Condensed Matter Physics (phy 771)
HW # 3 – solution
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① **Problem 3.1 Marder**

a) fcc: from table 3.1, we have

$\vec{a_1} = \frac{a}{2}(1,1,0)$, $\vec{a_2} = \frac{a}{2}(1,0,1)$, $\vec{a_3} = \frac{a}{2}(0,1,1)$

$$\Rightarrow \vec{b_1} = 2\pi \frac{\vec{a_2}\times\vec{a_3}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}} \quad ; \quad \vec{a_2}\times\vec{a_3} = \frac{a^2}{4}\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{vmatrix} = \frac{a^2}{4}(-1,-1,1)$$

and
$$\vec{a_1}\cdot\vec{a_2}\times\vec{a_3} = \frac{a}{2}(1,1,0)\cdot\frac{a^2}{4}(-1,-1,1)$$
$$= \frac{a^3}{8}(-1-1) = -a^3/4$$

$$\Rightarrow \vec{b_1} = 2\pi \frac{a^2/4\,(-1,-1,1)}{-a^3/4} = -\frac{2\pi}{a}(-1,-1,1) = \frac{4\pi}{a}\left(\tfrac{1}{2}, 1/2, -1/2\right)$$

similarly for $\vec{b_2}$ and $\vec{b_3}$

$$\vec{b_2} = 2\pi \frac{\vec{a_3}\times\vec{a_1}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}} = \frac{4\pi}{a}(+1/2, -1/2, +1/2) = \frac{4\pi}{a}\left(\tfrac{1}{2}, -1/2, 1/2\right)$$

and

$$\vec{b_3} = 2\pi \frac{\vec{a_1}\times\vec{a_2}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}} = \frac{4\pi}{a}(-1/2, 1/2, 1/2)$$

Note that $\vec{b_2}$ and $\vec{b_3}$ in table 3.1 are switched for fcc

$\Rightarrow \vec{b_1}, \vec{b_2}, \vec{b_3}$ form a bcc lattice with spacing $4\pi/a$

bcc: $\vec{a_1} = \frac{a}{2}(1,1,-1)$, $\vec{a_2} = \frac{a}{2}(-1,1,1)$, $\vec{a_3} = \frac{a}{2}(1,-1,1)$

$$\vec{b_1} = 2\pi \frac{\vec{a_2}\times\vec{a_3}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}}, \quad \vec{a_2}\times\vec{a_3} = \frac{a^2}{4}\begin{vmatrix} i & j & k \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{a^2}{2}(1,1,0)$$

and

$$\vec{a_1}\cdot\vec{a_2}\times\vec{a_3} = \frac{a}{2}(1,1,-1)\cdot\frac{a^2}{2}(1,1,0) = \frac{a^3}{4}(1+1+0) = \frac{a^3}{2}$$

$$\Rightarrow \vec{b_1} = 2\pi \frac{\frac{a^2}{2}(1,1,0)}{a^3/2} = \frac{2\pi}{a}(1,1,0) = \frac{4\pi}{a}\left(\frac{1}{2},\frac{1}{2},0\right)$$

$$\vec{b_2} = 2\pi \frac{\vec{a_3}\times\vec{a_1}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}}; \quad \vec{a_3}\times\vec{a_1} = \frac{a^2}{2}(0,1,1)$$

$$= 2\pi \frac{a^2/2\,(0,1,1)}{a^3/2} = \frac{2\pi}{a}(0,1,1) = \frac{4\pi}{a}\left(0,\frac{1}{2},1/2\right)$$

similarly

$$\vec{b_3} = 2\pi \frac{\vec{a_1}\times\vec{a_2}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}} = \frac{4\pi}{a}\left(\frac{1}{2},0,1/2\right)$$

Note that $\vec{b_2}$ and $\vec{b_3}$ are switched in table 3.1

$\Rightarrow \vec{b_1}, \vec{b_2}, \vec{b_3}$ form an fcc lattice with spacing $\frac{4\pi}{a}$

b) the reciprocal lattice vectors can be calculated from

$|\vec{K}| = \frac{2\pi}{d}$; d: separation between adjacent planes in the direct lattice.

for cubic lattices, $d = \frac{a}{\sqrt{h^2+k^2+l^2}}$; (h k l) are miller indices

$$\Rightarrow |\vec{K}| = \frac{2\pi}{a/\sqrt{h^2+k^2+l^2}} = \frac{2\pi}{a}\sqrt{h^2+k^2+l^2} \quad \text{---- (1)}$$

the shortest $\vec{K}$ corresponds to the smallest allowed (h k l) miller indices.

