Physics 140A-Problem Set 3 Answers

[1]

The source & the detector are located at distances $\gg$ than the interplanar spacing dimension, Moreover, Bragg's law demands <u>specular</u> reflection from the crystallographic planes

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[2]

A Compton's pattern cannot show a diffraction pattern. It is an inelastic process, the energy is not conserved, and therefore, when changing the angle, the Compton peak has a different wavelenght, so that there cannot be a defined phase relationship between the compton scattered waves.

FYI, just note that <u>any</u> Compton's experiment will show 2 peaks: one is shifted in λ according to $\Delta\lambda = \lambda_c(1-\cos\theta)$, the other is <u>NOT</u> λ-shifted, it corresponds to the elastic peak due to the scattering with electrons which are <u>bound</u>. This peak will show diffraction, being the elastic peak.

HERE IS AN EXAMPLE of COMPTON SCATTERING DATA ...

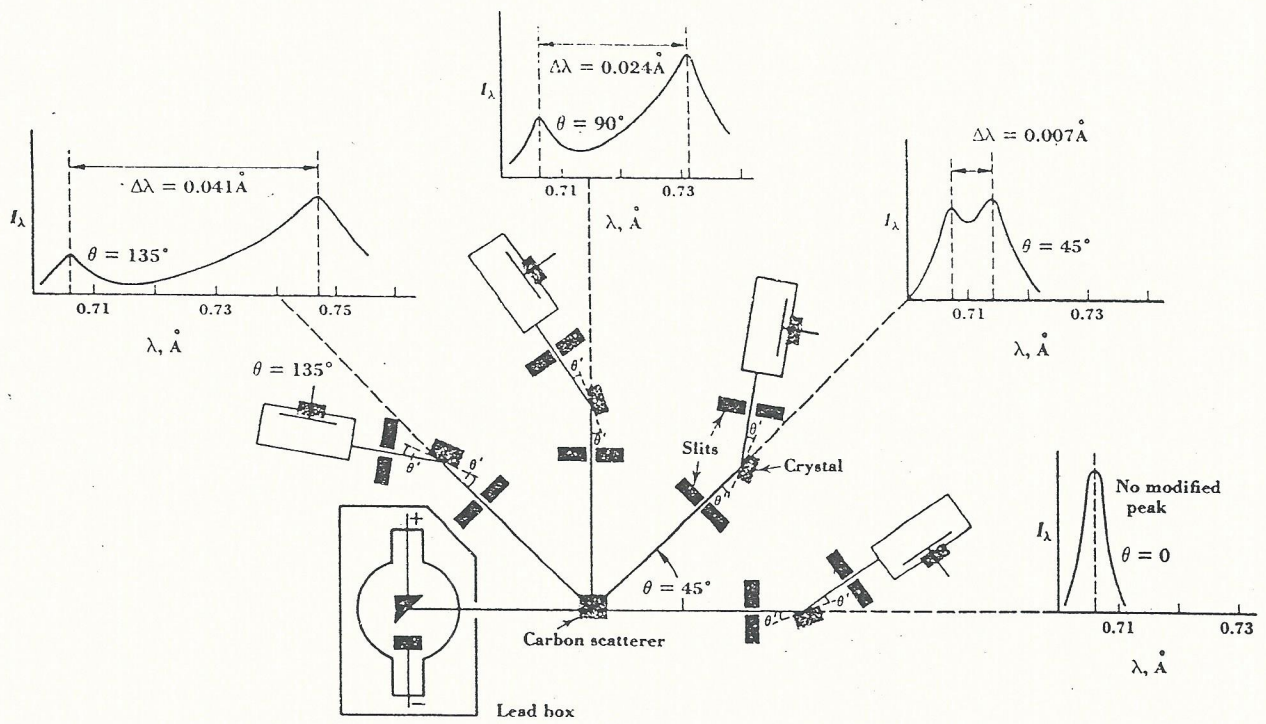

Fig. 7.15 The scattering of Mo $K\alpha$ x-rays ($\lambda = 0.707$ Å) at an angle θ gives rise to two peaks in the scattered radiation, one at the incident wavelength and the second at a wavelength greater by $\Delta\lambda = 0.024(1 - \cos\theta)$ Å. (*After A. W. Smith and J. N. Cooper, "Elements of Physics," 7th ed. Copyright* 1964. *McGraw-Hill Book Company. Used by permission.*)

[3]

Given a wave like $\vec{E} = \vec{E}(r)\, e^{i\omega t}$, we know E&M that $E^2 \propto$ intensity

i. $E^2 \propto \text{INTENSITY} = \frac{\text{ENERGY}}{\text{TIME} \cdot \text{SURFACE}}$

ii. $E^2 \propto \frac{1}{\text{surface}} \propto \frac{1}{r^2} \Rightarrow E \propto \frac{1}{r}$ √√

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[4] $\lambda_{Cu} = 1.54\ \text{Å}$

a) Bragg's law $\Rightarrow 2d\sin\theta = n\lambda$, take $n=1$ (first order) & get $d_{111} = \frac{\lambda}{2\sin\theta} = \frac{1.54}{2\cdot\sin(19.2)} = 2.34\ \text{Å}$

as a check, (111) planes are ⊥ to the reciprocal vector [111]

$\frac{2\pi}{d}$ is the shortest distance for the reciprocal vector along the direction ⊥ to the planes separated by d

NB $G_{111} = \frac{\sqrt{3}}{2} \cdot \frac{4\pi}{a}$

i. $d = \frac{2\pi}{|G_{111}|} = \frac{2\pi a}{2\sqrt{3}\pi} = \frac{a}{\sqrt{3}} \cong 2.34\ \text{Å}$

THIS IS DISCUSSED IN THE LAST PROBLEM, VERY IMPORTANT POINT

where I used the fact that 4.05 Å is Al lattice constant.

b) $M = 27 \Rightarrow$ 27 g of aluminum = 1 mole = N_a ATOMS

$\rho = 2.7\ \text{g/cm}^3 \Rightarrow$ 10 cm^3 contains N_a ATOMS, $V_{N_a} = 10\ \text{cm}^3$

$$\frac{N_a}{V_{Na}} = \frac{\#\text{ ATOMS IN CELL}}{\text{VOLUME of THE CELL}} = \frac{4}{a^3}$$

NB: here we are considering the conventional cubic cell, NOT THE PRIMITIVE cell.

$$N_a = \frac{4\,V_{Na}}{a^3} = \frac{4 \cdot 10\ cm^3}{(4{,}05)^3\ (\text{Å})^3} = \frac{40 \cdot (10^8)^3}{(4{,}05)^3} \cong 6{,}02 * 10^{23}\ \checkmark$$

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[5]

$$f_a = \int d\vec{r}\ \rho(\vec{r})\, e^{i\vec{s}\cdot\vec{r}}$$

let's choose first of all the incident direction along the $\hat{z}$ axis, so that $\vec{s}$ will be specified by the angle θ in spherical coordinates.

Then spherical symmetry for $\rho(\vec{r})$ means $\rho(\vec{r}) = \rho(|\vec{r}|) = \rho(r)$ i.e. NO AUGULAR DEPENDENCE.

$$d\vec{r} = d\theta d\phi dr \sin\theta\, r^2$$

$$\text{i.e.}\quad f_a = \int dr d\theta d\phi \sin\theta\, r^2 \rho(r)\, e^{i s r \cos\theta}$$

, where the integral is extended to the whole sphere of radius R

the integration over $d\phi$ yield 2π, so that

$$f_a = 2\pi \int_0^R dr\ r^2 \rho(r) \int_0^\pi \sin\theta\, e^{i s r \cos\theta}\, d\theta = 2\pi \int_0^R dr\ r^2 \rho(r) \left[\frac{i}{sr}\, e^{i s r \cos\theta} \Big|_0^\pi \right]$$

$$= 2\pi \int_0^R r^2 \rho(r) \frac{i}{sr} \left\{ e^{-isr} - e^{isr} \right\} = 4\pi \int_0^R r^2 \rho(r) \frac{\sin sr}{sr}\, dr \quad \checkmark$$

($e^{-isr} - e^{isr} = -2i\sin sr$)

[6]

2.20 $$f_{cR} = \sum_l f_{al}\, e^{i\vec{s}\cdot\vec{R}_l}$$

2.21 $$F = \sum_j f_{aj}\, e^{i\vec{s}\cdot\vec{\delta}_j}$$

2.22 $$S = \sum_l e^{i\vec{s}\cdot\vec{R}_l^{(c)}}$$

$\vec{R}_l$ in 2.20 is the position of the l-th atom. This can be specified if we know its position within the unit cell plus the position of the whole unit cell wrt the origin

$$\therefore \quad \vec{R}_l = \underbrace{\vec{R}_l^{\,c}}_{\substack{\text{POS'N}\\ l\text{-cell}}} + \underbrace{\vec{\delta}_l}_{\substack{\text{POS'N}\\ \text{of } l\text{-th}\\ \text{atom}}}$$

$$\therefore \quad f_{cR} = \sum_l f_{al}\, e^{i\vec{s}\cdot\vec{R}_l} = \sum_{l,j} f_{aj}\, e^{i\vec{s}\cdot[\vec{R}_l^{(c)} + \vec{\delta}_j]} =$$

$$= \underbrace{\sum_l e^{i\vec{s}\cdot\vec{R}_l^{(c)}}}_{S} \cdot \underbrace{\sum_j f_{aj}\, e^{i\vec{s}\cdot\vec{\delta}_j}}_{F} \quad \checkmark$$

[7]

$$\rho(r) = \frac{e^{-2r/a_0}}{\pi a_0^3}$$

use 2.17, i.e., $f_q = \int_0^R 4\pi r^2 \rho(r) \frac{\sin sr}{sr}\, dr$

$$f_q = \int_0^R 4\pi r^2 \frac{e^{-2r/a_0}}{\pi a_0^3} \frac{\sin sr}{sr}\, dr = \frac{4}{a_0^3 s} \int_0^\infty dr\, r \sin(sr)\, e^{-\frac{2r}{a_0}}$$

where we replaced the upper integration limit by ∞ since $\rho(r)$ dies off very fast.

