Assignment 1

pg. 25 #1

From Fig. 12: $\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$

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

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

Angle between $\vec{a}_1$ + $\vec{a}_2$ is θ.

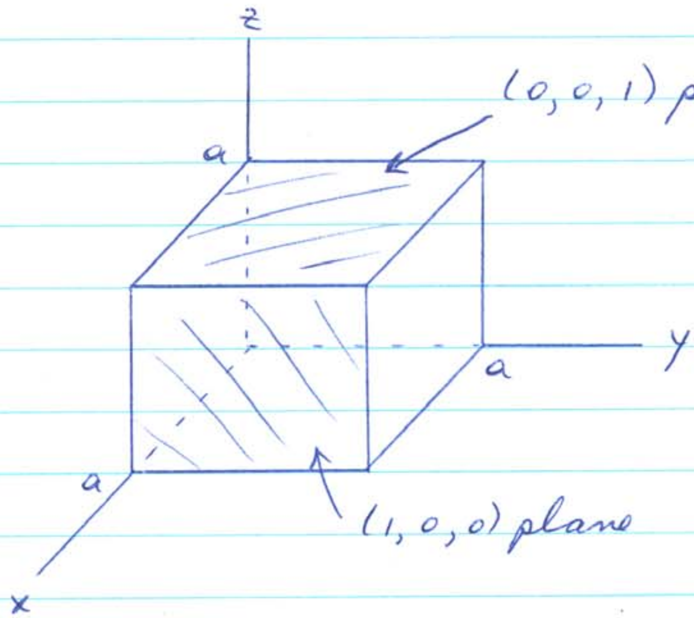
$$\cos\theta = \frac{\vec{a}_1 \cdot \vec{a}_2}{|\vec{a}_1||\vec{a}_2|}$$

$$= \frac{\left(\frac{a}{2}\right)^2(-1+1-1)}{\left(\frac{a}{2}\right)^2\sqrt{1+1+1}\,\sqrt{1+1+1}}$$

$$= -\frac{1}{3}$$

$\therefore$ $\theta = 109.5°$ is angle between tetrahedral bonds of diamond.

pg. 25 # 2.



Primitive vectors for simple cubic lattice are:

$$\vec{a} = a(1,0,0)$$
$$\vec{b} = a(0,1,0)$$
$$\vec{c} = a(0,0,1)$$

Primitive vectors for rhombohedral cell are:

$$\vec{a}' = \frac{a}{2}(1,1,0)$$
$$\vec{b}' = \frac{a}{2}(0,1,1)$$
$$\vec{c}' = \frac{a}{2}(1,0,1)$$

In terms of $\vec{a}'$, $\vec{b}'$, $\vec{c}'$, plane $(0,0,1)$ intersects at $(\infty, 2, 2)$
Inverting intersection points $\Rightarrow (0, \frac{1}{2}, \frac{1}{2}) \xrightarrow{\text{integerize}} (0,1,1)$.

$\therefore$ $(0,1,1)$ are Miller indices w.r.t. $\vec{a}'$, $\vec{b}'$, $\vec{c}'$ for $(0,0,1)$ plane.

Similarly $(1,0,1)$ " " $(1,0,0)$ " .

2a) Volume of Primitive Cell $V = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$

$$V = \left| \left(\frac{\sqrt{3}\,a}{2}, \frac{a}{2}, 0 \right) \cdot \left(\left(-\frac{\sqrt{3}\,a}{2}, \frac{a}{2}, 0 \right) \times (0, 0, c) \right) \right|$$

$$= a^2 c \left| \left(\frac{\sqrt{3}}{2}, \frac{1}{2}, 0 \right) \cdot \left(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0 \right) \right|$$

$$= \frac{\sqrt{3}}{2} a^2 c$$

b) Reciprocal lattice vectors are:

$$\vec{b}_1 = \frac{2\pi \; \vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$= \frac{2\pi \; ac \left(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0 \right)}{\frac{\sqrt{3}}{2} a^2 c}$$

$$= \frac{2\pi}{a} \left(\frac{1}{\sqrt{3}}, 1, 0 \right)$$

Similarly $\vec{b}_2 = \dfrac{2\pi \; \vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$

$$= \frac{2\pi}{a} \left(\frac{-1}{\sqrt{3}}, 1, 0 \right)$$

and $\vec{b}_3 = \dfrac{2\pi \; \vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$

$$= \frac{2\pi}{c} (0, 0, 1).$$

3) Volume of first Brillouin zone is:

$$V_B = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)$$

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

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

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

$$\therefore V_B = \frac{(2\pi)^3}{V_c} \quad \text{where } V_c \equiv \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$$

5) Structure Factor $S = \sum_{j=1}^{s} f_j \, e^{-i\vec{G}\cdot\vec{r}_j}$

$$\vec{r}_j \cdot \vec{G} = (x_j \vec{a}_1 + y_j \vec{a}_2 + z_j \vec{a}_3) \cdot (h \vec{b}_1 + k \vec{b}_2 + l \vec{b}_3)$$

$$= 2\pi (h x_j + k y_j + l z_j)$$

For diamond $f_j \equiv f$ (all carbon atoms)

$$\therefore S = f \left\{ \exp -2\pi i (0) + \exp -2\pi i \left(\frac{h+l}{2}\right) + \exp -2\pi i \left(\frac{k+l}{2}\right) + \exp -2\pi i \left(\frac{h+k}{2}\right) \right\} \cdot \left\{ 1 + \exp -2\pi i \left(\frac{h+k+l}{4}\right) \right\}$$

$$= f \left\{ 1 + (-1)^{h+l} + (-1)^{k+l} + (-1)^{h+k} \right\} \left(1 + \exp -\pi i \frac{(h+k+l)}{2} \right)$$

$\therefore S = 0$ if 1) $\exp -\frac{\pi i}{2} (h+k+l) = -1$

or $\frac{h+k+l}{2} = n \overbrace{\ }^{\text{odd}}$ integer

2) two of (h, k, l) are even and one odd or vice versa

$\therefore$ allowed reflections occur when $h+k+l = 4n$ and when all h, k, l are even or all odd.

6) Form Factor of Atomic H

$$f_H = \int n(\vec{\rho})\, e^{-i\vec{G}\cdot\vec{\rho}}\, d^3\rho$$

$$= \frac{1}{\pi a_0^3} \int e^{-2r/a_0}\, e^{-iGr\cos\theta}\, 2\pi r^2 \sin\theta\, d\theta\, dr$$

$$= \frac{2}{a_0^3} \int_0^\infty e^{-2r/a_0} \int_{u=-1}^{u=1} e^{-iGru}\, du\, r^2\, dr \qquad (u = \cos\theta)$$

$$= \frac{2}{a_0^3} \int_0^\infty e^{-2r/a_0} \left. \frac{e^{-iGru}}{-iGr} \right|_{-1}^{+1} r^2\, dr$$

$$= \frac{2}{a_0^3} \int_0^\infty e^{-2r/a_0}\, \frac{e^{-iGr} - e^{iGr}}{-iGr}\, r^2\, dr$$

$$= \frac{-2}{a_0^3\, iG} \int_0^\infty r\, e^{-2r/a_0} \left(e^{-iGr} - e^{iGr}\right) dr$$

Using $\int_0^\infty x\, e^{cx}\, dx = \frac{1}{c^2}$ provided $\mathrm{Re}\, c < 0$, we find:

$$f_H = \frac{16}{(4 + G^2 a_0^2)^2}.$$