from result of part a), we found that for an fcc lattice, the reciprocal lattice vectors $(\vec{b}_1, \vec{b}_2, \vec{b}_3)$ are all body-diagonal of type $\langle 111 \rangle$ directions, while for bcc lattice, the reciprocal lattice vectors are all of type $\langle 110 \rangle$ directions $\Rightarrow$ so

$$\underline{fcc}: |\vec{K}| = \frac{2\pi}{a}\sqrt{1^2+1^2+1^2} = \frac{2\pi}{a}\sqrt{3}$$

$$\underline{bcc}: |\vec{K}| = \frac{2\pi}{a}\sqrt{1^2+1^2+0^2} = \frac{2\pi}{a}\sqrt{2}$$

in vector form $\vec{K} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$

$$fcc(111): \vec{K} = \vec{b}_1 + \vec{b}_2 + \vec{b}_3$$
$$= \frac{2\pi}{a}(-1,-1,1) + \frac{2\pi}{a}(-1,1,-1) + \frac{2\pi}{a}(1,-1,-1)$$
$$= \frac{2\pi}{a}(-1,-1,-1) = \frac{4\pi}{a}(-1/2,-1/2,-1/2)$$

$$bcc(110) \quad \vec{K} = \vec{b}_1 + \vec{b}_2 = \frac{2\pi}{a}(0,1,1) + \frac{2\pi}{a}(1,-1,0)$$
$$= \frac{2\pi}{a}(1,0,1) = \frac{4\pi}{a}(-1/2, 0, 1/2)$$

we can further verify that the shortest reciprocal lattice vectors for fcc and bcc are <111> and <110> from results of structure factor calculations.

Recall that the allowed reflections for fcc lattice are given by miller indices (hkl) such that all are odd or all are even, resulting in allowed reflections of (111), (200), (220), ... The shortest $\vec{K}$ corresponds to the first reflection (111).

similarly for bcc, the condition of allowed reflections is given by $h+k+l =$ even only, giving (110), (200), (211), (220), ... allowed reflections. The first reflection (110) corresponds to the shortest $\vec{K}$ vector.

for Aluminum (Al); $a = 4.05 \text{Å}$ $\Rightarrow |\vec{K}| = \frac{2\pi}{a}\sqrt{3} = \frac{2\pi\sqrt{3}}{4.05}$
(fcc)

$$= 2.69 \text{Å}^{-1}$$

for Iron (Fe); $a = 2.87 \text{Å}$ $\Rightarrow |\vec{K}| = \frac{2\pi}{a}\sqrt{2}$
(bcc)

$$= \frac{2\pi\sqrt{2}}{2.87}$$

$$= 3.1 \text{Å}^{-1}$$

② a) $V_c = |\vec{a_1}\cdot(a_2 \times \vec{a_3})|$;

$V_R = \vec{b_1}\cdot(\vec{b_2}\times \vec{b_3})$; using $\vec{b_3} = 2\pi \dfrac{\vec{a_1}\times\vec{a_2}}{V_c}$

$= \vec{b_1}\cdot\left(\vec{b_2} \times \dfrac{2\pi}{V_c}(\vec{a_1}\times\vec{a_2})\right)$;

$= \dfrac{2\pi}{V_c}\vec{b_1}\cdot\left(\vec{b_2}\times(\vec{a_1}\times\vec{a_2})\right)$

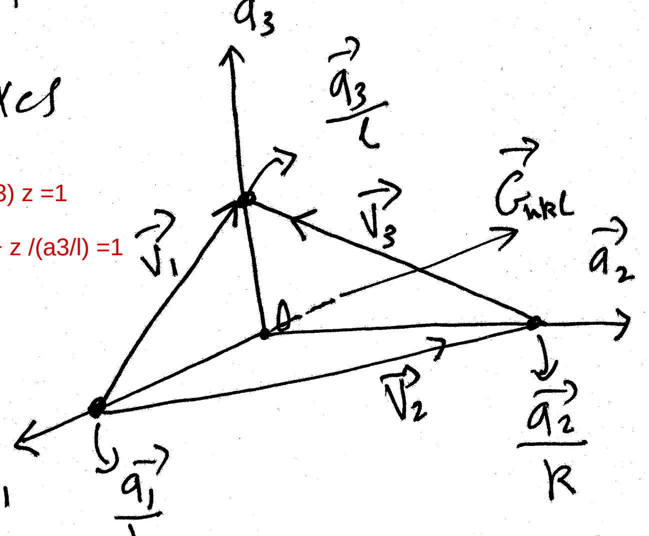
using $\vec{A}\times(\vec{B}\times\vec{C}) = (\vec{A}\cdot\vec{C})\vec{B} - (\vec{A}\cdot\vec{B})\vec{C}$, we get

$$V_R = \frac{2\pi}{V_c}\vec{b_1}\cdot\Big[\underbrace{(\vec{b_2}\cdot\vec{a_2})}_{2\pi}\vec{a_1} - \underbrace{(\vec{b_2}\cdot\vec{a_1})}_{\text{zero}}\vec{a_2}\Big]$$

