PHSX 886: Homework #2

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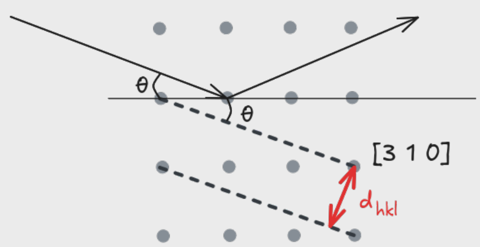
These 4 questions are from the "Elements of X-ray diffraction" book.

Problem 1

3-1 A transmission Laue pattern is made of a cubic crystal having a lattice parameter of 4.00Å. The x-ray beam is horizontal. The $[0\bar{1}0]$ axis of the crystal points along the beam towards the x-ray tube, the [100] axis points vertically upward, and the [001] axis is horizontal and parallel to the photographic film. The film is 5.00 cm from the crystal.

a) What is the wavelength of the radiation diffracted from the (310) planes?

Solution:



The (310) plane has normal in the direction of [3,1,0] and intercepts at $(\frac{1}{3}, 1, 0)$, at an angle $\tan^{-1}\left(\frac{1/3}{1}\right) = 18.4°$ below the horizontal.

The distance between planes is given by

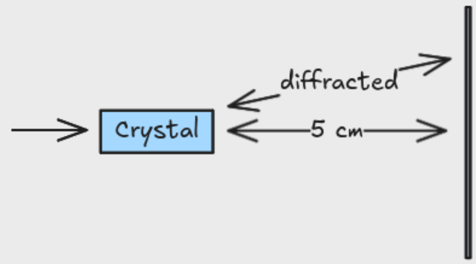
$$d_{hkl} = \frac{d}{\sqrt{h^2+k^2+l^2}} = \frac{4.0}{\sqrt{3^2+1^2}} = \frac{4}{\sqrt{10}}$$

I don't need to do anything complicated here, just apply the Bragg diffraction relation:

$$n\lambda = 2d\sin\theta$$
$$n\lambda = 2\left(\frac{4}{\sqrt{10}}\right)\sin(18.4°)$$
$$n\lambda \approx 0.526\text{Å}$$

b) Where will the 310 reflection strike the film?

Solution:



The outgoing angle is always 2θ, confirmed graphically in the figure in (a). We will just want the distance $d' = 5 \cdot \tan 24° \approx 2.2$ cm

For b), you can show it graphically and calculate the angle between the incident and diffracted beam.

Problem 2

3-3 Determine, and list in order of increasing angle, the values of 2θ and (hkl) for the first three lines (those of lowest 2θ values) on the powder patterns of substances with the following structures, the incident radiation being $\mathrm{Cu}K\alpha$:

a) simple cubic ($a = 3.00\text{Å}$),

Solution:

We know,

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

So we may have a set of lines with d_{hkl} given by

$$\frac{1}{d^2} = \frac{(h^2 + k^2 + \ell^2)}{a^2}$$

A table of the first few values is:

(hkl)	d_{hkl}
(100)	3.0
(110)	2.121
(111)	1.732

Which will net the following numeric solutions:

(hkl)	2θ
(100)	29.7
(110)	42.6
(111)	52.8

b) simple tetragonal ($a = 2.00\text{Å}, c = 3.00\text{Å}$),

Solution:

We will simply have different d_{hkl} for a tetragonal system:

$$d_{hk\ell} = \frac{1}{\sqrt{\frac{h^2+k^2}{a^2} + \frac{\ell^2}{c^2}}}$$

(hkl)	d_{hkl}	2θ
(100)	2.0	45.3
(110)	1.41	65.9
(111)	1.28	73.9
(200)	1.0	101.0
(210)	0.894	119.0

c) simple tetragonal ($a = 3.00\text{Å}, c = 2.00\text{Å}$),

Solution:

As in (b):

(hkl)	d_{hkl}	2θ
(100)	3.0	29.7
(110)	2.121	42.6
(111)	1.455	64.2
(200)	1.5	61.9
(210)	1.342	69.9

Note: Take the wavelength for $\mathrm{CuK}\alpha$ radiation to be 1.54Å.

Problem 3

4-5 A certain tetragonal crystal has four atoms of the same kind per unit cell, located at $0\frac{1}{2}\frac{1}{4}$, $\frac{1}{2}0\frac{1}{4}$, $\frac{1}{2}0\frac{3}{4}$, $0\frac{1}{2}\frac{3}{4}$. (Do not change axes.)

(a) Derive simplified expressions for F^2.

