Homework 2, due January 29, 1999

Problem 1. Ashcroft-Mermin 5.2

(a) $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a\sqrt{3}}{2}\hat{y}$, $\vec{a}_3 = c\hat{z}$

$\vec{a}_2 \times \vec{a}_3 = -\frac{ac}{2}\hat{y} + \frac{ac\sqrt{3}}{2}\hat{x}$

$\vec{a}_3 \times \vec{a}_1 = ac\hat{y}$

$\vec{a}_1 \times \vec{a}_2 = \frac{a^2\sqrt{3}}{2}\hat{z}$

$\vec{a}_1 \times \vec{a}_2 \cdot \vec{a}_3 = \frac{a^2c\sqrt{3}}{2}$

$\vec{b}_1 = \frac{2\pi}{a}(\hat{x} - \frac{1}{\sqrt{3}}\hat{y}) = -\frac{2\pi}{a\sqrt{3}}\hat{y} + \frac{2\pi}{a\sqrt{3}}\sqrt{3}\hat{x}$

$\vec{b}_2 = \frac{4\pi}{a\sqrt{3}}\hat{y}$

$\vec{b}_3 = \frac{2\pi}{c}\hat{z}$

The angle between the first two vectors is again 60 degrees, but they are rotated by 30 degrees compared to the original lattice.

(b) $c_{rec} = \frac{2\pi}{c}$, $a_{rec} = \frac{4\pi}{a\sqrt{3}}$

$(\frac{c}{a})_{rec} = \frac{\sqrt{3}}{2}(\frac{c}{a})^{-1}$

The c over a ratios are the same when

$(\frac{c}{a}) = \sqrt{\frac{\sqrt{3}}{2}}$

If the direct lattice is ideal $(\frac{c}{a}) = \frac{\sqrt{8}}{\sqrt{3}}$ and $(\frac{c}{a})_{rec} = \frac{3}{4\sqrt{2}}$

(c) Trigonal basis $\vec{a}_1 = a_0(x,1,1)$, $\vec{a}_2 = a_0(1,x,1)$,$\vec{a}_3 = a_0(1,1,x)$

The length of these vectors is $a = a_0\sqrt{2+x^2}$

The angle between the vectors is $\cos(\theta) = \frac{1}{a^2}\vec{a}_1 \cdot \vec{a}_2 = \frac{1+2x}{2+x^2}$

$\vec{a}_1 \times \vec{a}_2 = a_0^2(1-x, 1-x, x^2-1)$

$\vec{a}_1 \times \vec{a}_2 \cdot \vec{a}_3 = a_0^3(x(x^2-1) + 2(1-x)) = a_0^3(x-1)(x^2+x-2) =$

$a_0^3(x-1)^2(x+2)$

Hence $\vec{b}_3 = \frac{2\pi}{a_0(x-1)^2(x+2)}(1-x, 1-x, x^2-1)$ or

$\vec{b}_3 = \frac{2\pi}{a_0(1-x)(x+2)}(1,1,-(1+x))$

It is easy to see that (cyclic permutations)

$\vec{b}_1 = \frac{2\pi}{a_0(1-x)(x+2)}(-(1+x),1,1)$

$\vec{b}_2 = \frac{2\pi}{a_0(1-x)(x+2)}(1,-(1+x),1)$

This is again a trigonal lattice. The length of each vector is

$b = \frac{2\pi\sqrt{2+(1+x)^2}}{a_0(1-x)(x+2)} = \frac{2\pi\sqrt{2+x^2}\sqrt{2+(1+x)^2}}{a(1-x)(x+2)}$

$\cos(\theta') = \frac{-2(1+x)+1}{2+(1+x)^2} = -\frac{2x+1}{2+(1+x)^2}$

Compare

$\cos^{-1}(\theta) = \frac{2+x^2}{1+2x}$

and

$\cos^{-1}(\theta') = -\frac{x^2+2x+3}{2x+1}$

This shows

$\cos^{-1}(\theta) + \cos^{-1}(\theta') = \frac{-2x-1}{1+2x} = -1$

from which the required relation follows. Also

$2\cos(\theta)\cos(\theta') = -2\frac{1+2x}{2+x^2}\frac{2x+1}{2+(1+x)^2} = -2\frac{(1+2x)^2}{(2+x^2)(2x^2+2x+3}$

$1 + 2\cos(\theta)\cos(\theta') = \frac{(x-1)^2(x+2)^2}{(2+x^2)(2x^2+2x+3}$

which gives the required relation between a and b.

Problem 2. Ashcroft-Mermin 6.1

The formula to use is $K = 2k\sin(\frac{1}{2}\phi)$ where $k = \frac{2\pi}{\lambda}$.

(a) For the bcc structure the reciprocal lattice is fcc and the first four distances K are (see problem 4.7): $\frac{2\pi}{a}\sqrt{2}$, $\frac{2\pi}{a}\sqrt{4}$, $\frac{2\pi}{a}\sqrt{6}$, $\frac{2\pi}{a}\sqrt{8}$

For the fcc structure the reciprocal lattice is bcc and the first four distances K are $\frac{2\pi}{a}\sqrt{3}$, $\frac{2\pi}{a}\sqrt{4}$, $\frac{2\pi}{a}\sqrt{8}$, $\frac{2\pi}{a}\sqrt{11}$

For the diamond structure we have a bcc reciprocal lattice, but (see book) peaks at (2,0,0), (2,2,2), etc are extinguished $\frac{2\pi}{a}\sqrt{3}$, $\frac{2\pi}{a}\sqrt{8}$, $\frac{2\pi}{a}\sqrt{11}$, $\frac{2\pi}{a}\sqrt{16}$

