

Solutions

1. The coordinates of the nearest neighbors in diamond are:

$$\vec{r}_1 = \frac{a}{2} (\hat{x} + \hat{y} + \hat{z}) \quad \vec{r}_2 = \frac{a}{2} (\hat{x} - \hat{y} - \hat{z})$$

$$\vec{r}_3 = \frac{a}{2} (-\hat{x} + \hat{y} - \hat{z}) \quad \vec{r}_4 = \frac{a}{2} (-\hat{x} - \hat{y} + \hat{z})$$

We can find the angle between any 2 of these.

Use $\vec{r}_1 \cdot \vec{r}_2 = |\vec{r}_1| |\vec{r}_2| \cos \Theta$

$$\vec{r}_1 \cdot \vec{r}_2 = -\frac{a^2}{4}$$

$$|\vec{r}_1| |\vec{r}_2| = \frac{3a^2}{4}$$

$$\therefore \cos \Theta = -1/3$$

$$\rightarrow \Theta = 109.47^\circ$$

2. a)

We only have to show that \vec{G} is perpendicular to two vectors which are not parallel to each other but parallel to the plane considered. Let's call $\vec{a}, \vec{b}, \vec{c}$ the lattice translation vectors and $\vec{a}^*, \vec{b}^*, \vec{c}^*$ reciprocal lattice vectors. We have to show that

$$\vec{G} \cdot \left(\frac{1}{h} \vec{a} - \frac{1}{k} \vec{b} \right) = 0 \quad \text{and} \quad \vec{G} \cdot \left(\frac{1}{h} \vec{a} - \frac{1}{l} \vec{c} \right) = 0$$

$$\vec{G} \cdot \left(\frac{1}{h} \vec{a} - \frac{1}{k} \vec{b} \right) = \frac{1}{h} \vec{a} \cdot h \vec{a}^* - \frac{1}{k} \vec{b} \cdot k \vec{b}^*$$

$$= 2\pi(1-1) = 0$$

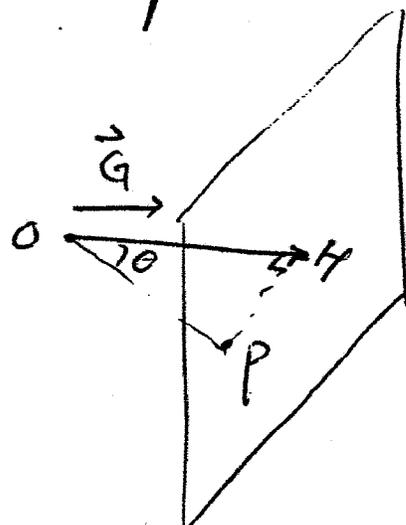
$$\vec{G} \cdot \left(\frac{1}{h} \vec{a} - \frac{1}{l} \vec{c} \right) = \frac{1}{h} \vec{a} \cdot h \vec{a}^* - \frac{1}{l} \vec{c} \cdot l \vec{c}^*$$

$$= 0$$

Therefore \vec{G} is perpendicular to (hkl)

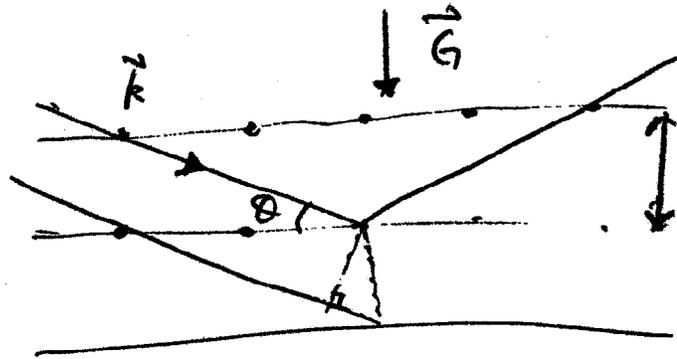
b) If we know a point lying on a plane, the distance from the origin to the plane is

$$\begin{aligned} OH &= OP \cos \theta \\ &= OP \cdot \frac{\vec{G} \cdot \vec{OP}}{|\vec{G}| OP} \\ &= \frac{\vec{G} \cdot \vec{OP}}{|\vec{G}|} = \frac{2\pi}{|\vec{G}|} \end{aligned}$$



if we take $\vec{OP} = \frac{1}{h} \vec{a}$.
 Hence the planes are separated by $\frac{2\pi}{|\vec{G}|}$

(c) $2\vec{k} \cdot \vec{G} = G^2$
 $\vec{k} \cdot \vec{G} = kG \cos(\pi/2 - \theta)$
 $= kG \sin \theta$



$\therefore 2kG \sin \theta = G^2$

$\therefore 2k \sin \theta = G$ $\dots \textcircled{*}$

Here G can be any reciprocal lattice vector which is perpendicular to the plane. Hence

$G = n \left(\frac{2\pi}{d} \right)$ n : integer.

