Homework 2 Solutions

1. O chap. 2   Q1

It is assumed that the detector is located very far away from the crystal.

2. O chap. 2   Q5.

The lattice structure factor S will be the same for diamond and silicon since they are both fcc, but the atomic form factors will be different.

3. O. chap. 2   Q9.

For crystal diffraction we need $\lambda \sim 1 \overset{\circ}{A} \equiv \lambda_0$

since we need $\lambda \sim$ interatomic spacing.

Using the de Broglie relation

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \quad \Rightarrow \quad \text{Needed:} \quad E = \frac{h^2}{2m\lambda_0^2}$$

$$m_{neutron} > m_{electron}$$

$$\Downarrow$$

$$E_{neutron} < E_{electron} \quad \left(E \sim \frac{1}{m}\right)$$

4. O chap. 2 Q 10.

For crystal diffraction to occur we would like

$$\lambda \sim d$$

where we note that from Bragg's law

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

there is no diffraction for $\lambda > 2d$ (since $\sin \theta \leq 1$) Thus visible green (~ 5100 Å) light could provide diffraction spots when scattered from a crystal with lattice constant $d \sim 5000$ Å ; this is three orders of magnitude greater than that of crystals we see in Nature

5. O. chapter 2 P1.

From (2.1) we have

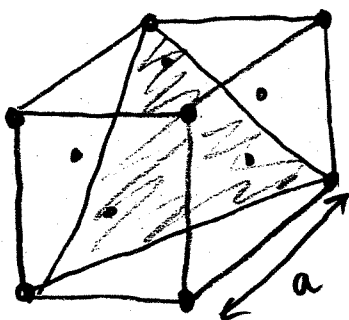$$V(kV) = \frac{12.3}{1.23} = 10 \quad kV = 10^4 V$$

$$\boxed{KE = eV = 10^4 eV}$$

6. O chapter 2   p. 3.

$\lambda = 1.54 \text{ Å}$

a) $\theta = 19.2°$ for (III) plane $\Rightarrow$ d_{111}

(III)

Bragg's Law

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

We assume $n = 1$

$$d = \frac{\lambda}{2\sin\theta} = \frac{1.54}{2\sin 19.2}$$

$$\boxed{d_{111} = 2.34 \text{ Å}}$$

b) $\rho = \dfrac{\#\ Al\ atoms}{Volume\ of\ unit\ cell} \times \dfrac{molecular\ weight\ of\ Al\ (g\text{-}atom)}{N\ (\#\ atoms\ in\ 1\ g\text{-}atom)}$

$\Downarrow$

$$N = \frac{\#\ Al\ atoms}{volume\ of\ unit\ cell} \times \frac{M(Al)}{\rho}$$

Al is fcc

- # atoms / unit cell

$$= \frac{8 \text{ enner atoms}}{8 \text{ cells}} + \frac{6 \text{ face atoms}}{2 \text{ cells}}$$

$$= 1 + 3 = 4 \text{ atoms / cell}$$

- $V = a^3$

For fcc lattice $\qquad d = \dfrac{a}{\sqrt{h^2 + k^2 + l^2}}$

$\downarrow$

$$a = d_{111} \sqrt{3} = 2.34 \sqrt{3} = 4.05 \text{ Å}$$

$\Downarrow$

$$N = \frac{4 \text{ atoms}}{(4.05 \times 10^{-8})^3 \text{ cm}^3} \times \frac{27 \text{ g}}{2.7 \text{ g/1 cm}^3}$$

$$= \frac{4}{(4.05)^3} \times 10^{25} \text{ atoms} = 6.02 \times 10^{23} \text{ atoms}$$