Sometimes it is not necessary to solve integrals to extract the physics behaviour: this is possible when you can convert by substitution of variables the integral to just a number, with the interesting physical quantities taken outside. This case is different though, can't take $sr = x$ & just get a # since the exp. factor

Need to solve the $\int$ either by computer or look @ $\int$ Tables

$$\int x^m e^{ax} [\sin bx]\, dx = \begin{cases} x^m e^{ax} \dfrac{a \sin bx - b \cos bx}{a^2 + b^2} \\ \quad - \dfrac{m}{a^2 + b^2} \int x^{m-1} e^{ax} (a \sin bx - b \cos bx)\, dx \\ \text{or} \\ e^{ax} \displaystyle\sum_{r=0}^{m} \frac{(-1)^r m! x^{m-r}}{\rho^{r+1}(m-r)!} \sin[bx - (r+1)\alpha] \\ \text{where} \\ \rho = \sqrt{a^2 + b^2}, \quad \rho \cos\alpha = a, \quad \rho \sin\alpha = b \end{cases}$$

This is what I found, this integral can be also found Tabulated

in our case ≡

$m = 1$

$b = s$

$a = -2/a_0$

nb you only need $m = 1$ here

538. $\int e^{ax} [\cos(bx)]\, dx = \dfrac{e^{ax}}{a^2 + b^2} [a \cos(bx) + b \sin(bx)]$

533. $\int e^{ax} [\sin(bx)]\, dx = \dfrac{e^{ax} [a \sin(bx) - b \cos(bx)]}{a^2 + b^2}$

$$\therefore \int x e^{ax} \sin bx\, dx = x e^{ax} \frac{a\sin bx - b\cos bx}{a^2+b^2} - \frac{1}{a^2+b^2}\int e^{ax}(a\sin bx - b\cos bx)$$

$$= x e^{ax} \frac{a\sin bx - b\cos bx}{a^2+b^2} - \frac{1}{a^2+b^2}\left\{ \frac{a e^{ax}[a\sin bx - b\cos bx]}{a^2+b^2} - \frac{b e^{ax}}{a^2+b^2}[a\cos bx + b\sin bx] \right\}$$

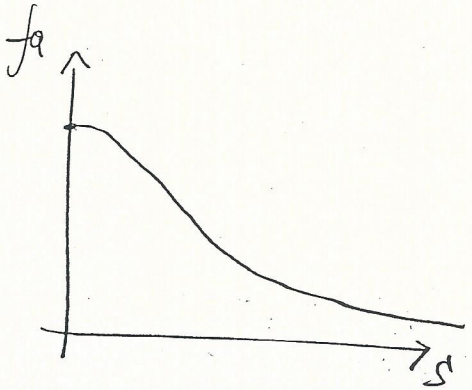
when evaluating from 0 to ∞, 1st term $\longrightarrow 0$

$$\int_0^\infty = \frac{2}{(a^2+b^2)^2} ab e^{ax}\cos bx = \frac{2}{\left(\frac{4}{a_0^2}+s^2\right)^2} \cdot \left(-\frac{2}{a_0}\right) s\, e^{-\frac{2r}{a_0}} \cos sr \Big|_0^\infty$$

$$= \frac{2}{\left(\frac{4}{a_0^2}+s^2\right)^2} \cdot \frac{2}{a_0} s \quad , \text{ and therefore } \Rightarrow$$

$$f_a = \frac{4}{a_0^3 \cdot 8} \cdot \frac{4s}{a_0} \cdot \frac{1}{\left[\left(\frac{2}{a_0}\right)^2 + s^2\right]^2} \quad \text{i.e.} \quad \text{const} \times \frac{1}{\left[(\text{const}' + s^2\right]^2}$$

this is the functional dependence you're interested in.

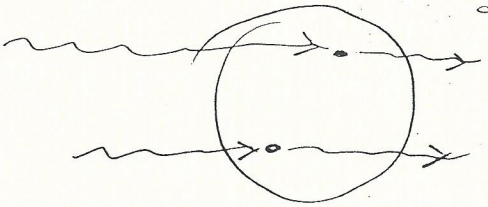


For back reflection the atomic scattering factor tends to become small because of DESTRUCTIVE INTERFERENCE

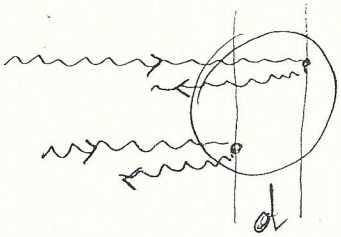
→

consider in fact a sphere, this being the volume of Radius $a_0 - 2a_0$ where you find the electron cloud

consider now 2 different points in the cloud. For forward scattering, there is <u>no</u> difference in the path.



For backward scattering, the difference in path is the greatest, equal to $2d$. Now, big deal, so what?



There's no problem if $2d$ is equal to an integer number of wavelenghts, you'd still have const. interference.

The point is that the dist. d is so small compared to the wavelenghts that this extra path results in a destructive int. effect.

In fact, say $\mathcal{E}_{x\text{-ray}} \cong 8{,}05$ keV (Cu $k\alpha$)

$$\lambda_{Cu} = 1{,}54\,\text{Å} > a_0 \sim d$$

[8]

Geometrical Structure Factor $F_{hkl} = \sum_j f_{aj} e^{i\vec{s}\cdot\vec{\delta}_j}$

$\vec{s}$, the change in wave vector, must be equal to a vector of the reciprocal lattice in order for scattering to be possible

$\vec{s} = \vec{G}_{hkl}$

If you consider the fcc lattice as a Bravais lattice, and it is, then scattering occur for values of $\vec{s}$ equal to the vectors of the reciprocal lattice, which is bcc. In this case, $\vec{\delta}_j = \vec{0}$ and the scattering factor is 1.

If you view the fcc lattice as a cubic lattice with a 4-atom basis, then we have to recall that we can take as the basis the vectors whose cartesian components are $(0,0,0)$; $(\frac{a}{2},\frac{a}{2},0)$; $(\frac{a}{2},0,\frac{a}{2})$; $(0,\frac{a}{2},\frac{a}{2})$

The reciprocal lattice is in this case composed by vectors of the form $\vec{G}_{hkl} = \frac{2\pi}{a}\left[h\hat{x} + k\hat{y} + l\hat{z}\right]$

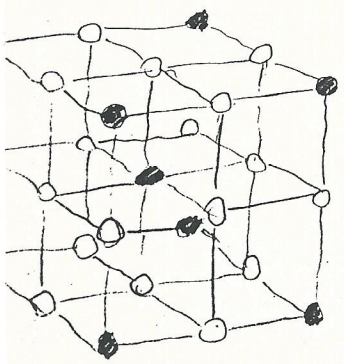
$$F_{hkl} = \sum_j f_{aj} e^{i\vec{s}\cdot\vec{\delta}_j} = f_{aj}\sum_j e^{i\vec{G}_{hkl}\cdot\vec{\delta}_j}$$ where f_{aj} has been factored out since it is a constant $\forall j$

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

hkl ALL EVEN $\Rightarrow F=4$; ONE EVEN, TWO ODD $\rightarrow F=0$

hkl " ODD $\Rightarrow F=4$; ONE ODD, TWO EVEN $\rightarrow F=0$

$\therefore$ for 14, just stated in prob. 13 = $F=0$ unless ALL EVEN OR ALL ODD



$\Rightarrow$ **(100) (110) (210) (211) ARE MISSING**

● = NOT MISSING
○ = MISSING $\Rightarrow$

SEE BEGINNING, WHEN CONSIDERING FORBIDDEN REFLECTION, YOUR CUBE TURNS OUT TO BE A BCC LATTICE, ... which is reciprocal of fcc

[9]

CsCl STRUCTURE, BCC with $f_{Cs} = 3 f_{Cl}$

CALCULATE F_{100}

$$F_{100} = \sum_j f_{aj} e^{i \vec{S} \cdot \vec{\delta}_j}$$

where now CsCl is bcc $\Rightarrow$ CUBIC CELL with A 2 point basis,

$d_1 = (0,0,0)$ OCCUPIED BY Cs

$d_2 = \left(\frac{a}{2}, \frac{a}{2}, \frac{a}{2}\right)$ OCCUPIED BY Cl

ARBITRARY, CAN BE THE OTHER WAY TOO...

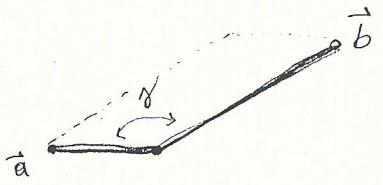
$$\vec{S} = \vec{G}_{100} = \frac{2\pi}{a} \hat{x}$$

$$F_{100} = f_{Cs} e^{i \cdot 0} + f_{Cl} e^{i \frac{2\pi}{a} \hat{x} \cdot \left[\frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z}\right]} =$$

$$= f_{Cs} + f_{Cl} e^{i \frac{2\pi}{a} \cdot \frac{a}{2}} = f_{Cs} + f_{Cl} e^{i\pi} = 2 f_{Cl} \quad \checkmark$$

No rule is, in fact, violated here: CsCl is simply NOT a BCC LATTICE, since the 2 ATOMIC species are different. It can be described as a cubic Bravais lattice with a 2-point basis, with the 2 BASIS ATOMS BEING NOW different.

