CMP PS3

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1 Crystal Structure

The diagram in the problem set shows a plan view of a structure of cubic ZnS (zinc blende) looking down the z axis. The numbers attached to some atoms represent the heights of the atoms above the $z = 0$ plane expressed as a fraction of the cube edge a. Unlabeled atoms are at $z = 0$ and $z = a$.

(a) What is the Bravais lattice type?

> The lattice is cubic, which restricts it to simple cubic, FCC or BCC. The actual type is then FCC, as there are atoms on the faces of the cube.

(b) Describe the basis.

> Given that we have said that the lattice type is FCC we need only describe the positions of one of each species of atom. Specifying any more would be unecessary. So we have Zn at $(0, 0, 0)$ and S at $\left(\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right)$.

(c) Given that $a = 0.541$nm, calculate the nearest-neighbour Zn-Zn, Zn-S and S-S distances.
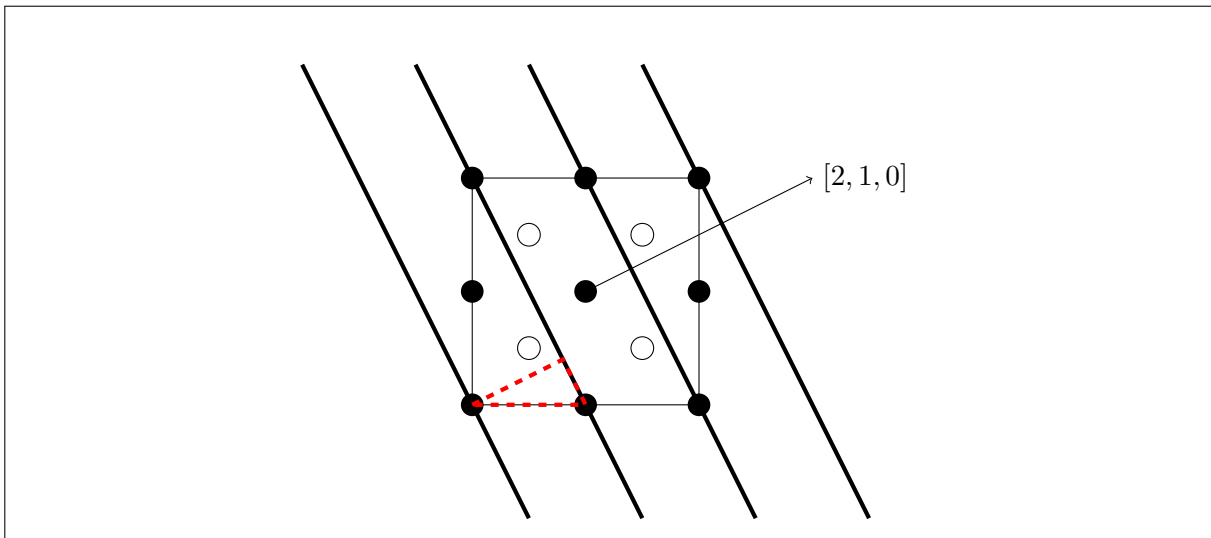
> In FCC the shortest distance between any two atoms is along the one of the planes. So
>
> $$d_{\text{Zn-Zn}} = d_{\text{S-S}} = \sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2 + 0^2} = \frac{a}{\sqrt{2}} = 0.383\text{nm}.$$
>
> The Zn-S distance is less simple. However, considering the Zn at $(1, 0, 0)$ and the S at $\left(\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right)$ it's clearly
>
> $$d_{\text{Zn-S}} = \sqrt{\left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2} = \frac{a\sqrt{3}}{4} = 0.234\text{nm}.$$

(d) Copy the drawing above and show the [210] direction and the set of (210) planes.

This number of planes arises as there must be two planes per unit cell along x and one plane per unit cell along y. Notice that all lattice points are not included so this is not a family of lattice planes.

(e) Calculate the spacing between adjacent (210) planes.

This question has been quite geometrical so let's use a geometrical method to find this distance. Consider the red triangle shown in the previous image. The sides are d, $\frac{d}{2}$ and $\frac{a}{2}$ where d is this distance between planes we're looking for. So

$$d = \frac{a}{\sqrt{5}} = 0.242\text{nm}.$$

This agrees with the formula we'll use later.

2 Directions and Spacings of Crystal Planes

Explain briefly what is meant by the terms "crystal planes" and "Miller indices".

A crystal plane is any plane which intersects and least three non-collinear lattice points (and hence an infinite number of lattice points). Non-collinear here meants that they don't lie in a straight line, which would clearly create some degeneracy as the plane's orientation would be ill-defined.

