_1, n_2 are zero or opposite

$\Rightarrow S_K = 0$ so we can find $S_K = 0$ points.

(3d). $\vec{K} = 0$, $n_1 = n_2 = 0$

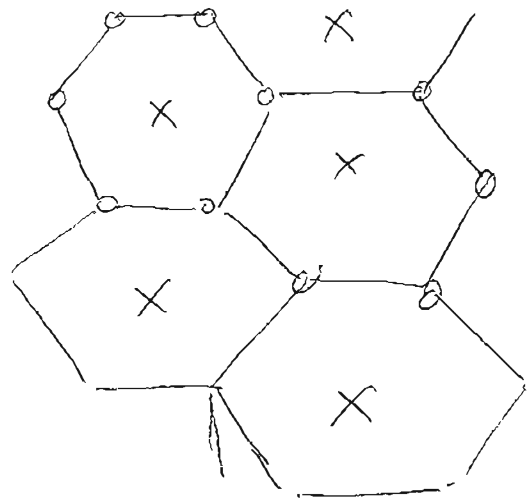
only n_3 is not zero. and n_3 is odd according to (3c)

$$S_K = 1 + e^{i\pi(2n_1 + 2n_2 + 3n_3)/3}$$

$$= 1 + e^{i\pi} = 0$$

(3e)

Remove all points $S_K = 0$



becomes honeycomb.

4)

a) $f_i = -\frac{1}{e} \int d\vec{r} \, e^{i\vec{k}\cdot r} \rho_i(\vec{r})$; $\rho_i(\vec{r}) = \sum_{j=1}^{m_i} (-Z_{ij} e)\, \delta(\vec{r} - \vec{b_{ij}})$

$= -\frac{1}{e} \sum_{j=1}^{m_i} e^{i\vec{k}\cdot\vec{b_{ij}}} (-Z_{ij} e)$

$= \sum_{j=1}^{m_i} Z_{ij} \, e^{i\vec{k}\vec{b_{ij}}}$.

b) $S_K = \sum_{i=1}^{n} f_i(\vec{k}) \, e^{i\vec{k} d_i}$

$= \sum_{i=1}^{n} \Big(\underbrace{\sum_{j=1}^{m_i} Z_{ij} \, e^{i\vec{k}\vec{b_{ij}}}}_{f_i(\vec{k})} \Big) e^{i\vec{k} d_i}$

We have a basis of many ions $(m_1 \ldots + m_n)$

$i = 1, \ldots, n$

each i : $j = 1, \ldots, n$.

$f_{ij} = Z_{ij}$

$S_K = \sum_{ij} Z_{ij} \, e^{i\vec{k}\vec{d_{ij}}} = \sum_{ij} Z_{ij} \, e^{i\vec{k}(\vec{b_{ij}} + \vec{d_i})}$

$\boxed{\S 5}$:

a) $\vec{d_1} = 0$, $d_2 = a/2\ \hat{x}$

$$\vec{k} = \sum_{i=1}^{3} n_i \vec{b_i} = \frac{4}{a} (\nu_1 \hat{x} + \nu_2 \hat{y} + \nu_3 \hat{z})$$

$$S_K = \sum_{j=1}^{2} f_j e^{i \vec{k} \vec{d_j}} = f_+ + f_- e^{i \frac{4\pi}{a} (\nu_1 \hat{x} + \nu_2 \hat{y} + \nu_3 \hat{z}) \frac{a}{2} \hat{x}}$$

$$S_K = f_+ + f_- e^{i 2\pi \nu_1}$$

ν_1 is integer : $S_K = f_+ + f_-$

if ν_1 is integer $+ \frac{1}{2}$ $S_K = f_+ - f_-$

if $f_+ = f_-$ and ν_i is integer $+ 1/2$ $\Rightarrow S_K = 0$

b) $$S_K = 1 + e^{i\pi \sum_{j=1}^{3} \nu_j}$$

$$S_K = f_+ + f_- e^{i\pi \sum \nu_j}$$

$$\Rightarrow S_K = f_+ \pm f_- \cdot i$$

if ν_j are integer $+ \frac{1}{2}$ $\Rightarrow \sum_j \nu_j =$ integer $+ 3/2$

$S_K = f_+ + f_-$: if $\sum \nu_j$ is even

$S_K = f_+ - f_-$ ———— odd

c)

NaCl :

$$\begin{cases} S_K = f_+ + f_- \\ S_K = f_+ - f_- \end{cases} \rightarrow \text{intensity} \quad \begin{matrix} |f_+ + f_-|^2 \\ |f_+ - f_-|^2 \end{matrix}$$

for zincblende s.

$$S_K = \begin{cases} f_+ \pm i f_- \\ f_+ + f_- \\ f_+ - f_- \end{cases} \quad \text{possible intensity} \quad \begin{matrix} |f_+|^2 + |f_-|^2 \\ |f_+ + f_-|^2 \\ |f_+ - f_-|^2 \end{matrix}$$