[10]



$|\vec{b}| = |2\vec{a}| = 2.5\,\text{Å}$

$|a| = 1.25\,\text{Å}$

$\gamma = 120°$

Look @ 2.35 in OMAR :

You are looking for $\vec{a}^*$ & $\vec{b}^*$ such that

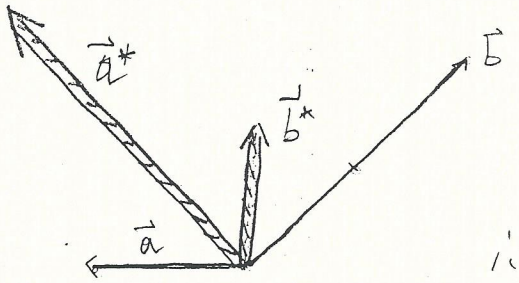
$\underline{a}^* \cdot \underline{a} = 2\pi$ $\quad$ $\underline{a}^* \cdot \underline{b} = 0$

$\underline{b}^* \cdot \underline{b} = 2\pi$ $\quad$ $\underline{b}^* \cdot \underline{a} = 0$

$\vec{a}^*$ & $\vec{b}^*$ must be perpendicular to $\underline{b}$ & $\underline{a}$ respectively

Moreover

$\underline{a}^* \cdot \underline{a} = \underline{b}^* \cdot \underline{b} = 2\pi$



$\therefore$ if $|\vec{a}| < |\vec{b}| \Rightarrow |\vec{a}^*| > |\vec{b}^*|$

You can summarize how to draw a reciprocal cell in 2D as follows :

- $\vec{a}^* \perp \vec{b}$; $\vec{b}^* \perp \vec{a}$
- if $|\vec{a}| \geq |\vec{b}| \Rightarrow |\vec{a}^*| \leq |\vec{b}^*|$

$\Rightarrow$ life is easier in 2D .....

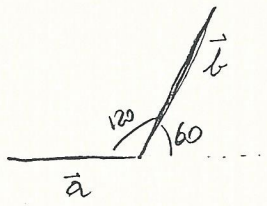
See also Fig. 2.7 p.48 in OMAR .... $\leftarrow$

You can of course find the same result with the conventional algorithm ...

$$\begin{cases} \vec{a}^* = \dfrac{2\pi}{A}\, \vec{b} \times \vec{n} \\ \vec{b}^* = \dfrac{2\pi}{A}\, \vec{n} \times \vec{a} \end{cases}$$

where A is the area of the cell and $\vec{n}$ is the normal unit vector to the $\vec{a}\hat{}\vec{b}$ plane

∴ in this case no need to take components,



$$|\vec{a}^*| = \frac{2\pi}{A}\left|\vec{b}\times\vec{n}\right| = \frac{2\pi}{A}\cdot b \quad , \text{ direction is } \perp \vec{b}$$

$$|\vec{b}^*| = \frac{2\pi}{A}\left|\vec{n}\times\vec{a}\right| = \frac{2\pi}{A}\cdot a \quad , \text{ direction } \perp \vec{a}$$

$$\therefore \quad |\vec{a}^*| = \frac{2\pi}{A}\cdot b = \frac{2\pi}{A}\cdot 2a = \frac{4\pi}{A}a$$

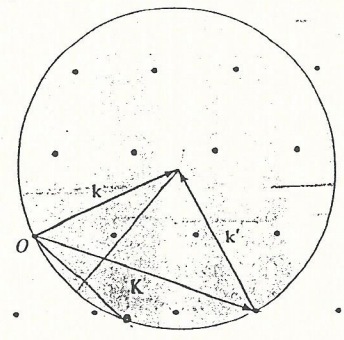
$$|\vec{b}^*| = \frac{2\pi}{A}\cdot a = \frac{2\pi}{A}a$$

$$\therefore \Rightarrow |\vec{a}^*| = 2|\vec{b}^*| \text{, to be compared to } |\vec{a}| = \frac{1}{2}|\vec{b}|$$

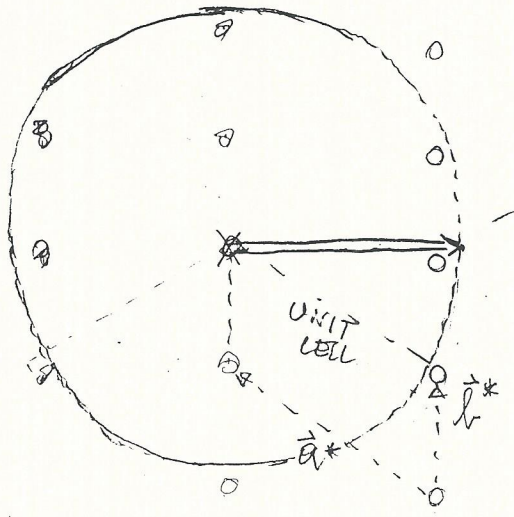
If you solve the exercise by taking components, you need to express $\vec{a}$ & $\vec{b}$ as a function of $\hat{x}, \hat{y}$ & $\hat{z}$, just take $\vec{n} \equiv \hat{z}$

AS REGARDS THE EWALD'S CONSTRUCTION, THE FOLLOWING FIGURE (from ASHCROFT - MERMIN (AM)) GIVES SOME DIRECTIONS:

Figure 6.7
The Ewald construction. Given the incident wave vector k, a sphere of radius k is drawn about the point k. Diffraction peaks corresponding to reciprocal lattice vectors K will be observed only if K gives a reciprocal lattice point on the surface of the sphere. Such a reciprocal lattice vector is indicated in the figure, together with the wave vector k′ of the Bragg reflected ray.



THEREFORE THE FIRST THING TO DO IS TO DRAW THE RECIPROCAL LATTICE POINTS



PICK THE ORIGIN
I CHOOSED THE POINT
⊗

THE INCIDENT WAVE VECTOR IS DIRECTED ALONG $\vec{a}$

THE MAGNITUDE of $\vec{k}_o$, (THE INCIDENT WAVE VECTOR) IS GIVEN BY

$|\vec{k}_o| = \frac{2\pi}{\lambda}$, where

$\lambda = \frac{12400}{(h\nu)(eV)}$ (Å) =

$o \longrightarrow \frac{\vec{a}}{|\vec{a}|}$

$\Rightarrow \quad \lambda = \frac{12400}{10080}$ Å $= 1.24$ Å $\quad \Rightarrow \quad K = \frac{2\pi}{\lambda} = \frac{2\pi}{1.24}$ Å^{-1} $\cong 5.067$ Å^{-1}

NEED TO KNOW $|\vec{b}^*| = \frac{2\pi}{A} \cdot a = \frac{2\pi}{ab\sin(120^\circ)} \cdot a \cong 2.9$ Å^{-1}

$ab\sin\gamma$ is THE AREA of THE UNIT CELL

$k_o \simeq 5.067$ Å^{-1}

$b^* \simeq 2.5$ Å^{-1}

$a^* = 2b^* \simeq 5.8$ Å^{-1} $\Rightarrow$ NEED TO DRAW IN SCALE!

$\frac{k_o}{b^*} = \frac{5.067}{2.9} \simeq 1.75 \Rightarrow$ THIS GIVES ME THE LENGHT of MY DRAWING $\Rightarrow k_o \simeq 2.75$ mm in the DRAWING

THE DRAWING IS "CLUMSY" ANYWAY YOU CAN TELL THAT THERE ARE NO SPOTS, JUST TAKE A LOOK @ THE RATIOS

$\frac{k_o}{a^*}$ & $\frac{k_o}{b^*}$, THEY ARE NOT INTEGER NUMBERS

ACTUALLY, IN 2D YOU GET ALWAYS REFLECTIONS, BUT THIS IS NOT COVERED IN 140A; SEE ADDENDUM FOR A BRIEF EXPLANATION, IF INTERESTED ASK DR. FADLEY ...

[11]

$a = 4\text{Å}$, $b = 6\text{Å}$, $c = 8\text{Å}$ $\quad \alpha = \beta = 90$, $\gamma = 120$

The following mathematical relations are useful in dealing with the reciprocal lattice:

$$\begin{aligned} \mathbf{a}^* \cdot \mathbf{a} &= 2\pi, & \mathbf{a}^* \cdot \mathbf{b} &= \mathbf{a}^* \cdot \mathbf{c} = 0, \\ \mathbf{b}^* \cdot \mathbf{b} &= 2\pi, & \mathbf{b}^* \cdot \mathbf{a} &= \mathbf{b}^* \cdot \mathbf{c} = 0, \\ \mathbf{c}^* \cdot \mathbf{c} &= 2\pi, & \mathbf{c}^* \cdot \mathbf{a} &= \mathbf{c}^* \cdot \mathbf{b} = 0. \end{aligned} \tag{2.35}$$

The first row of equations, for instance, can be established as follows: To prove the first of the equations, we substitute for $\mathbf{a}^*$ from (2.33) and find that

$$\mathbf{a}^* \cdot \mathbf{a} = \frac{2\pi}{\Omega_c} (\mathbf{b} \times \mathbf{c}) \cdot \mathbf{a}.$$

But $(\mathbf{b} \times \mathbf{c}) \cdot \mathbf{a}$ is also equal to the volume of the unit cell Ω_c, and hence $\mathbf{a}^* \cdot \mathbf{a} = 2\pi$, as required. The second two equations in the first row reflect the fact, already mentioned, that $\mathbf{a}^*$ is perpendicular to the plane formed by $\mathbf{b}$ and $\mathbf{c}$. The remainder of the equation in (2.35) can be established in a similar manner.

Examples of reciprocal lattices are shown in Fig. 2.7. Figure 2.7(a) shows a direct one-dimensional lattice and its reciprocal. Note that in this case $\mathbf{a}^*$ is parallel to $\mathbf{a}$, and that $a^* = 1/a$. Figure 2.7(b) shows a plane rectangular lattice and its reciprocal.† Three-dimensional examples are more complex, but the procedure for finding them is straightforward. One employs (2.33) to find the basis $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$, and then uses (2.34) to locate all the lattice points. It is evident, for instance, that the reciprocal of an sc lattice of edge a is also an sc lattice with a cube edge equal to $2\pi/a$ (Fig. 2.8).

