Physics 481: Solid State Physics - Homework Solutions 3

Homework 3.1

a) volume of primitive cell

$$V = \frac{a^3}{8} \begin{vmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{vmatrix} = \frac{a^3}{4}$$

$$\vec{b}_1 = \frac{2\pi}{V}(\vec{a}_2 \times \vec{a}_3) = \frac{2\pi}{a}\begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}$$

$$\vec{b}_2 = \frac{2\pi}{V}(\vec{a}_3 \times \vec{a}_1) = \frac{2\pi}{a}\begin{pmatrix} -1 \\ 1 \\ -1 \end{pmatrix}$$

$$\vec{b}_3 = \frac{2\pi}{V}(\vec{a}_1 \times \vec{a}_2) = \frac{2\pi}{a}\begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix}$$

b.c.c. lattice
lattice constant $\frac{4\pi}{a}$

$$\frac{d\sigma}{d\Omega} \sim N S(\vec{q})$$

delta peaks at $\vec{q} = \vec{K} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$

b) <u>conventional unit cell</u>

$\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = a\hat{y}$, $\vec{a}_3 = a\hat{z}$

<u>4 atom basis:</u>

$$\vec{v}_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \vec{v}_2 = \frac{a}{2}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \vec{v}_3 = \frac{a}{2}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \vec{v}_4 = \frac{a}{2}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$$

<u>reciprocal lattice</u>

$$\vec{b}_1 = \frac{2\pi}{a}\hat{x}, \quad \vec{b}_2 = \frac{2\pi}{a}\hat{y}, \quad \vec{b}_3 = \frac{2\pi}{a}\hat{z}$$

$$\Rightarrow \vec{q} = \vec{K} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$$
$$= \frac{2\pi}{a}(n_1\hat{x} + n_2\hat{y} + n_3\hat{z})$$

Modulation factor

$$F(\vec{q}) = \left| \sum_j e^{i\vec{q}\cdot\vec{v}_j} \right|^2$$

$$= \left| 1 + e^{i\pi(n_1+n_2)} + e^{i\pi(n_1+n_3)} + e^{i\pi(n_2+n_3)} \right|^2$$

$$= 4 + 2\cos\pi(n_1+n_2) + 2\cos\pi(n_1+n_3) + 2\cos\pi(n_2+n_3)$$

$$+ 2\cos\pi(n_2-n_3) + 2\cos\pi(n_1-n_3) + 2\cos\pi(n_1-n_2)$$

$F(\vec{q}) = 16$ if all n are even

or all n odd

$\Rightarrow$ b.c.c lattice with lattice constant

$\frac{4\pi}{a}$

Homework 3.2

scattering condition in powder method

$$q = 2k_0 \sin\Theta = 2k_0 \sin\frac{\vartheta}{2}$$

table of $\sin\frac{\vartheta}{2}$

A	B	C
0.36	0.249	0.365
0.416	0.35	0.596
0.588	0.429	0.701
0.69	0.497	0.843

ratios

A	B	C
1	1	1
1.155	1.41	1.633
1.633	1.72	1.92
1.917	2	2.31

Calculate shortest reciprocal lattice vectors

fcc : reciprocal lattice is bcc $\frac{2\pi}{a}\begin{pmatrix}-1\\-1\\1\end{pmatrix}, \frac{2\pi}{a}\begin{pmatrix}-1\\1\\-1\end{pmatrix}, \frac{2\pi}{a}\begin{pmatrix}1\\-1\\-1\end{pmatrix}$

$n_1 = 1, n_2, n_3 = 0 \quad |\vec{K}_1| = \frac{2\pi}{a}\sqrt{3}$

$n_1 = 2, n_2, n_3 = 0 \quad |\vec{K}_2| = \frac{2\pi}{a}\, 2\sqrt{3}$

$n_1 = 1, n_2 = 1, n_3 = 0 \quad \frac{2\pi}{a}\begin{pmatrix}2\\0\\0\end{pmatrix} \quad |\vec{K}_3| = \frac{2\pi}{a}\cdot 2$

$n_1 = 1, n_2 = 1 \; n_3 = 1 \quad \frac{2\pi}{a}\begin{pmatrix}-1\\-1\\-1\end{pmatrix} \quad |\vec{K}_4| = \frac{2\pi}{a}\cdot\sqrt{3}$

$n_1 = 1, n_1 = -1 \quad \frac{2\pi}{a}\begin{pmatrix}0\\2\\2\end{pmatrix} \quad |\vec{K}_5| = \frac{2\pi}{a}\, 2\sqrt{2}$

$n_1 = 1 \quad n_2 = +1, n_3 = -1 \quad \frac{2\pi}{a}\begin{pmatrix}-3\\1\\1\end{pmatrix} \quad |\vec{K}_6| = \frac{2\pi}{a}\sqrt{11}$

ratios:

1
1.155
1.633
1.915
2

A

$\boxed{4}$

bcc: reciprocal lattice is fcc $\frac{2\pi}{a}\begin{pmatrix}1\\1\\0\end{pmatrix}$ $\frac{2\pi}{a}\begin{pmatrix}1\\0\\1\end{pmatrix}$ $\frac{2\pi}{a}\begin{pmatrix}0\\1\\1\end{pmatrix}$

n_1	n_2	n_3		
1	0	0	$\lvert\vec{K}_1\rvert = \frac{2\pi}{a}\sqrt{2}$	
1	1	0	$\vec{K}_2 = \frac{2\pi}{a}(2,1,1)$	$\lvert\vec{K}_2\rvert = \frac{2\pi}{a}\sqrt{6}$
1	−1	0	$\vec{K}_3 = \frac{2\pi}{a}(0\ 1\ -1)$	$\lvert\vec{K}_3\rvert = \frac{2\pi}{a}\sqrt{2}$
1	1	1	$\vec{K}_4 = \frac{2\pi}{a}(2\ 2\ 2)$	$\vec{K}_4 = \frac{2\pi}{a}\sqrt{12}$
1	1	−1	$\vec{K}_5 = \frac{2\pi}{a}(2,0\ 0)$	$\vec{K}_5 = \frac{2\pi}{a}\,2$
2	0	0	$\lvert\vec{K}_6\rvert = \frac{2\pi}{a}\,2\sqrt{2}$	

ratios: 1, 1.414, 1.73, 2 $\Rightarrow$ B

leaves diamond for C (extinctions compare with f.c.c.)

5) fcc $\frac{2\pi}{a}\sqrt{3} = 2k_0 \cdot 0.36 = 2\frac{2\pi}{\lambda}\cdot 0.36$

$$a = \frac{\sqrt{3}}{2}\frac{\lambda}{0.36} = 3.608\,\mathring{A}$$

bcc $\frac{2\pi}{a}\sqrt{2} = 2\frac{2\pi}{\lambda}\cdot 0.249$

$$a = \frac{\sqrt{2}}{2}\frac{\lambda}{0.249} = 4.260\,\mathring{A}$$

diamond $a = \frac{\sqrt{3}}{2}\frac{\lambda}{0.365} = 3.559\,\mathring{A}$