$$\boxed{N = 6.02 \times 10^{23} \text{ atoms}}$$

7. Kittel chapter 2 # 1

The plane (hkl) is defined by the intercepts

$$\frac{\vec{a_1}}{h}, \quad \frac{\vec{a_2}}{k}, \quad \frac{\vec{a_3}}{l}$$

(a) We take 2 vectors in this plane

$$\vec{A} = \frac{\vec{a_1}}{h} - \frac{\vec{a_2}}{k}$$

$$\vec{B} = \frac{\vec{a_1}}{h} - \frac{\vec{a_3}}{l}$$

$$\Downarrow$$

$$\vec{G} = h\vec{a_1} + k\vec{a_2} + l\vec{a_3}$$

$$\vec{G} \cdot \vec{A} = 0$$

$$\vec{G} \cdot \vec{B} = 0$$

$\Rightarrow$ G must be perpendicular to (hkl)

(b) Let $\hat{n}$ be the unit normal to the plane

$$\Downarrow$$

interplanar spacing is $\dfrac{\hat{n} \cdot \vec{a_1}}{h} = d(hkl)$

However

$$\hat{n} = \frac{\vec{G}}{|\vec{G}|}$$

$$\Downarrow$$

$$d(hkl) = \frac{\vec{G} \cdot \vec{a_1}}{h|\vec{G}|} = \frac{2\pi}{|G|}$$

(c) For a simple cubic lattice

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

$$\Downarrow$$

$$\frac{1}{d^2} = \frac{G^2}{4\pi^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

$$\Downarrow$$

$$\boxed{d^2 = \frac{a^2}{h^2 + k^2 + l^2}}$$

8. Kittel chapter 2 p.2

Hexagonal lattice
$$\vec{a}_1 = \frac{\sqrt{3}}{2} a\hat{x} + \frac{a}{2} \hat{y}$$

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

$$\vec{a}_3 = c\hat{z}$$

(a) Cell volume $= \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

$$= \vec{a}_1 \cdot \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ -\frac{\sqrt{3}}{2}a & \frac{a}{2} & 0 \\ 0 & 0 & c \end{vmatrix}$$

$$= \left(\frac{\sqrt{3}}{2} a\hat{x}\right) \cdot \left(\frac{ac}{2} \hat{x}\right)$$

$$+ \left(\frac{a}{2} \hat{y}\right) \cdot \left(\frac{\sqrt{3}}{2} ac\, \hat{y}\right)$$

$$= \frac{2\sqrt{3}}{4} a^2 c = \frac{\sqrt{3}}{2} a^2 c.$$

(1)

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

$$= \frac{2\pi}{\frac{\sqrt{3}}{2} a^2 c} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ -\frac{\sqrt{3}}{2} a & \frac{a}{2} & 0 \\ 0 & 0 & c \end{vmatrix}$$

$\Downarrow$

$$\boxed{\vec{b}_1 = \frac{2\pi}{\sqrt{3} a} \hat{x} + \frac{2\pi}{a} \hat{y}}$$

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

$$= \frac{4\pi}{\sqrt{3} a^2 c} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & c \\ \frac{\sqrt{3}}{2} a & \frac{a}{2} & 0 \end{vmatrix}$$

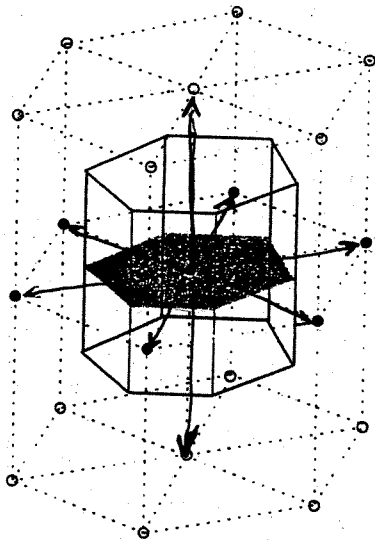$$\boxed{\vec{b}_2 = +\frac{2\pi}{a} \left(-\frac{1}{\sqrt{3}} \hat{x} + \hat{y} \right)}$$

$$\vec{A}_3 = \frac{2\pi}{V_c} (\vec{a}_1 \times \vec{a}_2)$$

$$= \frac{4\pi}{\sqrt{3}\, a^2 c} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\sqrt{3}}{2} a & \frac{a}{2} & 0 \\ -\frac{\sqrt{3}}{2} a & \frac{a}{2} & 0 \end{vmatrix}$$