We can similarly establish that the reciprocal of a bcc is an fcc lattice, and vice versa (see the problem section). One may extend the argument to other crystal systems. When we realize that the reciprocal lattice is a lattice in its own right, and that it possesses the same rotational symmetry as the direct lattice, we see that the reciprocal lattice always falls in the same crystal system as its direct lattice (see Table 1.1). Thus the reciprocals for monoclinic, triclinic,... and hexagonal lattices are also monoclinic, triclinic,... and hexagonal, respectively. (Note, however, that the two lattices need not have the same Bravais structure within the same system; see the bcc and fcc examples above.)

FROM OMAR, P. 47 ....

BEFORE LAUNCHING YOURSELF IN LENGHTY ALGEBRA CALCULATION, TRY TO GET A FEELING OF YOU ARE GOING TO GET

→ WHAT LATTICE ARE YOU DEALING WITH ?

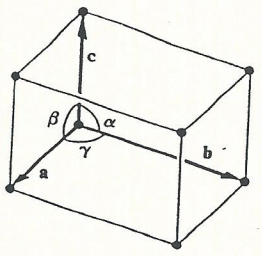
LOOK @ TABLE 1.1 @ P. 9 IN OMAR

if $a \neq b \neq c$, $\alpha = \beta = 90 \neq \gamma$

$\Rightarrow$ MONOCLINIC

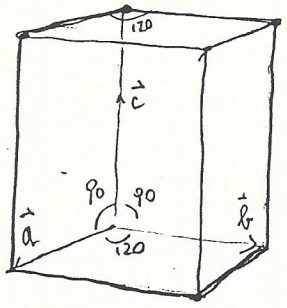
LOOK @ P. 8 ....

FROM OMAR, P. 7, ABOUT THE CONVENTIONS ....



$\Rightarrow$

$a = 4\text{Å}$, $b = 6\text{Å}$, $c = 8\text{Å}$ $\Rightarrow$
$b = \frac{3}{2}a$, $c = 2a$



YOU THEREFORE EXPECT THE RECIPROCAL LATTICE TO BE MONOCLINIC AS WELL

RECALL THE FORMULAS FOR THE RECIPROCAL LATTICE VECTORS:

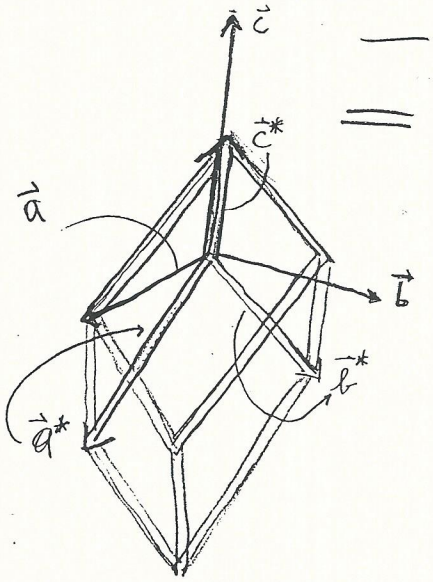
$$\vec{a}^* = \frac{2\pi}{\Omega}(\vec{b}\times\vec{c}) \quad ; \quad \vec{b}^* = \frac{2\pi}{\Omega}(\vec{c}\times\vec{a}) \quad ; \quad \vec{c}^* = \frac{2\pi}{\Omega}(\vec{a}\times\vec{b})$$

Ω = VOLUME OF THE CELL.

BEFORE DOING MATH THEN .....

1) $\vec{a}^*$ MUST BE $\perp$ $\hat{bc}$ PLANE
   $\vec{b}^*$ $\parallel$ $\perp$ $\hat{ac}$ PLANE
   $\vec{c}^*$ $\parallel$ $\perp$ $\hat{ab}$ PLANE

2) SINCE $\vec{a}^*\cdot\vec{a} = \vec{b}^*\cdot\vec{b} = \vec{c}^*\cdot\vec{c} = 2\pi$ = CONSTANT $\Rightarrow$
   if $a<b<c \Rightarrow a^* > b^* > c^*$



—— = DIRECT LATTICE

═══ = RECIPROCAL

I GUESS THERE WILL BE A POINT IN THE PROBLEM WHERE WE'LL BE ASKED TO WRITE DOWN THE BASIS VECTORS IN CARTESIAN COMPONENTS, BUT, IN GENERAL, SEE IF YOU CAN CALCULATE THE VECTORS LENGHT WITH SIMPLE VECTOR ALGEBRA.

$$\Omega = (\underbrace{\vec{a}\times\vec{b}}_{\text{AREA PARALL.}})\cdot\vec{c} = ab\sin\gamma\cdot c = \quad (\times \text{ HEIGHT})$$

$$\Omega = abc\sin\gamma = a\cdot\frac{3}{2}a\cdot 2a\sin\gamma = 3\sin\gamma\, a^3 \simeq$$

$$\Omega \simeq 2.56\, a^3 \simeq 166.27\ \text{Å}^3 \quad \checkmark$$

$$\vec{b}\times\vec{c} = bc\sin\alpha\alpha = \frac{3}{2}a\cdot 2a = 3a^2$$
$$\vec{c}\times\vec{a} = ac\sin\beta = a\cdot 2a = 2a^2$$
$$\vec{a}\times\vec{b} = ab\sin\gamma = \frac{3}{2}\sin\gamma\, a^2 = \frac{3\sqrt{3}}{4}a^2$$

$$|\vec{a}^*| = \frac{2\pi}{\Omega}|\vec{b}\times\vec{c}| = \frac{2\pi}{3\sin\gamma\, a^3}\cdot 3a^2 = \frac{2\pi}{\sin\gamma}\cdot\frac{1}{a} = \frac{2\pi\cdot 2}{\sqrt{3}}\frac{1}{a} = \frac{4\pi}{\sqrt{3}}\frac{1}{a}$$

$$|\vec{b}^*| = \frac{2\pi}{\Omega}|\vec{c}\times\vec{a}| = \frac{2\pi}{3\sin\gamma\, a^3}\cdot 2a^2 = \frac{4}{3}\pi\frac{1}{\sin\gamma}\frac{1}{a} = \frac{4}{3}\pi\frac{2}{\sqrt{3}}\frac{1}{a} = \frac{8\pi}{3\sqrt{3}}\frac{1}{a}$$

$$|c^*| = \frac{2\pi}{\Omega}|\vec{a}\times\vec{b}| = \frac{2\pi}{3\sin\gamma\, a^3}\cdot\frac{3}{2}\sin\gamma\, a^2 = \frac{\pi}{a}$$

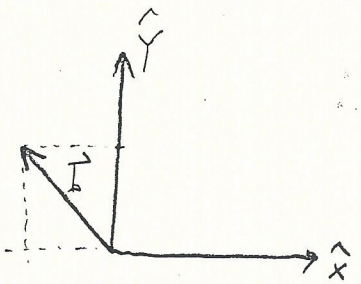
SO YOU CAN SEE THAT

$$c^* < b^* < a^*$$

NOW WE CAN CALCULATE THE RECIPROCAL LATTICE VECTORS AGAIN BY CONSIDERING THEIR CARTESIAN COMPONENTS.

TAKE $\vec{a} = a\hat{x}$, $\vec{c} = c\hat{z}$ $\Rightarrow$

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



$$\vec{b}\times\vec{c} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ -\frac{b}{2} & \frac{\sqrt{3}b}{2} & 0 \\ 0 & 0 & c \end{vmatrix} = \frac{\sqrt{3}}{2}bc\hat{x} + \frac{bc}{2}\hat{y} = 3a^2\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right)$$

$$\vec{c}\times\vec{a} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & c \\ a & 0 & 0 \end{vmatrix} = ac\hat{y} = 2a^2\hat{y}$$

b

FROM ASHCROFT – MERMIN

VOLUME OF THE RECIPROCAL LATTICE PRIMITIVE CELL

If v is the volume[5] of a primitive cell in the direct lattice, then the primitive cell of the reciprocal lattice has a volume $(2\pi)^3/v$. This is proved in Problem 1.

OF COURSE, YOU CAN TAKE THE RECIPROCAL LATTICE VECTORS & CALCULATE $(\vec{a}^* \times \vec{b}^*) \cdot \vec{c}^*$
THIS WAY THOUGH, YOU HAVE TO CALCULATE THE RECIPROCAL LATTICE VECTORS,

THE FOLLOWING PROBLEM FROM A-M HIGHLIGHTS THIS QUESTION, GUIDING THROUGH THE PROOF OF THIS SORT OF THEOREM

---

1. (a) Prove that the reciprocal lattice primitive vectors defined in (5.3) satisfy

$$\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3) = \frac{(2\pi)^3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}. \tag{5.15}$$

(*Hint:* Write $\mathbf{b}_1$ (but not $\mathbf{b}_2$ or $\mathbf{b}_3$) in terms of the $\mathbf{a}_i$, and use the orthogonality relations (5.4).)

(b) Suppose primitive vectors are constructed from the $\mathbf{b}_i$ in the same manner (Eq. (5.3)) as the $\mathbf{b}_i$ are constructed from the $\mathbf{a}_i$. Prove that these vectors are just the $\mathbf{a}_i$ themselves; i.e., show that

$$2\pi \frac{\mathbf{b}_2 \times \mathbf{b}_3}{\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3)} = \mathbf{a}_1, \quad \text{etc.} \tag{5.16}$$

(*Hint:* Write $\mathbf{b}_3$ in the numerator (but not $\mathbf{b}_2$) in terms of the $\mathbf{a}_i$, use the vector identity $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = \mathbf{B}(\mathbf{A} \cdot \mathbf{C}) - \mathbf{C}(\mathbf{A} \cdot \mathbf{B})$, and appeal to the orthogonality relations (5.4) and the result (5.15) above.)