Solution:

The resultant wave scattered by all the atoms of the unit cell is called the *structure factor* and is designated by the symbol F. It is obtained by simply adding together all the waves scattered by the individual atoms. In general, this equation is given by:

$$F_{hkl} = \sum_{1}^{N} f_n e^{2\pi\imath(hu_n + kv_n + \ell w_n)}$$

Which in the case given simplifies to

$$F = f\left(e^{2\pi i(0+\frac{k}{2}+\frac{\ell}{4})}\right) = f\left(e^{\pi i(k+\frac{\ell}{2})}\right) \qquad \text{(Atom 1)}$$
$$F = f\left(e^{2\pi i(\frac{h}{2}+0+\frac{\ell}{4})}\right) = f\left(e^{\pi i(h+\frac{\ell}{2})}\right) \qquad \text{(Atom 2)}$$
$$F = f\left(e^{2\pi i(\frac{h}{2}+0+\frac{3\ell}{4})}\right) = f\left(e^{\pi i(h+\frac{3\ell}{2})}\right) \qquad \text{(Atom 3)}$$
$$F = f\left(e^{2\pi i(0+\frac{k}{2}+\frac{3\ell}{4})}\right) = f\left(e^{\pi i(k+\frac{3\ell}{2})}\right) \qquad \text{(Atom 4)}$$

The sum of these is then the actual wave scattered:

$$F = f\left[e^{\pi i\left(k+\frac{\ell}{2}\right)} + e^{\pi i\left(h+\frac{\ell}{2}\right)} + e^{\pi i\left(h+\frac{3\ell}{2}\right)} + e^{\pi i\left(k+\frac{3\ell}{2}\right)}\right]$$

This may be factored a bit to get a nicer complex conjugate

$$F = f\cdot e^{\pi i\ell/2}\left[e^{\pi ik} + e^{\pi ih} + e^{\pi ih}\cdot e^{\pi i\ell} + e^{\pi ik}\cdot e^{\pi i\ell}\right]$$
$$F = f\cdot e^{\pi i\ell/2}\left[e^{\pi ik}\left(1+e^{\pi i\ell}\right) + e^{\pi ih}\left(1+e^{\pi i\ell}\right)\right]$$
$$F = f\cdot e^{\pi i\ell/2}\left(1+e^{\pi i\ell}\right)\left[e^{\pi ik} + e^{\pi ih}\right]$$

And the magnitude will be this times the complex conjugate, which is

$$|F|^2 = f^2\cdot\left|1+e^{\pi i\ell}\right|^2\cdot\left|e^{\pi ik}+e^{\pi ih}\right|^2$$

As an exercise, I'll also write this in terms of sinusoidal functions:

Let $x = \pi\ell$.

$$\begin{aligned}\left|1+e^{ix}\right|^2 &= \left(1+e^{ix}\right)\left(1+e^{-ix}\right)\\ &= 1+e^{ix}+e^{-ix}+1\\ &= 2+2\cos x\\ &= 4\cos^2\left(\frac{x}{2}\right)\end{aligned}$$

because $1+\cos x = 2\cos^2(x/2)$.

So

$$\left|1+e^{\pi i\ell}\right|^2 = 4\cos^2\left(\frac{\pi\ell}{2}\right)$$

For the other term,

$$
\begin{aligned}
&\text{Let } a = \pi k, b = \pi h. \\
\left|e^{ia} + e^{ib}\right|^2 &= \left(e^{ia} + e^{ib}\right)\left(e^{-ia} + e^{-ib}\right) \\
&= 2 + e^{i(a-b)} + e^{-i(a-b)} \\
&= 2 + 2\cos(a-b) \\
&= 4\cos^2\left(\frac{a-b}{2}\right) \\
&= 4\cos^2\left(\frac{\pi(k-h)}{2}\right)
\end{aligned}
$$

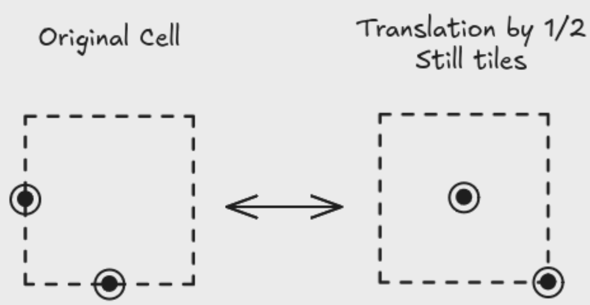
The product will then be

$$
|F|^2 = 16 f^2 \cos^2\left(\frac{\pi\ell}{2}\right)\cos^2\left(\frac{\pi(k-h)}{2}\right)
$$

(b) What is the Bravais lattice of this crystals?

Solution:

Carefully inspecting the basis vectors reveals there is a translation symmetry by a factor of 1/2, which implies the atoms can be centered in the cell. This is graphically confirmed in the below figure



(c) What are the values of F^2 for the $100, 002, 111$, and 011 reflections?