$= \dfrac{2\pi}{V_c}\vec{b_1}\cdot\left[2\pi\vec{a_1}\right]$; when $\vec{b_i}\cdot\vec{a_j} = 2\pi\delta_{ij}$

$= \dfrac{(2\pi)^2}{V_c}\underbrace{\vec{b_1}\cdot\vec{a_1}}_{2\pi} = \dfrac{(2\pi)^3}{V_c}$ ✓

b) consider The (hkl) Plane shown in figure.



The plane intercepts the three axes at $\dfrac{\vec{a_1}}{h}$, $\dfrac{\vec{a_2}}{k}$, $\dfrac{\vec{a_3}}{l}$.

equation of the plane is
(h/a1) x + (k/a2) y+ (l/a3) z =1

(or x /(a1/h) + y /(a2/k)+ z /(a3/l) =1

$\vec{G}_{hkl} = h\vec{b_1} + k\vec{b_2} + l\vec{b_3}$

the reciprocal lattice vector, $\vec{G}_{hkl}$, can be shown to be normal to the (hkl) plane by taking the dot product of $\vec{G}_{hkl}$ with $\vec{v_1}, \vec{v_2}, \vec{v_3}$, where

$\vec{U_1}, \vec{U_2}, \vec{U_3}$ are three vectors in the plane

$$\vec{U_1} = \frac{\vec{a_3}}{l} - \frac{\vec{a_1}}{h}, \quad \vec{U_2} = \frac{\vec{a_2}}{k} - \frac{\vec{a_1}}{h}, \quad \vec{U_3} = \frac{\vec{a_3}}{l} - \frac{\vec{a_2}}{k}$$

$$\Rightarrow \vec{U_1} \cdot \vec{G}_{hkl} = \left(\frac{\vec{a_3}}{l} - \frac{\vec{a_1}}{h}\right) \cdot (h\vec{b_1} + k\vec{b_2} + l\vec{b_3})$$

$$= \vec{a_3} \cdot \vec{b_3} - \vec{a_1} \cdot \vec{b_1} = 2\pi - 2\pi = \text{zero},$$

where I used $\vec{a_i} \cdot \vec{b_j} = 2\pi \delta_{ij}$

similarly, one find

$$\vec{U_2} \cdot \vec{G}_{hkl} = 0 \quad \text{and} \quad \vec{U_3} \cdot \vec{G}_{hkl} = 0$$

See that any other combination of $\vec{U_1}, \vec{U_2}, \vec{U_3}$ will give a vector in the plane that is also normal to $\vec{G}_{hkl}$, for example try

$$(\vec{U_1} + \vec{U_2} + \vec{U_3}) \cdot \vec{G}_{hkl} = \left(\frac{2\vec{a_3}}{l} - \frac{2\vec{a_1}}{h}\right) \cdot (h\vec{b_1} + k\vec{b_2} + l\vec{b_3})$$

$$= 2\vec{a_3} \cdot \vec{b_3} - 2\vec{a_1} \cdot \vec{b_1} = \text{zero}$$

$$= 4\pi - 4\pi$$

c)