(c) Prove that the volume of a Bravais lattice primitive cell is

$$v = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|, \tag{5.17}$$

where the $\mathbf{a}_i$ are three primitive vectors. (In conjunction with (5.15) this establishes that the volume of the reciprocal lattice primitive cell is $(2\pi)^3/v$.)

from PART a)

i) $\Omega = \frac{3\sqrt{3}}{2} a^3 \Rightarrow \Omega^{REC} = \frac{(2\pi)^3}{\Omega} = \frac{(2\pi)^3}{3\sqrt{3}} \cdot \frac{2}{a^3}$

$\Omega \equiv 166{,}27\ \text{Å}^3$, $\Omega^{REC} \simeq 1{,}49\ \text{Å}^{-3}$

$$\vec{a}\times\vec{b} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ a & 0 & 0 \\ -\frac{b}{2} & \frac{\sqrt{3}}{2}b & 0 \end{vmatrix} = \frac{\sqrt{3}}{2}ab\,\hat{z} = \frac{\sqrt{3}}{2}\frac{3}{2}a^2\hat{z} = \frac{3\sqrt{3}}{4}a^2\hat{z}$$

$\therefore \quad |\vec{b}\times\vec{c}| = 3a^2$, $|\vec{c}\times\vec{a}| = 2a^2$, $|\vec{a}\times\vec{b}| = \frac{3\sqrt{3}}{4}a^2$ as before ....

since $\frac{2\pi}{\Omega} = \frac{2\pi\cdot 2}{3\sqrt{3}a^3} = \frac{4\pi}{3\sqrt{3}a^3}$, $\Rightarrow$

$$\vec{a}^* = \frac{2\pi}{\Omega}(\vec{b}\times\vec{c}) = \frac{4\pi}{3\sqrt{3}}\cdot\frac{1}{a^2}\cdot 3a^2\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right) = \frac{4\pi}{\sqrt{3}}\frac{1}{a}\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right)$$

$$\vec{b}^* = \frac{2\pi}{\Omega}(\vec{c}\times\vec{a}) = \frac{4\pi}{3\sqrt{3}}\frac{1}{a^3}2a^2\hat{y} = \frac{8\pi}{3\sqrt{3}}\frac{1}{a}\hat{y}$$

$$\vec{c}^* = \frac{2\pi}{\Omega}(\vec{a}\times\vec{b}) = \frac{4\pi}{3\sqrt{3}}\frac{1}{a^3}\cdot\frac{3\sqrt{3}}{4}a^2\hat{z} = \frac{\pi}{a}\hat{z}$$

WHICH CONFIRM THE INITIAL CONSIDERATIONS, i.e. $\vec{a}^* \not\perp \vec{b}^* \perp \vec{c}^*$

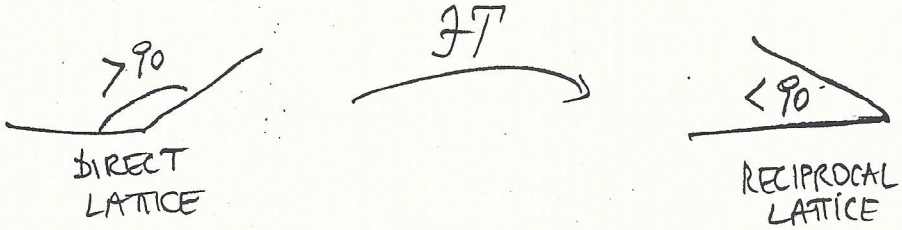
NOTE THAT $\vec{a}^*\cdot\vec{b}^* = \frac{4\pi}{\sqrt{3}}\cdot\frac{1}{a}\cdot\frac{1}{2}\cdot\frac{8\pi}{3\sqrt{3}}\cdot\frac{1}{a} = \frac{16\pi^2}{9}\frac{1}{a^2}$

$= |\vec{a}^*|\cdot|\vec{b}^*|\sin\gamma'$, where γ' is THE ANGLE BETWEEN $\vec{a}^*$ & $\vec{b}^*$

$$\frac{16}{9}\pi^2\frac{1}{a^2} = \frac{4\pi}{\sqrt{3}}\frac{1}{a}\cdot\frac{8\pi}{3\sqrt{3}}\frac{1}{a}\cdot\sin\gamma' = \frac{32\pi^2}{9}\frac{1}{a^2}\sin\gamma' \Rightarrow$$

$$\frac{16}{9}\pi^2\frac{1}{a^2} = \frac{32\pi^2}{9}\frac{1}{a^2}\sin\gamma' \Rightarrow \sin\gamma' = 1/2 \Rightarrow$$

i.e. ACUTE ANGLE NOW BETWEEN a^* & b^* $\Rightarrow$



c) THIS CAN BE TRICKY!

DO NOT USE THE FORMULA (1.5) ON p. 16 in OMAR! THAT FORMULA IS VALID ONLY if THE AXES ARE ORTHOGONAL

WE SHALL USE INSTEAD (2.38) @ p.50 IN OMAR

INTERPLANAR DISTANCE $d_{hkl} = \frac{2\pi}{G_{hkl}}$ WHERE $G_{hkL} = |\vec{G}_{hkL}|$

$\vec{G}_{hkL}$ IS THE SHORTEST VECTOR IN THE RECIPROCAL LATTICE PERPENDICULAR TO THE PLANE (hkL)

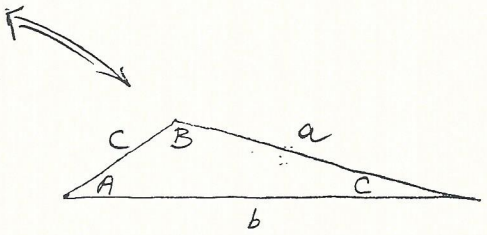
SEE FOR THE LAST PROBLEM A DETAIL EXPLANATION OF THIS TOPIC

LET'S FIRST DETERMINE THE DISTANCE WITH ELEMENTARY GEOMETRY

RECALL SOME BASIC GEOMETRY

Plane Triangle Formulas

In the following, A, B, C denote the angles of any plane triangle, a, b, c the corresponding opposite sides, and $s = \frac{1}{2}(a + b + c)$.



Radius of inscribed circle:

$$r = \sqrt{\frac{(s-a)(s-b)(s-c)}{s}}$$

Radius of circumscribed circle:

$$R = \frac{a}{2\sin A} = \frac{b}{2\sin B} = \frac{c}{2\sin C}$$

Law of sines:

$$\frac{a}{\sin A} = \frac{b}{\sin B} = \frac{c}{\sin C}$$

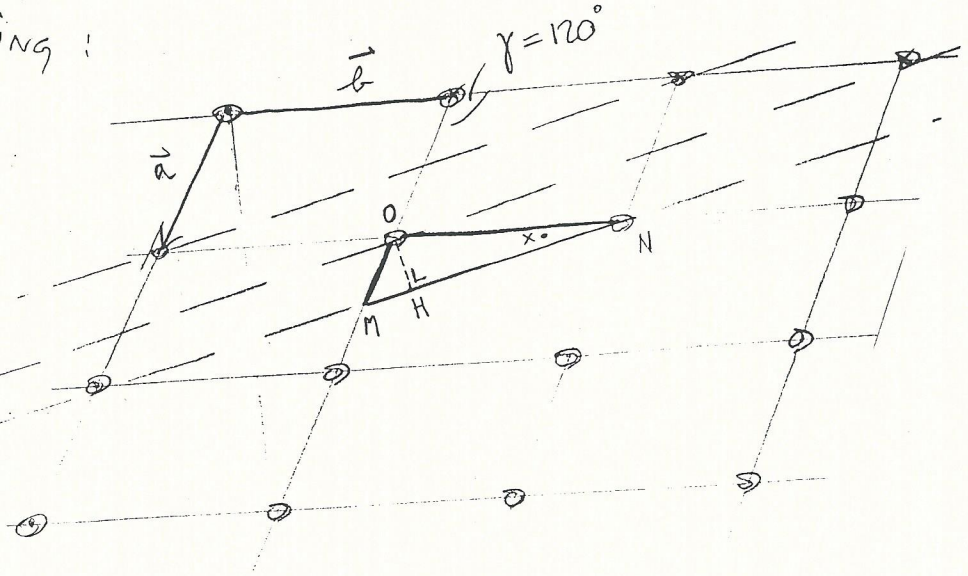
Law of cosines:

$$a^2 = b^2 + c^2 - 2bc\cos A, \quad \cos A = \frac{b^2 + c^2 - a^2}{2bc}$$

$$b^2 = c^2 + a^2 - 2ca\cos B, \quad \cos B = \frac{c^2 + a^2 - b^2}{2ca}$$

$$c^2 = a^2 + b^2 - 2ab\cos C, \quad \cos C = \frac{a^2 + b^2 - c^2}{2ab}$$

THE PLANE (210) INTERCEPTS THE AXES IN $\frac{1}{2}, 1, \infty$, SO YOU HAVE THE FOLLOWING DRAWING :



∞ MEANS THAT THE $\hat{z}$ AXIS IS NOT INTERCEPTED

$\overline{OH}$ is d_{210}

$\overline{OM} = a/2$, $\overline{ON} = b = \frac{3a}{2}$

$d_{210} = b \sin x$

FROM THE LAW of SINES $\Rightarrow$ $\sin x = \frac{\overline{OM}}{\overline{MN}} \sin\gamma$;

$\overline{MN}$ IS GIVEN BY THE LAW of COSINES APPLIED TO $M\hat{O}N$

$\overline{MN}^2 = \overline{OM}^2 + \overline{ON}^2 - 2\,\overline{OM}\cdot\overline{ON}\cos\gamma = \frac{13}{4}a^2$