$\therefore \textcircled{*}$ becomes $2d \sin \theta = n\lambda$

3. a)

The basis atoms are drawn in solid circles.

Their coordinates are

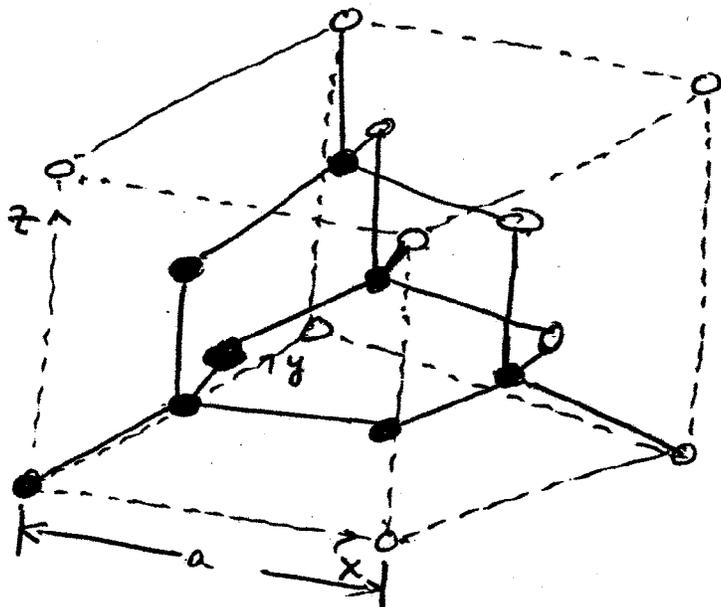
$$a(0, 0, 0),$$

$$a\left(\frac{1}{2}, \frac{1}{2}, 0\right), a\left(\frac{1}{2}, 0, \frac{1}{2}\right)$$

$$a\left(0, \frac{1}{2}, \frac{1}{2}\right), a\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right),$$

$$a\left(\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right), a\left(\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right)$$

$$a\left(\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right).$$



The structure factor is given by

$$S_G = \sum_j f_j \exp(-i \vec{G} \cdot \vec{r}_j)$$

The reciprocal lattice vectors are based on

$$\left\{ \frac{2\pi}{a} \hat{x}, \frac{2\pi}{a} \hat{y}, \frac{2\pi}{a} \hat{z} \right\}$$

Let $\vec{G} = \frac{2\pi}{a} (v_1 \hat{x} + v_2 \hat{y} + v_3 \hat{z})$. Then S_G is given by

$$S_G = f \left\{ 1 + \exp(-i\pi(v_1+v_2)) + \exp(-i\pi(v_2+v_3)) \right. \\ + \exp(-i\pi(v_1+v_3)) + \exp\left(-\frac{i\pi}{2}(v_1+v_2+v_3)\right) \\ + \exp\left(-\frac{i\pi}{2}(3v_1+3v_2+v_3)\right) \\ + \exp\left(-\frac{i\pi}{2}(3v_1+v_2+3v_3)\right) \\ \left. + \exp\left(-\frac{i\pi}{2}(v_1+3v_2+3v_3)\right) \right\}$$

$$\begin{aligned}
 &= f \left\{ 1 + e^{-i\pi(v_1+v_2)} + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_1+v_3)} \right. \\
 &\quad \left. + e^{-i\pi/2(v_1+v_2+v_3)} \right\} \times \left\{ 1 + e^{-i\pi(v_1+v_2)} + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_1+v_3)} \right\} \\
 &= f \left(1 + e^{-i\pi/2(v_1+v_2+v_3)} \right) \\
 &\quad \times \left\{ 1 + e^{-i\pi(v_1+v_2)} + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_1+v_3)} \right\} \\
 &\quad \dots \rightarrow \text{Answer}
 \end{aligned}$$

b)

$$1 + e^{-i\pi/2(v_1+v_2+v_3)} = 0 \text{ if } v_1+v_2+v_3 = 4n+2.$$

$$1 + e^{-i\pi(v_1+v_2)} + e^{-i\pi(v_2+v_3)} + e^{-i\pi(v_1+v_3)} = 0 \quad (n \text{ integer})$$

unless all of indices are even or odd.