A, shift the origin one unit along $+y$ axis, so

x'	y'	z'
$\frac{1}{2}$	$-1/2$	∞
2	-2	0

$$\Rightarrow (hkl) = (2\ {-2}\ 0) = (2\bar{2}0)$$

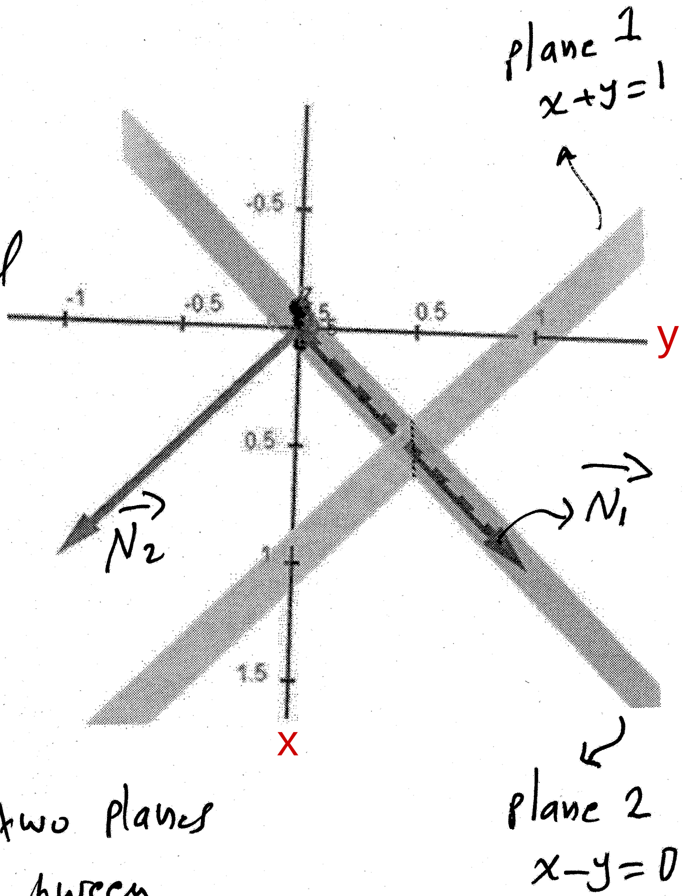
B

x	y	z
1	$1/2$	$1/2$
1	2	2

$$\Rightarrow (hkl) = (1\,2\,2)$$

(3)

(a) compare with the general equation of a plane $hx + ky + lz = d$, where $(h\,k\,l)$ are Miller indices that represent the normal vector to the plane



$\Rightarrow$ Plane 1: $(h_1 k_1 l_1) = (1\,1\,0)$

$\Rightarrow \vec{N_1} = (1,1,0)$

Plane 2: $(h_2 k_2 l_2) = (1\,-1\,0)$

$\Rightarrow \vec{N_2} = (1,-1,0)$

(b) Now the angle between the two planes is the same as the angle between the two normals $\Rightarrow$

$\vec{N_1}\cdot\vec{N_2} = |\vec{N_1}|\,|\vec{N_2}|\cos\theta \Rightarrow \cos\theta = \dfrac{\vec{N_1}\cdot\vec{N_2}}{|\vec{N_1}|\,|\vec{N_2}|} = \dfrac{(1,1,0)\cdot(1,-1,0)}{\sqrt{2}\,\sqrt{2}}$

$= \dfrac{1-1}{2} = 0 \Rightarrow \theta = \dfrac{\pi}{2}$

(c) to determine the parametric eq^{ns} of the line of intersection, we need a point on the line and a parallel vector $\vec{A}$

$\Rightarrow$ to find a point on the line, substitute eq^n of plane 2 $(x_0 = y_0)$ into the eq^n of plane 1 $(x_0 + y_0 = 1)$ $\Rightarrow 2x_0 = 1 \Rightarrow x_0 = 1/2$

$\Rightarrow y_0 = 1/2$

$\Rightarrow (x_0, y_0, z_0) = (1/2, 1/2, 0) = \vec{r_0}$

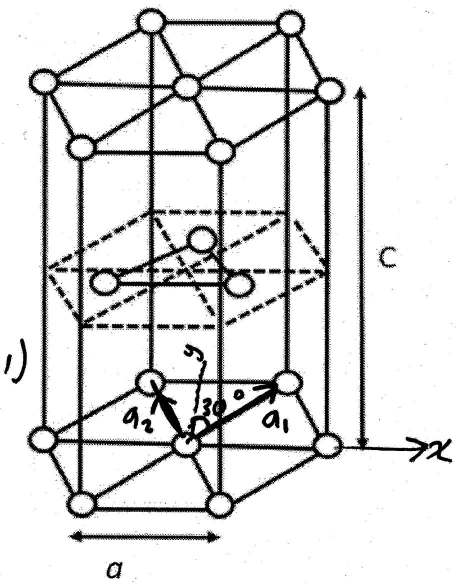
Now to find a parallel vector, use $\vec{A} = \vec{N_1}\times\vec{N_2}$

$\Rightarrow \vec{A} = \vec{N_1}\times\vec{N_2} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 1 & 1 & 0 \\ 1 & -1 & 0 \end{vmatrix} = -2\hat{k} = (0,0,-2)$, so the equation of line now reads $\vec{r} = \vec{r_0} + \vec{A}t$

$\Rightarrow (x,y,z) = (1/2, 1/2, 0) + (0,0,-2)t \Rightarrow \left.\begin{array}{l} x = 1/2 \\ y = 1/2 \\ z = -2t \end{array}\right\}$ Parametric equations of the line of intersection

(4) problem 3.2 Marder

a) according to table 3.1 in textbook, the primitive vectors of the direct lattice of simple hexagonal are