$\therefore \quad \sin x = \frac{a}{2}\cdot\frac{\sqrt{3}}{2}\cdot\frac{2}{\sqrt{13}}\frac{1}{a} = \frac{\sqrt{3}}{2\sqrt{13}}$, SO THAT

$$d_{210} = b\sin x = \frac{3a}{2}\cdot\frac{\sqrt{3}}{2\sqrt{13}} = \frac{3\sqrt{3}}{4\sqrt{13}}a$$

NOW SEE if WE GET THE SAME ANSWER BY CALCULATING

$d_{hkL} = \frac{2\pi}{G_{hkL}}$

WHAT is $|G_{210}|$? BE CAREFULL, THIS is NOT AN ORTHOGONAL SYSTEM, SO YOU CAN'T SAY $G_{210} = \sqrt{5}$

$G_{210} = (\vec{G}_{210}\cdot\vec{G}_{210})^{1/2} = \left[(2\vec{a}^* + \vec{b}^*)\cdot(2\vec{a}^* + \vec{b}^*)\right]^{1/2} =$

$= \left[4a^{*2} + b^{*2} + 4\,\vec{a}^*\cdot\vec{b}^*\right]^{1/2}$, where $a^* = |\vec{a}^*|$, $b^* = |\vec{b}^*|$

FROM PART a) $\rightarrow$ $a^* = \frac{4\pi}{\sqrt{3}}\frac{1}{a}$, $b^* = \frac{8\pi}{3\sqrt{3}}\frac{1}{a}$, $a^* \cdot b^* = \frac{16}{9}\pi^2 \frac{1}{a^2}$

SO THAT

$$G_{210}^2 = \left[4 \cdot \frac{16\pi^2}{3} + \frac{64\pi^2}{27} + 4 \cdot \frac{16}{9}\pi^2\right]\frac{1}{a^2} = \frac{832}{27}\frac{\pi^2}{a^2}$$

$$G_{210} = \frac{8\sqrt{13}}{3\sqrt{3}}\frac{\pi}{a}$$

$$d_{210} = \frac{2\pi}{G_{210}} = \frac{2\pi \cdot 3\sqrt{3}}{8\sqrt{13}\,\pi}\,a = \frac{3\sqrt{3}}{4\sqrt{13}}\,a \quad \checkmark$$

CALCULATE NOW USING THE CARTESIAN COMPONENTS :

$$G_{210}^2 = \vec{G}_{210} \cdot \vec{G}_{210} = \left[2 \cdot \frac{4\pi}{\sqrt{3}}\frac{1}{a}\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right) + \frac{8\pi}{3\sqrt{3}}\frac{1}{a}\hat{y}\right] \cdot \left[\text{SAME THING}\right] =$$

$$= 4 \cdot \frac{16\pi^2}{3}\frac{1}{a^2} + \frac{64\pi^2}{27}\frac{1}{a^2} + 2 \cdot \frac{2 \cdot 4\pi}{\sqrt{3}}\frac{1}{a}\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right) \cdot \frac{8\pi}{3\sqrt{3}}\frac{1}{a}\hat{y} =$$

$$= \left(\frac{64\pi^2}{3} + \frac{64\pi^2}{27} + \frac{16\pi}{\sqrt{3}} \cdot \frac{8\pi}{3\sqrt{3}} \cdot \frac{1}{2}\right)\frac{1}{a^2} =$$

$$= \left(\frac{9 \cdot 64 + 64 + 16 \cdot 43}{27}\right)\frac{\pi^2}{a^2} = \frac{832}{27}\frac{\pi^2}{a^2}$$

$$d_{210} = \frac{2\pi}{G_{210}} = \frac{3\sqrt{3}}{4\sqrt{13}}\,a \quad \checkmark$$

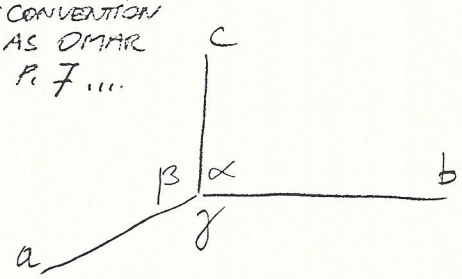
YOU PROBABLY NOTICED THAT THERE IS FULL CONSISTENCY BETWEEN THE SPACING CALCULATED WITH BASIC GEOMETRY & WITH $\frac{2\pi}{\text{GIVE}}$.

THIS IS A GENERAL FORMULA from WARREN, (X-RAY Diff.)

To conform to the usual crystallographic notation, we let

$$a_1 = a, \quad \alpha_{23} = \alpha,$$
$$a_2 = b, \quad \alpha_{31} = \beta,$$
$$a_3 = c, \quad \alpha_{12} = \gamma.$$

SAME CONVENTION AS OMAR P. 7 ....



Combining Eqs. (2.6) and (2.7) and changing to the usual crystallographic notation, we obtain

$$\frac{1}{d_{hkl}^2} = \frac{1}{(1 + 2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma)} \times \left\{ \frac{h^2\sin^2\alpha}{a^2} + \frac{k^2\sin^2\beta}{b^2} + \frac{l^2\sin^2\gamma}{c^2} + \frac{2hk}{ab}(\cos\alpha\cos\beta - \cos\gamma) + \frac{2kl}{bc}(\cos\beta\cos\gamma - \cos\alpha) + \frac{2lh}{ac}(\cos\gamma\cos\alpha - \cos\beta) \right\}. \quad (2.8)$$

NB. THIS IS JUST ANOTHER CHECK. THE PROOF OF THIS FORMULA IS BEYOND UNDERGRADUATE CLASSES....

NO NEED TO MEMORIZE THIS!

$\frac{1}{d_{210}^2}$ = USE ABOVE FORMULA WITH $L=0$, $h=2$, $k=1$, FOR MONOCLINIC TAKE $\alpha=\beta=90$, $\gamma=120$, $\cos\alpha=\cos\beta=0$, $\sin\alpha=\sin\beta=1$

$$\frac{1}{d_{210}^2} = \frac{1}{1-\cos^2\gamma}\left\{\frac{4}{a^2} + \frac{1}{b^2} - \frac{4}{ab}\cos 120\right\} = \frac{1}{\sin^2\gamma}\left\{\frac{4}{a^2} + \frac{1}{b^2} + \frac{2}{ab}\right\} =$$

$$= \frac{4}{3}\frac{1}{a^2}\left(4 + \frac{4}{9} + \frac{4}{3}\right) = \frac{4\cdot 52}{27}\frac{1}{a^2} \Rightarrow d_{210} = \sqrt{\frac{27}{13\cdot 16}}\,a = \frac{3\sqrt{3}}{4\sqrt{13}}\,a$$

SAME AS WE GOT!

RECIPROCAL LATTICE IS COOL, THAT'S WHY WE USE IT!

d)

USE BRAGG'S LAW HERE

$$2d_{210}\sin\theta_{210} = n\lambda \Rightarrow$$

$$\theta_{210} = \arcsin\left(\frac{n\lambda}{2d_{210}}\right)$$

e)

FIRST BRILLOUIN ZONE

The Wigner-Seitz primitive cell (page 73) of the reciprocal lattice is known as the *first Brillouin zone*. As the name suggests, one also defines higher Brillouin zones,

→ THE FOLLOWING DEFINES THE W-S-CELL

WIGNER-SEITZ PRIMITIVE CELL

One can always choose a *primitive* cell with the full symmetry of the Bravais lattice. By far the most common such choice is the *Wigner-Seitz cell*. The Wigner-Seitz cell about a lattice point is the region of space that is closer to that point than to any other lattice point.[10] ~~Because of the translational symmetry of the Bravais lattice,~~

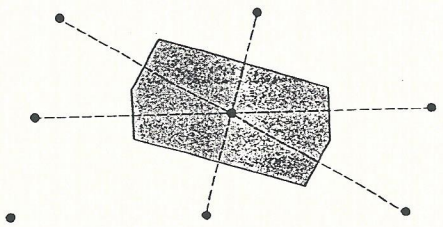
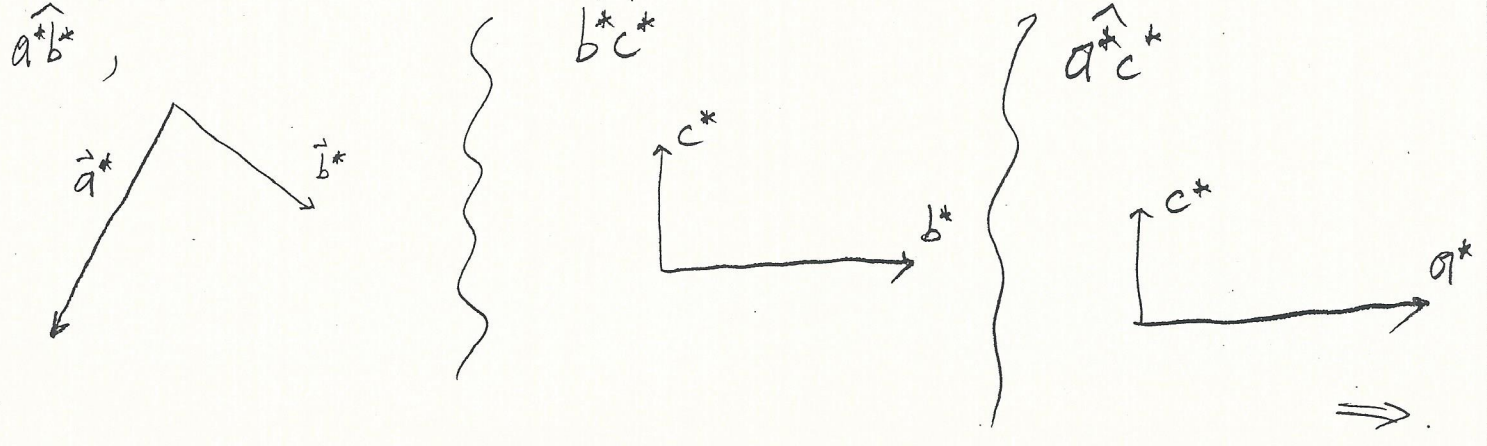


Figure 4.14
The Wigner-Seitz cell for a two-dimensional Bravais lattice. The six sides of the cell bisect the lines joining the central points to its six nearest neighboring points (shown as dashed lines). In two dimensions the Wigner-Seitz cell is always a hexagon unless the lattice is rectangular (see Problem 4a).