This gives

bcc: $\sin(\frac{1}{2}\phi_2) = \sqrt{2}\sin(\frac{1}{2}\phi_1)$,

$\sin(\frac{1}{2}\phi_3) = \sqrt{3}\sin(\frac{1}{2}\phi_1)$, $\sin(\frac{1}{2}\phi_4) = \sqrt{4}\sin(\frac{1}{2}\phi_1)$

fcc: $\sin(\frac{1}{2}\phi_2) = \sqrt{\frac{4}{3}}\sin(\frac{1}{2}\phi_1)$,

$\sin(\frac{1}{2}\phi_3) = \sqrt{\frac{8}{3}}\sin(\frac{1}{2}\phi_1)$, $\sin(\frac{1}{2}\phi_4) = \sqrt{\frac{11}{3}}\sin(\frac{1}{2}\phi_1)$

diamond: $\sin(\frac{1}{2}\phi_2) = \sqrt{\frac{8}{3}}\sin(\frac{1}{2}\phi_1)$,

$\sin(\frac{1}{2}\phi_3) = \sqrt{\frac{11}{3}}\sin(\frac{1}{2}\phi_1)$, $\sin(\frac{1}{2}\phi_4) = \sqrt{\frac{16}{3}}\sin(\frac{1}{2}\phi_1)$

Therefore

	ϕ_1	ϕ_2	ϕ_3	ϕ_4
bcc	28.8	41.2	51.0	59.7
bcc	42.2	61.2	77.1	92.1
bcc	42.8	62.1	78.4	93.7
fcc	28.8	33.4	47.9	56.9
fcc	42.2	49.1	72.0	87.2
fcc	42.8	49.8	73.1	88.6
diamond	28.8	47.9	56.9	70.1
diamond	42.2	72.0	87.2	112.5
diamond	42.8	73.1	88.6	114.8

and A=fcc, B=bcc, C=diamond.

(b) We have $\lambda = 1.5Ang$. Using

$K_1 = 2k\sin(\frac{1}{2}\phi_1)$ and $k = \frac{2\pi}{\lambda}$ we get

bcc $K_1 = \frac{2\pi}{a}\sqrt{2}$ or $a = \frac{2\pi}{K_1}\sqrt{2} = \frac{\lambda}{2\sin(\frac{1}{2}\phi_1)}\sqrt{2}$

fcc $K_1 = \frac{2\pi}{a}\sqrt{3} = \frac{\lambda}{2\sin(\frac{1}{2}\phi_1)}\sqrt{3}$

diamond $K_1 = \frac{2\pi}{a}\sqrt{3} = \frac{\lambda}{2\sin(\frac{1}{2}\phi_1)}\sqrt{3}$

which leads to

structure A (fcc) $a = 3.6Ang$

structure B (bcc) $a = 4.3Ang$

structure C (diamond) $a = 3.6Ang$

(c) Now we go back to an fcc structure and the second peak shows, therefore the angles would be 42.8 , 49.8 , 73.2 , 89.0

Problem 3. Ashcroft-Mermin 6.3

(a) We have $\vec{d} = \frac{1}{3}\vec{a}_1 + \frac{1}{3}\vec{a}_2 + \frac{1}{2}\vec{a}_3$ (use figure 4.20)

and $\vec{K} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$ with $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$

In standard notation:

$\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{a\sqrt{3}}{2}\hat{y}$, $\vec{a}_3 = c\hat{z}$ and

$\vec{b}_1 = \frac{a'\sqrt{3}}{2}\hat{x} - \frac{a'}{2}\hat{y}$,$\vec{b}_2 = a'\hat{y}$, $\vec{b}_3 = c'\hat{z}$

This gives

$S_{\vec{K}} = 1 + e^{i\vec{K}\cdot\vec{d}} = 1 + e^{2\pi i(\frac{m_1}{3}+\frac{m_2}{3}+\frac{m_3}{2})}$

or

$S_{\vec{K}} = 1 + e^{\frac{\pi}{3}i(2m_1+2m_2+3m_3)}$

and $2m_1 + 2m_2 + 3m_3$ can take all integer values.

(b) This is the plane given by $m_3 = 0$, in which case

$S_{\vec{K}} = 1 + e^{\frac{2\pi}{3} i(m_1+m_2)}$

and this is never zero, since that would require $m_1 + m_2 = \frac{3}{2}(1 + 2k)$ with k integer. This is not possible.

(c) $S_{\vec{K}} = 0$ requires $2m_1 + 2m_2 + 3m_3 = 3 + 6k$, k integer. This has solutions only when m_3 is odd.

(d) These are the points $\vec{K} = m_3\vec{b}_3$ with m_3 odd. We have for these points $S_{\vec{K}} = 1 + e^{\frac{\pi}{3} i3m_3} = 1 + e^{i\pi m_3}$ which is zero.

(e) Take, for example, the case $m_3 = 1$. The points left in this plane form a two dimensional structure given by $\vec{P} = m_1\vec{b}_1 + m_2\vec{b}_2$ with $m_1 + m_2 = 3k+1$ or $m_1 + m_2 = 3k + 2$, k integer.

The collection of all points $\vec{P} = m_1\vec{b}_1 + m_2\vec{b}_2$ forms a triangular net, since $\vec{b}_1$ and $\vec{b}_2$ have equal lengths and have a 120 degree angle.

The collection of points $\vec{P} = m_1\vec{b}_1 + m_2\vec{b}_2$ with $m_1 + m_2 = 3k$, k integer also form a triangular net, with basis vectors $\vec{b}_1 + 2\vec{b}_2$ and $2\vec{b}_1 + \vec{b}_2$.

From Figure 4.17 we see that the collection of all heavy dots and centers of the hexagons form a triangular net and that the collection of center points forms a triangular net with one third of the points, identical to our situation. Therefore, the set of remaining points is a honeycomb net.