$\vec{a}_1 = a(1/2, \frac{\sqrt{3}}{2}, 0)$, $\vec{a}_2 = a(-1/2, \frac{\sqrt{3}}{2}, 0)$; $\vec{a}_3 = c(0,0,1)$

$V_p = |\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|$

$$\vec{a}_2 \times \vec{a}_3 = ac \begin{vmatrix} i & j & k \\ -1/2 & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{vmatrix} = ac\left(\frac{\sqrt{3}}{2}, 1/2, 0\right)$$

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

$$\Rightarrow \vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{|\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3|} = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{V_p} = \frac{2\pi\, ac\left(\frac{\sqrt{3}}{2}, 1/2, 0\right)}{a^2 c \frac{\sqrt{3}}{2}}$$

$$= \frac{4\pi}{\sqrt{3}\, a}\left(\frac{\sqrt{3}}{2}, 1/2, 0\right), \text{ and}$$

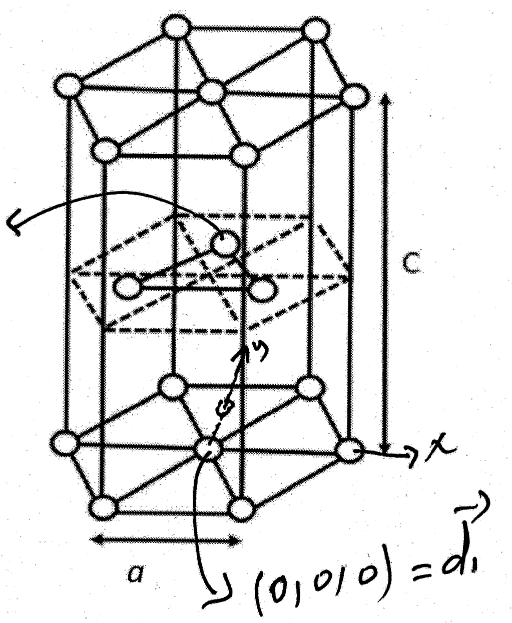
$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{V_p} \quad ; \quad \vec{a}_3 \times \vec{a}_1 = ac\left(-\frac{\sqrt{3}}{2}, 1/2, 0\right)$$

$$= 2\pi \frac{ac\left(-\frac{\sqrt{3}}{2}, 1/2, 0\right)}{a^2 c \frac{\sqrt{3}}{2}} = \frac{4\pi}{\sqrt{3}\, a}\left(-\frac{\sqrt{3}}{2}, 1/2, 0\right)$$

Note that in table 3.1, the signs of x and y components of $\vec{b}_2$ are switched mistakenly.

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{V_p} \quad ; \quad \vec{a}_1 \times \vec{a}_2 = a^2 \frac{\sqrt{3}}{2}(0, 0, 1)$$

$$\Rightarrow \vec{b}_3 = \frac{2\pi\, a^2 \frac{\sqrt{3}}{2} (0,0,1)}{a^2 c \frac{\sqrt{3}}{2}} = \frac{2\pi}{c}(0,0,1)$$



This verifies the reciprocal lattice vectors as given in table 3.1. We see that the reciprocal lattice vectors $\vec{b}_1, \vec{b}_2, \vec{b}_3$ also form hexagonal lattice but rotated at 30° w.r.t the direct lattice primitive vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$. To verify this, it is enough to take $\vec{a}_1 \cdot \vec{b}_1 = 2\pi \Rightarrow |\vec{a}_1||\vec{b}_1| \cos\theta = 2\pi$

$$\Rightarrow \cos\theta = \frac{2\pi}{|\vec{a}_1|\,|\vec{b}_1|} = \frac{2\pi}{a\sqrt{\frac{1}{4}+3/4} \cdot \frac{4\pi}{\sqrt{3}a}\sqrt{\frac{3}{4}+\frac{1}{4}}} = \frac{2\pi}{4\pi}\sqrt{3} = \frac{\sqrt{3}}{2}$$

$$\Rightarrow \theta = 30^\circ$$

b) there are two basis located at $\vec{d}_1 = (0,0,0)$ and $\vec{d}_2$ using eq^n 2.6b, $\vec{d}_2 = \frac{1}{3}\vec{a}_1 + \frac{1}{3}\vec{a}_2 + \frac{\vec{a}_3}{2}$, $\vec{a}_3 = c$

$$\Rightarrow \vec{d}_2 = \frac{a}{3}(1/2, \frac{\sqrt{3}}{2}, 0) + \frac{a}{3}(-1/2, \frac{\sqrt{3}}{2}, 0) + \frac{c}{2}(0,0,1)$$

$$= (0, a\frac{\sqrt{3}}{2}, \frac{c}{2}) = (0, \frac{a}{\sqrt{3}}, \frac{c}{2})$$

$$\therefore \vec{d}_1 = (0,0,0) \text{ and } \vec{d}_2 = (0, \frac{a}{\sqrt{3}}, \frac{c}{2})$$