Miller indices are the indices, h, k and l, describing sets of crystal planes in a given lattice by a vector in the reciprocal lattice with coordinates h, k and l

$$\boldsymbol{G} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3.$$

In more physical terms these are planes oriented such that one encounters h lattice planes if one traverse the unit cell along x, k planes along y and l along z. We may think about placing them similarly to the diagram in the previous question, with one passing through the origin and the next passing through the points $\frac{\boldsymbol{a}_1}{h}$, $\frac{\boldsymbol{a}_2}{k}$ and $\frac{\boldsymbol{a}_3}{l}$. We can use this to construct a vector orthogonal to the plane,

$$\boldsymbol{n} \propto \left(\frac{\boldsymbol{a}_1}{h} - \frac{\boldsymbol{a}_2}{k}\right) \times \left(\frac{\boldsymbol{a}_1}{h} - \frac{\boldsymbol{a}_3}{l}\right)$$

$$\boldsymbol{n} \propto \frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{kl} + \frac{\boldsymbol{a}_3 \times \boldsymbol{a}_1}{lh} + \frac{\boldsymbol{a}_1 \times \boldsymbol{a}_2}{hk}.$$

We then notice from the general definition of reciprocal lattice vectors in a later question that, upon factoring out $\frac{1}{hkl}$, this vector is exactly along the reciprocal lattice vector

$$\boldsymbol{n} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$$

(where in this last step we chose the proportionality to keep the form simple). This argument is completely independent of the basis (they could even be non-orthogonal).

Show that the general direction $[hkl]$ in a cubic crystal is normal to the planes with Miller indices (hkl).

The reciprocal lattice vectors $\boldsymbol{b}_i$ are defined such that

$$\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}.$$

Now, the direction $[hkl]$ is given by the real lattice vector

$$\boldsymbol{R} = h\boldsymbol{a}_1 + k\boldsymbol{a}_2 + l\boldsymbol{a}_3.$$

To check if this is parallel to $\boldsymbol{G}$ we dot the two, (using that $b_i = \frac{2\pi}{a_i}$ in a system with orthogonal axes)

$$\frac{\boldsymbol{R} \cdot \boldsymbol{G}}{RG} = \frac{2\pi(h^2 + k^2 + l^2)}{\sqrt{h^2 a_1^2 + k^2 a_2^2 + l^2 a_3^2} \times \sqrt{\left(h\frac{2\pi}{a_1}\right)^2 + \left(k\frac{2\pi}{a_2}\right)^2 + \left(l\frac{2\pi}{a_3}\right)^2}}.$$

Therefore, if $a_1 = a_2 = a_3$ then this evaluates to 1 and these vectors are indeed parallel.

Is the same true in general for an orthorhombic crystal?

The above formula cannot be satisfied for all h, k and l if all the a_i are not equal.

Show that the spacing d of the (hkl) set of planes in a cubic crystal with lattice parameter a is

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

The lattice planes intersect the axes at $\frac{a_x}{h}$, $\frac{a_y}{k}$ and $\frac{a_z}{l}$ and the previous plane runs through $(0,0,0)$. Thus, we want to project any vector from $(0,0,0)$ to the plane onto the unit normal $\frac{n}{n}$ and this will give us the distance to that plane. So

$$d = \frac{a_x}{h} \cdot \frac{n}{n} = \frac{1}{n} = \frac{1}{\sqrt{\left(\frac{h}{a_x}\right)^2 + \left(\frac{k}{a_y}\right)^2 + \left(\frac{l}{a_z}\right)^2}}.$$

Therefore, we reproduce the stated result when $a_x = a_y = a_z = a$.

What is the generalisation of this formula for an orthorhombic crystal?

See above.

3 Reciprocal Lattice

(a) Define the term Reciprocal Lattice.

> The reciprocal lattice is the set of vectors $\boldsymbol{G}$ which satisfy
>
> $$\boldsymbol{G} \cdot \boldsymbol{R} = 2\pi n$$
>
> for any integer n where $\boldsymbol{R}$ is a vector of the real lattice.

Show that if a lattice in three dimensions has primitive lattice vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ and $\boldsymbol{a}_3$ then primitive lattice vectors for the reciprocal lattice can be taken as

$$\boldsymbol{b}_1 = 2\pi \frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)},$$

$$\boldsymbol{b}_2 = 2\pi \frac{\boldsymbol{a}_3 \times \boldsymbol{a}_1}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)},$$

$$\boldsymbol{b}_3 = 2\pi \frac{\boldsymbol{a}_1 \times \boldsymbol{a}_2}{\boldsymbol{a}_1 \cdot (\boldsymbol{a}_2 \times \boldsymbol{a}_3)}.$$

What is the proper formula in two dimensions?