Solution:

(hkl)	$\|F\|^2$
(100)	0
(002)	$16f^2$
(111)	0
(011)	0

Problem 4

4-6 Derive simplified expressions for F^2 for the wurtzite form of ZnS , including the rules governing observed reflections. This crystal is hexagorial and contains 2 ZnS per unit cell, located in the following positions:

$$\begin{aligned} \text{Zn:} &\quad 0\,0\,0,\ \tfrac{1}{3}\,\tfrac{2}{3}\,\tfrac{1}{2}, \\ \text{S:} &\quad 0\,0\,\tfrac{3}{8},\ \tfrac{1}{3}\,\tfrac{2}{3}\,\tfrac{7}{8} \end{aligned}$$

Note that these positions involve a common translation, which may be factored out of the structure-factor equation.

Solution:
As before, the structure factor will be the sum of all scattered waves:

$$\begin{aligned} F_1 &= f_{\text{Zn}} \\ F_2 &= f_{\text{Zn}} e^{2\pi i\left(\frac{h}{3}+\frac{2k}{3}+\frac{\ell}{2}\right)} &&= f_{\text{Zn}} e^{\pi i\left(\frac{2h}{3}+\frac{4k}{3}+\ell\right)} \\ F_3 &= f_{\text{S}} e^{2\pi i\left(\frac{3\ell}{8}\right)} &&= f_{\text{S}} e^{\pi i\left(\frac{3\ell}{4}\right)} \\ F_4 &= f_{\text{S}} e^{2\pi i\left(\frac{h}{3}+\frac{2k}{3}+\frac{7\ell}{8}\right)} &&= f_{\text{S}} e^{\pi i\left(\frac{2h}{3}+\frac{4k}{3}+\frac{7\ell}{4}\right)} \end{aligned}$$

Then, we will have a sum:

$$\begin{aligned} F &= f_{\text{Zn}}\left(1+e^{\pi i\left(\frac{2h}{3}+\frac{4k}{3}+\ell\right)}\right) + f_{\text{S}}\left(e^{\pi i\left(\frac{3\ell}{4}\right)} + e^{\pi i\left(\frac{2h}{3}+\frac{4k}{3}+\frac{7\ell}{4}\right)}\right) \\ &= f_{\text{Zn}}\left(1+\xi e^{\pi i\ell}\right) + f_{\text{S}}\left(e^{\frac{3\pi i\ell}{4}} + \xi e^{\frac{7\pi i\ell}{4}}\right) && \xi \equiv e^{\frac{2\pi i}{3}(h+k)} \\ &= f_{\text{Zn}}\left(1+\xi e^{\pi i\ell}\right) + f_{\text{S}} e^{\frac{3\pi\ell}{4}}\left(1+\xi e^{\pi i\ell}\right) \\ &= \left(1+\xi e^{\pi i\ell}\right)\left(f_{\text{Zn}} + f_{\text{S}} e^{\frac{3\pi i\ell}{4}}\right) \end{aligned}$$

Magnitude will then be:

$$|F|^2 = \left|1+\xi e^{\pi i\ell}\right|^2 \left|f_{\text{Zn}} + f_{\text{S}} e^{\frac{3\pi i\ell}{4}}\right|^2, \qquad \xi \equiv e^{\frac{2\pi i}{3}(h+k)}$$

There will be no reflections when $|F|^2$ is zero, i.e. when $|1+e^{\frac{2\pi i}{3}(h+k)}e^{\pi i\ell}|^2 = -1 = e^{n\pi i}$ for any odd integer n. Inspection of the exponential terms reveals we specifically require:

$$\frac{2}{3}(h+k)+\ell = \text{odd integer}$$

All other cases will give some intensity of reflected wave, the textbook goes into detail on all cases:

$h+2k$	1	F^2
$3n$	$2p+1$ (as $1,3,5,7,\ldots$)	0
$3n$	$8p$ (as $8,16,24,\ldots$)	$4\left(f_{\text{Zn}}+f_{\text{S}}\right)^2$
$3n$	$4(2p+1)$ (as $4,12,20,28,\ldots$)	$4\left(f_{\text{Zn}}-f_{\text{S}}\right)^2$
$3n$	$2(2p+1)$ (as $2,6,10,14,\ldots$)	$4\left(f_{\text{Zn}}^2+f_{\text{S}}^2\right)$
$3n\pm1$	$8p\pm1$ (as $1,7,9,15,17,\ldots$)	$3\left(f_{\text{Zn}}^2+f_{\text{S}}^2-\sqrt{2}\,f_{\text{Zn}}f_{\text{S}}\right)$
$3n\pm1$	$4(2p+1)\pm1$ (as $3,5,11,13,\ldots$)	$3\left(f_{\text{Zn}}^2+f_{\text{S}}^2+\sqrt{2}\,f_{\text{Zn}}f_{\text{S}}\right)$
$3n\pm1$	$8p$	$\left(f_{\text{Zn}}+f_{\text{S}}\right)^2$
$3n\pm1$	$4(2p+1)$	$\left(f_{\text{Zn}}-f_{\text{S}}\right)^2$
$3n\pm1$	$2(2p+1)$	$f_{\text{Zn}}^2+f_{\text{S}}^2$

n and p are any integers, including zero.

Problem 4 continued on next page...