Physics 560A HW 2 solutions

1) <u>3.1</u> a) Reciprocal to bcc lattice:

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \frac{2\pi}{a}(\hat{y} + \hat{z})$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \frac{2\pi}{a}(\hat{x} + \hat{z})$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \frac{2\pi}{a}(\hat{x} + \hat{y})$$

$\Rightarrow$ fcc lattice

Reciprocal to fcc lattice:

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

$$\vec{b}_2 = \frac{2\pi}{a}(\hat{x} - \hat{y} + \hat{z})$$

$$\vec{b}_3 = \frac{2\pi}{a}(\hat{x} + \hat{y} - \hat{z})$$

$\Rightarrow$ bcc lattice

3.1 b) Al = fcc

shortest $\vec{G}$s are the 8 vectors

$\frac{2\pi}{a}(\pm\hat{x} \pm \hat{y} \pm \hat{z})$ $a = 4.05\,\mathring{A}$

miller indices: ⟨111⟩

Fe = bcc shortest $\vec{G}$s are the

$a = 2.87\,\mathring{A}$

12 vectors:

$\frac{2\pi}{a}(\pm\hat{y} \pm \hat{z})$, $\frac{2\pi}{a}(\pm\hat{x} \pm \hat{y})$, $\frac{2\pi}{a}(\pm\hat{x} \pm \hat{z})$

miller indices: ⟨110⟩

Be = hcp = simple hexagonal with basis of two atoms and $\frac{c}{a} = \sqrt{\frac{8}{3}}$

Shortest $\vec{G}$s are $\pm\frac{2\pi}{c}\hat{z}$ $c = 3.58\,\mathring{A}$

Miller indices: (001) $(00\bar{1})$

~~3.2 a) using Wyckoff's convention~~

$\cancel{\vec{a}_1 = \sqrt{3}\frac{a}{2}\hat{x} + \frac{a}{2}\hat{y}}$ $\cancel{\vec{a}_2 = -\frac{\sqrt{3}}{2}a\hat{x} + \frac{a}{2}\hat{y}}$

$\cancel{\vec{a}_3 = c\hat{z}}$ $\cancel{\vec{b}_1 = 2\pi\frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot\vec{a}_2\times\vec{a}_3} = \frac{2\pi}{\sqrt{3}a}\hat{x} + \frac{2\pi}{a}\hat{y}}$

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

3.2 a)

$$\vec{b}_1 = \frac{2\pi\, \vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \frac{4\pi}{\sqrt{3}\, a^2 c} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ a/2 & \frac{a\sqrt{3}}{2} & 0 \\ 0 & 0 & c \end{vmatrix}$$

$$= \frac{2\pi}{a}\hat{x} - \frac{2\pi}{\sqrt{3}\, a}\hat{y}$$

$$\vec{b}_2 = \frac{2\pi\, \vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \frac{4\pi}{\sqrt{3}\, a^2 c} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & c \\ a & 0 & 0 \end{vmatrix}$$

$$= \frac{4\pi}{\sqrt{3}\, a}\hat{y}$$

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

b) $$F(\vec{G}) = \left| \sum_{\ell} e^{i \vec{G} \cdot \vec{v}_\ell} \right|^2$$

$$\vec{v}_1 = (0, 0, 0) \qquad \vec{v}_2 = \left(\frac{a}{2} \quad \frac{a}{2\sqrt{3}} \quad \frac{c}{2} \right)$$

$$\vec{G} = n_1 \vec{b}_1 + n_2 \vec{b}_2 + n_3 \vec{b}_3$$

$$\vec{G} \cdot \vec{v}_2 = n_1 \vec{b}_1 \cdot \vec{v}_2 + n_2 \vec{b}_2 \cdot \vec{v}_2 + n_3 \vec{b}_3 \cdot \vec{v}_2$$

$$\vec{b}_1 \circ \vec{V}_2 = \begin{pmatrix} \frac{2\pi}{a} & \frac{-2\pi}{\sqrt{3}a} & 0 \end{pmatrix} \begin{pmatrix} \frac{a}{2} \\ \frac{a}{2\sqrt{3}} \\ \frac{c}{2} \end{pmatrix} = \frac{2\pi}{3}$$

$$\vec{b}_2 \circ \vec{V}_2 = \frac{4\pi}{\sqrt{3}a} \frac{a}{2\sqrt{3}} = \frac{2\pi}{3}$$

$$\vec{b}_3 \circ \vec{V}_2 = \pi$$

$$F(\vec{G}) = \left| 1 + e^{i\frac{\pi}{3}(2n_1 + 2n_2 + 3n_3)} \right|^2$$

c) $2n_1 + 2n_2 + 3n_3 = 3(2n+1)$

If n_1 and n_2 are multiples of 3 (including 0) and n_3 is odd, then $F(\vec{G}) = 0$.

Physics 560 Homework # 2

Solutions (continued)

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3) a) The plane (hkl) intersects the axes $\vec{a}_1$, $\vec{a}_2$, & $\vec{a}_3$ at $kl\,\vec{a}_1$, $hl\,\vec{a}_2$, & $hk\,\vec{a}_3$.

The normal to the plane is the cross product

$$hkl\,\vec{n} = (hl\,\vec{a}_2 - kl\,\vec{a}_1) \times (hk\,\vec{a}_3 - kl\,\vec{a}_1)$$

$$\vec{n} = h\,(\vec{a}_2 \times \vec{a}_3) + k\,(\vec{a}_3 \times \vec{a}_1) + l\,(\vec{a}_1 \times \vec{a}_2)$$

Now $\vec{G} = \dfrac{2\pi\,\vec{n}}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$, thus

$\vec{G} \perp (hkl)$.

b) Let $\vec{r}_1$ and $\vec{r}_2$ be nearest points in two neighboring planes parallel to (hkl). $\vec{r}_1$ and $\vec{r}_2$ are points in the Bravais lattice, and so is

$$\vec{d} = \vec{r}_2 - \vec{r}_1 .$$

The distance between planes is

$$d = |\vec{d}| .$$

But $e^{i\vec{G}\cdot\vec{d}} = 1$ by the definition of a reciprocal lattice vector. Thus

$$\vec{G}\cdot\vec{d} = |\vec{G}|\, d \cos\theta = 2\pi n .$$

We showed that $\theta = 0$ in part (a). Thus $|\vec{G}| d = 2\pi n$.

The shortest reciprocal lattice vector in the direction $\hat{G}$ satisfies this relation with $n=1$. Q.E.D.

c) In the s.c. lattice,

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

$$\vec{G} = \frac{2\pi}{a}(h\hat{x} + k\hat{y} + l\hat{z})$$

$$|\vec{G}| = \frac{2\pi}{a}\sqrt{h^2+k^2+l^2}$$

$$d^2 = \frac{(2\pi)^2}{G^2} = \frac{a^2}{h^2+k^2+l^2}$$

4) Volume of Brillouin Zone

$$V_{BZ} = |\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)|$$

$$= \left(\frac{2\pi}{V_c}\right)^3 (\vec{a}_2 \times \vec{a}_3) \cdot [(\vec{a}_3 \times \vec{a}_1) \times (\vec{a}_1 \times \vec{a}_2)]$$

$$= \left(\frac{2\pi}{V_c}\right)^3 (\vec{a}_2 \times \vec{a}_3) \cdot \underbrace{[\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)]}_{V_c} \vec{a}_1$$

$$= \frac{(2\pi)^3 V_c^2}{V_c^3} = \frac{(2\pi)^3}{V_c} \qquad \text{Q.E.D.}$$