Now $S(\vec{G}) = \sum_{l'=1}^{2} f_{l'} e^{i\vec{G}\cdot\vec{d_{l'}}} = f_1 + f_2 e^{i\vec{G}\cdot\vec{d_2}}$, but $f_1 = f_2 = f$

$= f\left[1 + e^{i\vec{G}\cdot\vec{d_2}}\right]$, need to find $\vec{G}$ first

Now $\vec{G} = n_1\vec{b_1} + n_2\vec{b_2} + n_3\vec{b_3}$

$= n_1 \frac{4\pi}{\sqrt{3}a}\left(\frac{\sqrt{3}}{2}, 1/2, 0\right) + n_2 \frac{4\pi}{\sqrt{3}a}\left(-\frac{\sqrt{3}}{2}, 1/2, 0\right) + n_3 \frac{2\pi}{c}(0,0,1)$

$= \left(n_1 \frac{2\pi}{a} - n_2 \frac{2\pi}{a},\ n_1 \frac{2\pi}{\sqrt{3}a} + n_2 \frac{2\pi}{\sqrt{3}a},\ n_3 \frac{2\pi}{c}\right)$

$= \left(\frac{2\pi}{a}(n_1 - n_2),\ \frac{2\pi}{\sqrt{3}a}(n_1 + n_2),\ n_3 \frac{2\pi}{c}\right)$

$\Rightarrow \vec{G}\cdot\vec{d_2} = \left(\frac{2\pi}{a}(n_1-n_2),\ \frac{2\pi}{\sqrt{3}a}(n_1+n_2),\ n_3\frac{2\pi}{c}\right)\cdot\left(0, \frac{a}{\sqrt{3}}, \frac{c}{2}\right)$

$= \frac{2\pi}{3}(n_1+n_2) + n_3\pi = \frac{\pi}{3}\left[2(n_1+n_2) + 3n_3\right]$

$\Rightarrow S(\vec{G}) = f\left[1 + e^{i\frac{\pi}{3}[2(n_1+n_2)+3n_3]}\right]$

$\Rightarrow F_{\vec{q}} = F_{\vec{G}} = |S(\vec{G})|^2 = |f|^2 \left|1 + e^{i\frac{\pi}{3}[2(n_1+n_2)+3n_3]}\right|$

for simplicity take $f = 1 \Rightarrow$

$$F_{\vec{G}} = \left|1 + e^{i\frac{\pi}{3}[2(n_1+n_2)+3n_3]}\right| \quad \text{------ (1)}$$

Extinction occurs when $F_{\vec{G}}$ = zero and hence no reflections observed. Therefore, for $F_{\vec{G}}$ to be zero, and based on equation (1),

$$e^{i\frac{\pi}{3}[2(n_1+n_2)+3n_3]} = -1 \quad , \text{ or}$$

$$e^{i\pi\left[\frac{2(n_1+n_2)}{3}+n_3\right]} = -1 \quad , \text{ and this occurs when}$$

$$\cos\pi\left[\frac{2(n_1+n_2)}{3}+n_3\right] + i\sin\pi\left[\frac{2(n_1+n_2)}{3}+n_3\right] = -1$$

equating real parts gives

$$\cos\pi\left[\frac{2(n_1+n_2)}{3}+n_3\right] = -1$$ and this happens

when $\frac{2(n_1+n_2)}{3}+n_3 = \text{odd}$ i.e $1, 3, 5, 7, \ldots$

one choice is (n_1+n_2) is multiple of 3 and

n_3 odd.