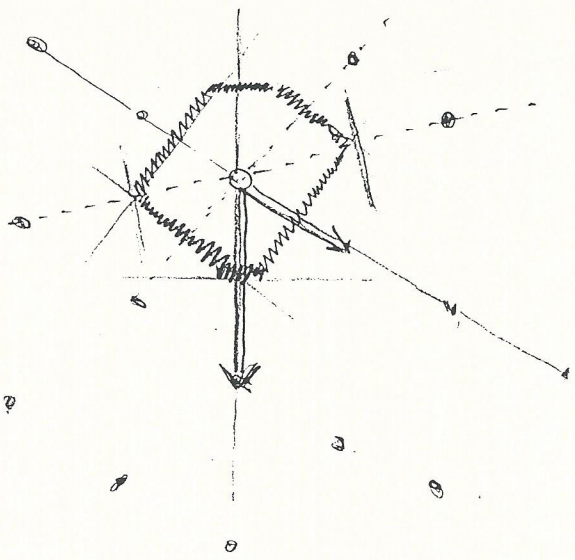
GOING BACK TO THE DRAWING OF THE RECIPROCAL LATTICE VECTOR IN PART a), IN THE PLANES a^*b^*, b^*c^* & a^*c^* WE HAVE



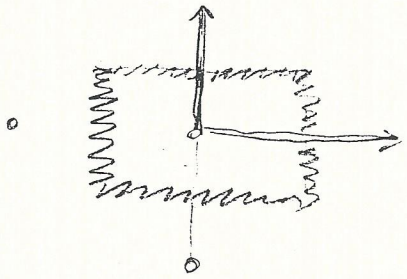
⇒

THEREFORE,

$\hat{a}^*b^*$ PLANE



FOR THE OTHER TWO PLANES



[12]

AS ALREADY MENTIONED IN PROBLEM [4] AND [11], THE DETERMINATION OF THE INTERPLANAR DISTANCES d_{hkl} BETWEEN (hkl) PLANES DESERVES PARTICULAR ATTENTION

WITH THE FOLLOWING FEW EXPLANATIONS, WE WILL ARGUE THAT THERE IS A PROFOUND CONNECTION BETWEEN THE INTERPLANAR DISTANCES AND THE VECTORS OF THE RECIPROCAL LATTICE.

THE INTERPLANAR DISTANCES d_{hkl} PLAY A FOUNDAMENTAL RULE IN BRAGG'S LAW, THEREFORE IT IS VERY IMPORTANT TO TRY TO CLARIFY THIS POINT.

THE USE OF THE RECIPROCAL LATTICE PROVIDES A SYSTEMATIC WAY TO DETERMINE d_{hkl}, PARTICULARLY WHEN THE CRYSTAL STRUCTURES ARE SO COMPLEX THAT A GEOMETRICAL DETERMINATION BECOMES VERY DIFICULT TO ACHIEVE.

THIS IS TAKEN FROM ASHCROFT - MERMIN

Fig 0

Given a particular Bravais lattice, a *lattice plane* is defined to be any plane containing at least three noncollinear Bravais lattice points. Because of the translational symmetry of the Bravais lattice, any such plane will actually contain infinitely many lattice points, which form a two-dimensional Bravais lattice within the plane. Some lattice planes in a simple cubic Bravais lattice are pictured in Figure 5.3.

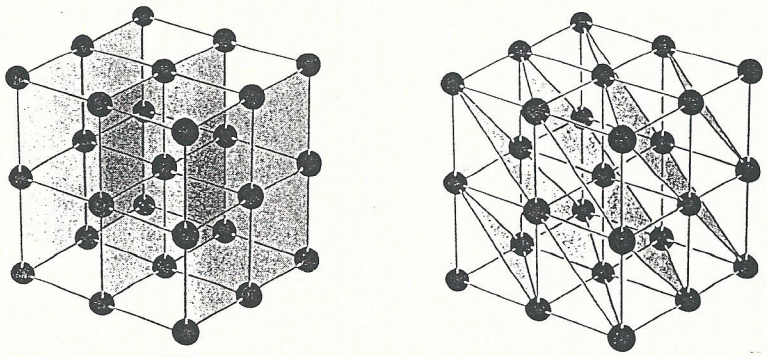


Figure 5.3
Some lattice planes (shaded) in a simple cubic Bravais lattice; (a) and (b) show two different ways of representing the lattice as a family of lattice planes.

By a *family of lattice planes* we mean a set of parallel, equally spaced lattice planes, which together contain all the points of the three-dimensional Bravais lattice. Any lattice plane is a member of such a family. Evidently the resolution of a Bravais lattice into a family of lattice planes is far from unique (Figure 5.3). The reciprocal lattice provides a very simple way to classify all possible families of lattice planes, which is embodied in the following theorem:

⇒ For any family of lattice planes separated by a distance d, there are reciprocal lattice vectors perpendicular to the planes, the shortest of which have a length of $2\pi/d$. Conversely, for any reciprocal lattice vector **K**, there is a family of lattice planes normal to **K** and separated by a distance d, where $2\pi/d$ is the length of the shortest reciprocal lattice vector parallel to **K**.

IT BECOMES CLEAR THAT A KNOWLEDGE OF THE RECIPROCAL LATTICE IS OF FUNDAMENTAL IMPORTANCE

IMPORTANT EXAMPLES

The *simple cubic* Bravais lattice, with cubic primitive cell of side a, has as its reciprocal a simple cubic lattice with cubic primitive cell of side $2\pi/a$. This can be seen, for example, from the construction (5.3), for if

$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = a\hat{\mathbf{y}}, \quad \mathbf{a}_3 = a\hat{\mathbf{z}}, \tag{5.10}$$

then

$$\mathbf{b}_1 = \frac{2\pi}{a}\hat{\mathbf{x}}, \quad \mathbf{b}_2 = \frac{2\pi}{a}\hat{\mathbf{y}}, \quad \mathbf{b}_3 = \frac{2\pi}{a}\hat{\mathbf{z}}. \tag{5.11}$$

The *face-centered cubic* Bravais lattice with conventional cubic cell of side a has as its reciprocal a body-centered cubic lattice with conventional cubic cell of side $4\pi/a$. This can be seen by applying the construction (5.3) to the fcc primitive vectors (4.5). The result is

$$\mathbf{b}_1 = \frac{4\pi}{a}\frac{1}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}} - \hat{\mathbf{x}}), \quad \mathbf{b}_2 = \frac{4\pi}{a}\frac{1}{2}(\hat{\mathbf{z}} + \hat{\mathbf{x}} - \hat{\mathbf{y}}), \quad \mathbf{b}_3 = \frac{4\pi}{a}\frac{1}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}}) \tag{5.12}$$

This has precisely the form of the bcc primitive vectors (4.4), provided that the side of the cubic cell is taken to be $4\pi/a$.

The *body-centered cubic* lattice with conventional cubic cell of side a has as its reciprocal a face-centered cubic lattice with conventional cubic cell of side $4\pi/a$. This can again be proved from the construction (5.3), but it also follows from the above result for the reciprocal of the fcc lattice, along with the theorem that the reciprocal of the reciprocal is the original lattice.

It is left as an exercise for the reader to verify (Problem 2) that the reciprocal to a *simple hexagonal* Bravais lattice with lattice constants c and a (Figure 5.1a) is another

THEREFORE BCC → FCC

FCC → BCC

DIRECT RECIPROCAL

where $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ are three orthogonal unit vectors, then a set of primitive vectors for the body-centered cubic lattice could be (Figure 4.6)

$$\mathbf{a}_1 = a\hat{\mathbf{x}}, \quad \mathbf{a}_2 = a\hat{\mathbf{y}}, \quad \mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}}).$$

Fig 1

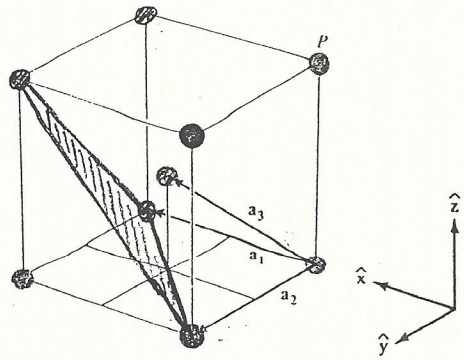


Figure 4.6
Three primitive vectors, specified in Eq. (4.3), for the body-centered cubic Bravais lattice. The lattice is formed by taking all linear combinations of the primitive vectors with integral coefficients. The point P, for example, is $P = -\mathbf{a}_1 - \mathbf{a}_2 + 2\mathbf{a}_3$.

A symmetric set of primitive vectors for the face-centered cubic lattice (see Figure 4.9) is

$$\mathbf{a}_1 = \frac{a}{2}(\hat{y} + \hat{z}), \quad \mathbf{a}_2 = \frac{a}{2}(\hat{z} + \hat{x}), \quad \mathbf{a}_3 = \frac{a}{2}(\hat{x} + \hat{y}).$$

Figure 4.9
A set of primitive vectors, as given in Eq. (4.5), for the face-centered cubic Bravais lattice. The labeled points are $P = \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$, $Q = 2\mathbf{a}_2$, $R = \mathbf{a}_2 + \mathbf{a}_3$, and $S = -\mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$.