Hence the condition to get reflection is

$$\left(v_1+v_2+v_3 \neq 4n+2 \right) \text{ and } \left\{ \begin{array}{l} \text{all of indices are even} \\ \text{or all of indices are odd} \end{array} \right.$$

$$\equiv \left[\left(v_1+v_2+v_3 \neq 4n+2 \right) \text{ and (all of indices are even)} \right. \\ \left. \text{for any integer } n \right]$$

$$\text{or } \left[\left(v_1+v_2+v_3 \neq 4n+2 \right) \text{ and (all of indices are odd)} \right. \\ \left. \text{for any integer } n \right]$$

$$\equiv \left[\left(v_1+v_2+v_3 = 4n \right) \text{ and (all of indices are even)} \right. \\ \left. \text{for any integer } n \right]$$

or (all of indices are odd)

4. Germanium has diamond structure with $a = 5.65 \text{ \AA}$ when we think of the structure as a simple cubic structure.

$$\vec{G} = h_1 \vec{b}_1 + h_2 \vec{b}_2 + h_3 \vec{b}_3 \quad \text{where}$$

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

$$\therefore |\vec{G}| = \frac{2\pi}{a} (h_1^2 + h_2^2 + h_3^2)^{1/2}$$

$$\therefore d = \frac{2\pi}{G} = \frac{a}{(h_1^2 + h_2^2 + h_3^2)^{1/2}}$$

Bragg condition is

$$2d \sin \theta = \lambda$$

i) (111) plane

$$d = \frac{a}{\sqrt{3}} = 3.262 \text{ \AA}$$

$$\sin \theta = \left(\frac{\lambda}{2d} \right) = (0.236)$$

$$\therefore \theta = 13.65^\circ$$

$$\theta_c = 76.35^\circ$$

ii) (220) plane

$$d = \frac{a}{2\sqrt{2}} = 1.978 \text{ \AA}$$

$$\sin \theta = n \left(\frac{\lambda}{2d} \right) = (0.385)$$

$$\theta = 22.64^\circ$$

$$\theta_c = 67.36^\circ$$

iii) (311) plane

$$d = \frac{a}{\sqrt{11}} = 1.704 \text{ \AA}$$

$$\sin \theta = \left(\frac{\lambda}{2d} \right) = (0.452)$$

$$\theta = 26.9^\circ$$

$$\theta_c = 63.1^\circ$$

iv) (400)

$$d = \frac{a}{4} = 1.41 \text{ \AA}$$

$$\theta = 33.1^\circ$$

$$\theta_c = 56.9^\circ$$

5. Atomic form factor is given by

$$f^p = \int dV n_j(\vec{p}) \exp(-i \vec{G} \cdot \vec{p})$$

$$= \int_0^{2\pi} \int_0^\pi \int_0^\infty r^2 \sin \theta dr d\theta d\phi \cdot n(r) \exp(-i G r \cos \theta)$$

in spherical coordinates

$$= 2\pi \int_0^\infty r^2 dr \frac{1}{\pi a_0^3} \exp\left(-\frac{2r}{a_0}\right) \int_{-1}^1 dx \exp(i G r x)$$

$$x = \cos \theta$$

$$= \frac{2}{a_0^3} \int_0^\infty r^2 dr \exp\left(-\frac{2r}{a_0}\right) \frac{e^{-i G r} - e^{i G r}}{-i G r}$$

$$= \frac{4}{G a_0^3} \text{Im} \int_0^\infty dr \left[r \exp\left(-\frac{2r}{a_0}\right) e^{i G r} \right]$$

$$= \frac{4}{G a_0^3} \text{Im} \left[\frac{1}{\left(\frac{2}{a_0} - i G\right)^2} \right]$$

$$= \frac{4}{G a_0^3} \cdot \frac{\frac{4G}{a_0}}{\left(\frac{4}{a_0^2} + G^2\right)^2}$$

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

Note) $\int_0^\infty r \exp(-(a+bi)r) dr = \frac{1}{(a+bi)^2} \quad (a > 0)$