5 Problem 3.3 Marder

a) $\vec{k}_0 = \frac{2\pi}{a}\left(\frac{5}{2}, 0, 0\right)$

$\vec{k} = \frac{2\pi}{a}\left(\frac{3}{2}, 2, 0\right)$, thus

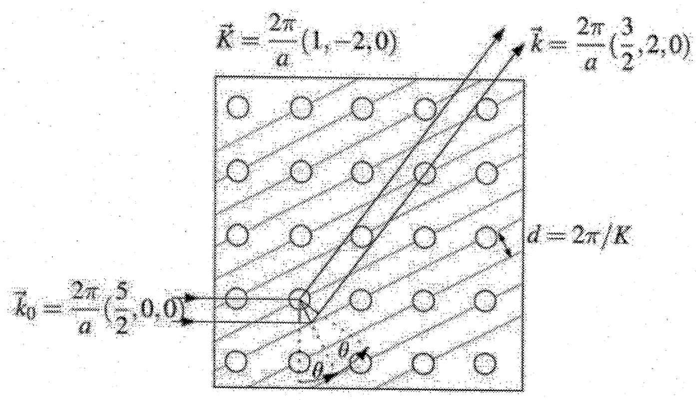


Fig 3.2

$$\vec{q} = \vec{k}_0 - \vec{k}$$

$$= \frac{2\pi}{a}\left(\frac{5}{2}, 0, 0\right) - \frac{2\pi}{a}\left(\frac{3}{2}, 2, 0\right)$$

$$= \frac{2\pi}{a}(1, -2, 0)$$

b) constructive interference occurs when scattering vector $\vec{q}$ is a reciprocal lattice vector, i.e $\vec{q} = \vec{K}$ (sometimes I use $\vec{K}$ and $\vec{G}$ interchangably i.e $\vec{K} = \vec{G}$)

$$\Rightarrow |\vec{q}| = |\vec{K}|$$

$$2 k_0 \sin\theta = \frac{2\pi}{d}$$

; but $|\vec{K}| = \frac{2\pi}{d}$ is the shortest reciprocal lattice vector that corresponds to first-order diffraction ($n=1$). in general $|\vec{K}| = n\frac{2\pi}{d}$.

i.e $\vec{K}$ is an integral multiple of the shortest reciprocal lattice vector parallel to $\vec{K}$.

in general

$$\Rightarrow 2 k_0 \sin\theta = n\frac{2\pi}{d};$$

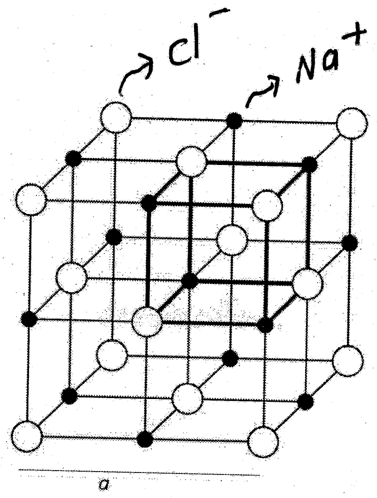
with $k_0 = \frac{2\pi}{\lambda}$, we get

$$2\frac{\cancel{2\pi}}{\lambda}\sin\theta = n\frac{\cancel{2\pi}}{d}$$

$$\Rightarrow \boxed{2d\sin\theta = n\lambda}$$

(6)

The NaCl lattice is an fcc lattice with 4 Na^{+1} ions and 4 Cl^- ions located at



Cl^- : $(0,0,0), (1/2,1/2,0), (1/2,0,1/2), (0,1/2,1/2)$

Na^+: $(\frac{1}{2},0,0), (0,1/2,0), (0,0,1/2), (1/2,1/2,1/2)$

$$S(q) = \sum_{l'=1}^{8} f_{l'} \, e^{2\pi i (h x_{l'} + k y_{l'} + l z_{l'})}$$

$$= f_{Cl}\left[1 + e^{i\pi(h+k)} + e^{i\pi(h+l)} + e^{i\pi(k+l)}\right]$$

$$+ f_{Na}\left[e^{i\pi h} + e^{i\pi k} + e^{i\pi l} + e^{i\pi(h+k+l)}\right]$$

Now using $e^{i\pi m} = (-1)^m$, we get

$$S(q) = f_{Cl}\left[1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l}\right]$$

$$+ f_{Na}\left[(-1)^h + (-1)^k + (-1)^l + (-1)^{h+k+l}\right]$$

$$= f_{Cl}\left[1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l}\right]$$