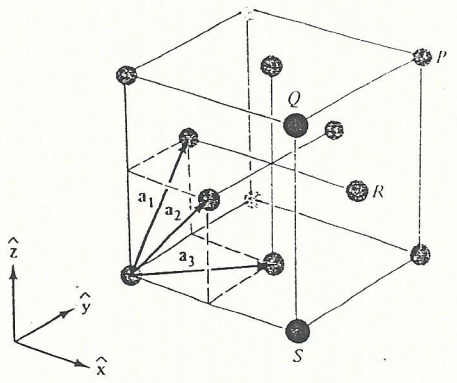


Fig 2

IN PROBLEM 4 YOU ARE ASKED TO DETERMINE d_{111} FOR A fcc LATTICE

$d_{111} = \frac{2\pi}{G_{111}}$, WHERE G_{111} IS THE MAGNITUDE OF THE SHORTEST VECTOR IN THE RECIPROCAL SPACE ⊥ TO (111) PLANES

YOU HAVE fcc. WHAT'S THE RECIPROCAL? ⇒ bcc

NOW, WHAT IS THE SHORTEST VECTOR IN A bcc LATTICE ALONG [111]?

IT IS THE VECTOR $\vec{a}_3^*$ IN (fig. 1);

∴ $G_{111} = \frac{(\text{LENGHT of CUBE})}{2}(\hat{x}+\hat{y}+\hat{z})$; LENGHT of CUBE for bcc RECIPROCAL of fcc of SIDE a $\equiv \frac{4\pi}{a}$ (see IMPORTANT EXAMPLES)

∴ $G_{111} = \frac{4\pi}{a} \cdot \frac{1}{2} \cdot \sqrt{3}$, $d_{111} = \frac{2\pi}{G_{111}} = \frac{2\pi}{2\pi}\frac{a}{\sqrt{3}} = \frac{a}{\sqrt{3}}$ ✓

nb. DO NOT USE (1,5) p. 16 IN OMAR!

$$d_{hkl} = \frac{1}{\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right]^{1/2}}$$

THE FACT THAT THIS GIVES YOU THE CORRECT RESULT FOR d_{111} IN fcc IS .... LUCK!, BECAUSE d_{111} IN fcc & SIMPLE CUBIC ARE THE SAME.

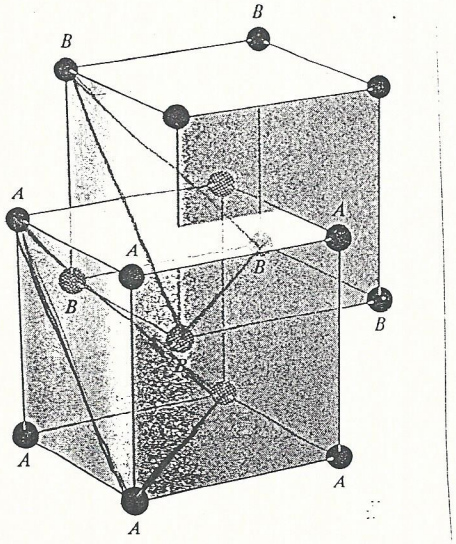
THINK ABOUT THE REASON WHY IN ALL THE PROBLEMS YOU HAD IT WAS EXPLICITELY GIVEN THAT THE STRUCTURE WAS fcc.

IF YOU USE (1,5) p. 16 YOU WOULD GET THE SAME RESULT FOR SIMPLE CUBIC, fcc AND BCC, AND THIS CAN'T BE

TRY TO CALCULATE d_{111} FOR BCC., FOR EXAMPLE.

(1,5) WOULD GIVE $\frac{a}{\sqrt{3}}$,

WHILE AN INSPECTION of THE figure SHOWS THAT d_{111} IS HALF of d_{111} FOR fcc OR SIMPLE CUBIC (SEE fig 8(b) FOR SIMPLE CUBIC)



INFACT, THE RECIPROCAL OF BCC IS fcc, AND THE SIDE IS $\frac{4\pi}{a}$

WHAT IS THE SHORTEST LATTICE VECTOR IN fcc ALONG [111]? ⇒ (Fig 2) ⇒ VECTOR CONNECTING THE ORIGIN WITH P, i.e, THE CUBE DIAGONAL

i.e $G_{111} = \sqrt{3} \cdot \frac{4\pi}{a}$, $d^{bcc}_{111} = \frac{2\pi}{G_{111}} = \frac{2\pi a}{4\pi\sqrt{3}} = \frac{a}{2\sqrt{3}} = \frac{1}{2} d^{fcc}$ ✓✓

NOW BACK TO PROBLEM 25 IN OMAR ....

fcc, $a = 3{,}25$ Å, $K.E_{BEAM} = 150$ eV $= V$

(2,55) ⇒ $\lambda = \sqrt{\frac{150}{V(eV)}} = 1$ Å

RECALL BRAGG'S LAW ⇒ $2 d_{hkl} \sin\theta_{hkl} = n\lambda$

$$\sin\theta_{hkl} = \frac{\lambda}{2 d_{hkl}}$$, where we consider 1st order

HERE THE IDEA IS THAT $\sin\theta_{hkl} \propto \frac{1}{d_{hkl}} \propto G_{hkl}$

LOOK @ THE RECIPROCAL LATTICE for fcc (WHICH IS BCC WITH SIDE $\frac{4\pi}{a}$) AND CHOOSE THE SHORTEST ONES ...

LOOK @ (FIG 1) $\Rightarrow$ THE SHORTEST IS a_3^* ,
THE SECOND ONE IS a_1^* OR a_2^*

$$|\vec{a}_3^*| = \frac{\sqrt{3}}{2} \cdot \frac{4\pi}{a} = \frac{2\sqrt{3}\,\pi}{a} \quad ; \quad |\vec{a}_1^*| = |\vec{a}_2^*| = \frac{4\pi}{a}$$

$\vec{a}_3^*$ ALONG [111] , $\vec{a}_1^*$ ALONG [100] , $\vec{a}_2^*$ ALONG [010]
(I COULD ALSO CONSIDER [001] , THERE IS SYMMETRY ...)

$$\sin\theta_{hkl} = \frac{\lambda}{2 d_{hkl}} = \frac{\lambda G_{hkl}}{2 \cdot 2\pi} = \frac{\lambda G_{hkl}}{4\pi}$$

$$\sin\theta_{111} = \frac{\lambda |\vec{a}_3^*|}{4\pi} = \frac{\lambda}{4\pi} \cdot \frac{2\sqrt{3}\pi}{a} = \frac{\sqrt{3}}{2}\frac{\lambda}{a} \simeq 0.26 \Rightarrow \theta_{111} \simeq 15.45^\circ$$

$$\left.\begin{matrix}\sin\theta_{100} \\ \sin\theta_{010} \\ \sin\theta_{001}\end{matrix}\right\} = \frac{\lambda}{4\pi} \cdot \frac{4\pi}{a} = \frac{\lambda}{a} \simeq 0.30 \Rightarrow \left.\begin{matrix}\theta_{100} \\ \theta_{010} \\ \theta_{001}\end{matrix}\right\} \simeq 17.92^\circ$$

ADDENDUM

momentum parallel to the surface and its validity can be seen in Fig. 3.8. Eqn (3.13b) amounts to the conservation of energy used here because it is an elastic scattering process under consideration.

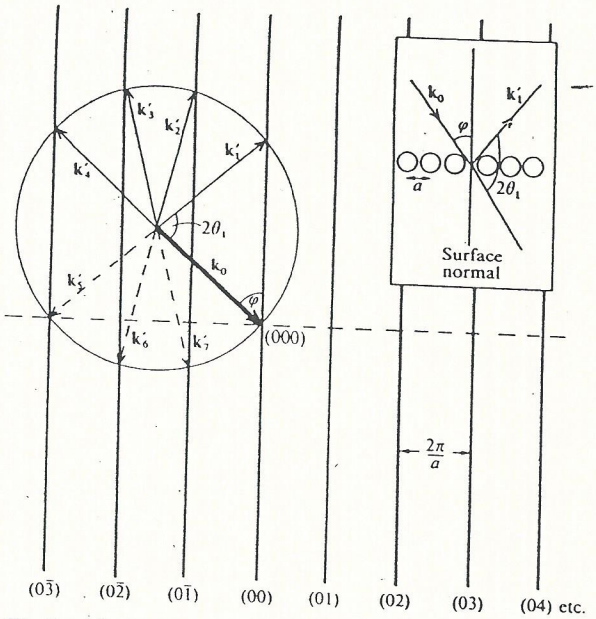


FIG. 3.8. The Ewald sphere construction (e.g. Wormald 1973) applied to diffraction from a square net of atoms of side a. In the case drawn seven elastically scattered diffracted beams can be generated by incident wavevector $\mathbf{k}_0$ arriving at an angle of incidence ϕ to the surface normal. Four beams are shown back-scattered from the surface; three beams are shown transmitted into the solid. More than this number of beams will occur because only that part of reciprocal space in the plane of the paper can be drawn. *Inset*. Real space diagram of the specular beam $\mathbf{k}_1'$.

IF YOU ARE IN 2D, YOU HAVE TO REALIZE THAT THE RECIPROCAL LATTICE HAS A DIMENSION WHICH EXTENDS INFINITELY ALONG $\vec{c}^*$.

IN PROBLEM [10] WE OUTLINE THAT IF IN THE DIRECT LATTICE YOU HAVE $|\vec{a}| \gtrless |\vec{b}|$ $\Rightarrow$ IN RECIPROCAL SPACE $|\vec{a}^*| \lessgtr |\vec{b}^*|$

SO IN 2D, $|\vec{c}| = 0 \Rightarrow |\vec{c}^*| \to \infty$

THIS GIVE RISE NOT TO POINTS ANY MORE, BUT "RODS", WHICH ALWAYS INTERSECT THE EWALD SPHERE, SO THAT YOU ALWAYS HAVE SPOT. THIS IS WHAT HAPPENS IN THE DIFFRACTION FOR ELECTRONS @ LOW ENERGIES (L.E.E.D)