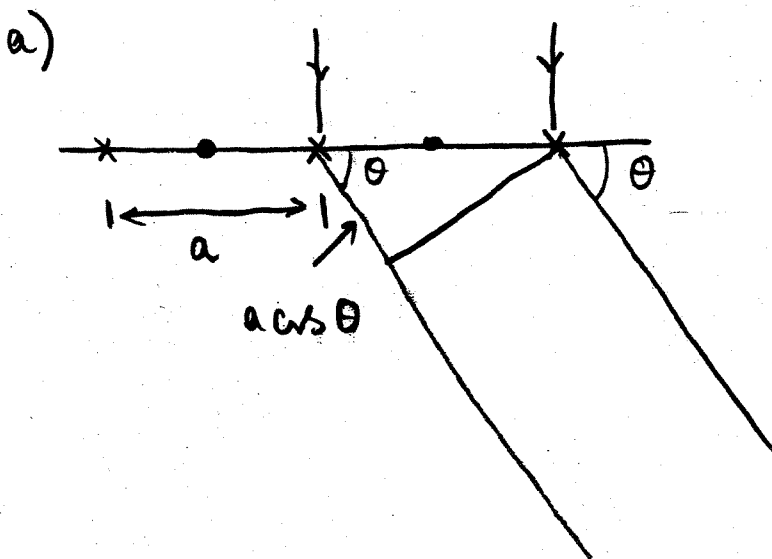$$\boxed{\vec{A}_3 = \frac{2\pi}{c} \hat{z}}$$

(c)

The reciprocal lattice is shown as dots and is shifted by an angle of $30°$ from the real-space lattice. The shaded BZ is also shown; it is oriented w/ the real space lattice (shifted from the reciprocal lattice by $30°$).

9. Kittel chap. 2 # 7

Let $x = A$, $\bullet = B$.

a)

Constructive interference iff

$$n\lambda = a\cos\theta$$

b) $S_G = \sum_j f_j \, e^{-i2\pi \nu_1 x_j}$

$\qquad = f_A + f_B \, e^{-i\nu_1 \pi}$

$x_A = 0$

$x_B = \frac{1}{2}$

ν_1 even $\qquad e^{-i\nu_1\pi} = +1$

ν_1 odd $\qquad e^{-i\nu_1\pi} = -1$.

Therefore

$$S_G = f_A - f_B \qquad \nu_1 \text{ odd}$$

$$A_G = f_A + f_B \qquad \nu_2 \text{ even}$$

$$\Downarrow$$

$$I \propto |S_G|^2 = \begin{cases} |f_A - f_B|^2 & \nu_1 \text{ odd} \\ \\ |f_A + f_B|^2 & \nu_1 \text{ even} \end{cases}$$

c) $f_A = f_B$.

No reflection w/ ν_1 odd

Same reflections as for monatomic lattice

w/ $a/2$ lattice spacing.

10. Key points of Doner et al. paper.

- Key result: oblate spheroids (M+Ms)
  pack differently (more densely) than
  do spheres when poured randomly
  and shaken

- Extensions of work w/ more experiments
  on spheroids w/ different aspect ratios
  and w/ computer simulations ⟹
  random packing densities approach
  those of perfectly ordered arrangements
  of spheres.

- Use MRI to check that there was no
  periodic ordering in center

- Always assumed that periodic orderings are
  denser than random ones ⟹ true for
  spheres but may not be the case for all
  spheroids

- Shape change sphere → spheroids leads to
  major change in random in random packing
  densities (such shape changes have minimal
  effects on non-random packing)