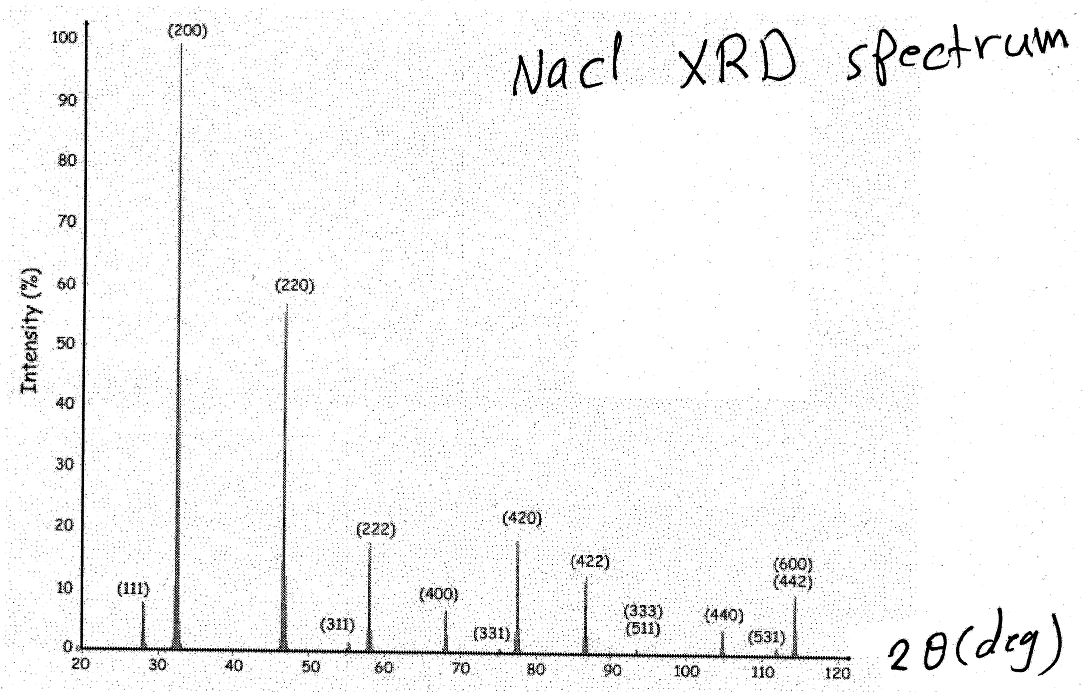
$$+ f_{Na}(-1)^h\left[1 + (-1)^{k-h} + (-1)^{l-h} + (-1)^{k+l}\right]$$

but $(-1)^{k+h} = (-1)^{k-h}$; proof: $(-1)^{k-h} \times \frac{(-1)^{2h}}{(-1)^{2h}} = \frac{(-1)^{k+h}}{1} = (-1)^{k+h}$ and $(-1)^{h+l} = (-1)^{l-h}$

$$\Rightarrow S(q) = f_{Cl}\left[1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l}\right]$$

$$+ f_{Na}(-1)^h\left[1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l}\right]$$

$$= \left[f_{Cl} + f_{Na}(-1)^h\right]\left[1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l}\right]$$



$$\Rightarrow S(q) = \begin{cases} 4(f_{Cl}+f_{Na}) \; ; & h,k,l \text{ are all even} \\ 4(f_{Cl}-f_{Na}) \; ; & h,k,l \text{ are all odd} \\ 0 \; ; & \text{mixed indices} \end{cases}$$ (Extinction)

the modulation factor $F_q = |S(q)|^2$

$$F_{\vec{q}} = \begin{cases} 16\,(f_{Cl}+f_{Na})^2 \; ; & h,k,l \text{ are all even} \\ 16\,(f_{Cl}-f_{Na})^2 \; ; & h,k,l \text{ are all odd} \\ 0 \; ; & \text{mixed indices} \end{cases}$$

it can be demonstrated from the above spectrum that the lattice is an fcc lattice as all reflections are either all even or all odd. in addition, we see that reflections of odd indices are much smaller than reflections of even indices, confirming the calculated intensity $I \propto F_{\vec{q}}$

7)

```
(*Here I am using Mathematica to plot the function |∑_q|^2 =
(Sin[qaN/2]^2)/(Sin[qa/2]^2) for N=30... see figure 3.3 in textbook*)
```

In[39]:=

```
(*Define the function with N=30 and a=1*)a = 1; n = 30; function[q_] := (Sin[q a n / 2] ^2) / (Sin[q a / 2] ^2);

(*note that the symbole N can not be used as it is preserved symbole in mathematica*)
(*Plot the function over a suitable range of q*)
Plot[function[q], {q, 0, 10 π}, (*Exclude singularities*) PlotRange → {0, 1000}, (*Focus on peaks*)
 AxesLabel → {"\!\(\*
StyleBox[\"q\",\nFontSize->24]\)", "\!\(\*
StyleBox[\"|\",\nFontSize->24]\)\!\(\*
StyleBox[UnderscriptBox[
  RowBox[{\" \", \"∑\"}], \"q\"],\nFontSize->24]\)\!\(\*
StyleBox[\" \",\nFontSize->24]\)\!\(\*
StyleBox[SuperscriptBox[\"|\", \"2\"],\nFontSize->24]\)"}, (*Label axes*) PlotLabel → " N=30",
 PlotPoints → 100, LabelStyle → Directive[Black, Bold, 16], (*Smooth the curve*) ImageSize → 800]
```

Out[40]=