> We can simply dot each $\boldsymbol{b}_i$ with $\boldsymbol{a}_i$ and recall that $\boldsymbol{a}_i \cdot (\boldsymbol{a}_j \times \boldsymbol{a}_k) = \boldsymbol{a}_k \cdot (\boldsymbol{a}_i \times \boldsymbol{a}_j)$ (because the levi-civita symbol is cyclic). Therefore, trivially $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi \delta_{ij}$. As such, any reciprocal lattice vector
>
> $$\boldsymbol{G} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$$
>
> dotted with any real lattice vector
>
> $$\boldsymbol{R} = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a_3}$$
>
> must give $2\pi \times$ an integer.
> In 2D replace $\boldsymbol{a}_3$ with $\hat{\boldsymbol{z}}$.

Define "tetragonal" and "orthorhombic" lattices. For an orthorhombic lattice, show that $|\boldsymbol{b}_j| = \frac{2\pi}{|\boldsymbol{a}_j|}$. Hence, show that the length of the reciprocal lattice vector $\boldsymbol{G} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_3$ is equal to $\frac{2\pi}{d}$, where d is the spacing of the (hkl) planes (see question 3.2).

> A tetragonal lattice has its lattice vectors orthogonal and the magnitude of two are equal - the lattice has a four-fold rotational symmetry about one axis and two-fold rotational symmetry about the other two.
> An orthorhombic lattice has its lattice vectors orthogonal but no sides of the unit cell of equal length - the lattice has two-fold rotational symmetry about each axis.
> For a general orthorhombic lattice $\boldsymbol{a}_j \times \boldsymbol{a}_k = a_j a_k \frac{\boldsymbol{a}_i}{a_i}$ (assuming $i \neq j \neq k$). Therefore,
>
> $$\boldsymbol{b}_i = 2\pi \frac{a_j a_k \frac{\boldsymbol{a}_i}{a_i}}{a_i a_j a_k} = 2\pi \frac{\boldsymbol{a}_i}{a_i^2}.$$

Therefore, indeed $b_i = \frac{2\pi}{a_i}$.

All the $\boldsymbol{b}_i$ are orthogonal so the length of $\boldsymbol{G}$ is

$$G = 2\pi \sqrt{\left(\frac{h}{a_1}\right)^2 + \left(\frac{k}{a_2}\right)^2 + \left(\frac{l}{a_3}\right)^2}.$$

By inspection this is simply $\frac{2\pi}{d}$.

4 Reciprocal Lattice and X-ray Scattering

A two-dimensional rectangular crystal has a unit cell with sides $a_1 = 0.468$nm and $a_2 = 0.342$nm. A colimated beam of monochromatic X-rays with wavelength 0.166nm is used to examine the crystal.

(a) Draw to scale a diagram of the reciprocal lattice.

The recirpocal lattice is also a rectangle but with inverse lattice spacings, $b_i = \frac{2\pi}{a_i}$. So

$(0,3)$ $(1,3)$ $(2,3)$ $(3,3)$

$(0,2)$ $(1,2)$ $(2,2)$ $(3,2)$

$(0,1)$ $(1,1)$ $(2,1)$ $(3,1)$

$(0,0)$ $(1,0)$ $(2,0)$ $(3,0)$
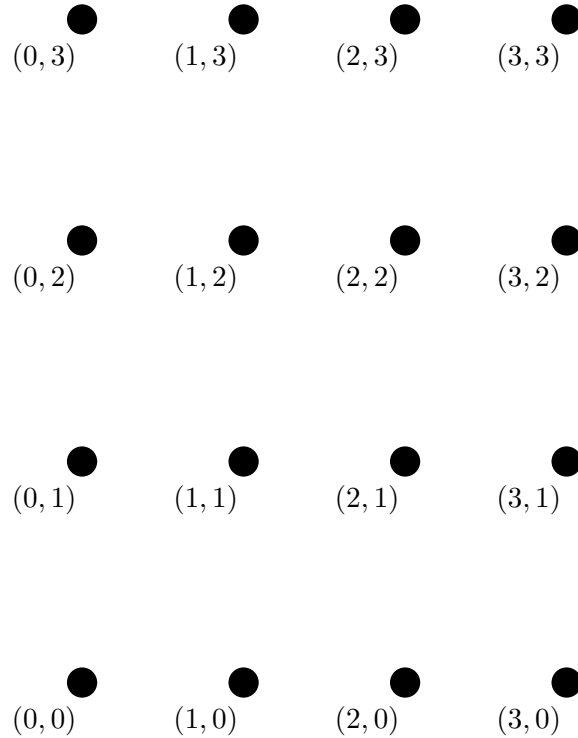
Label the reciprocal lattice points for indices in the range $0 \leq h \leq 3$ and $0 \leq k \leq 3$.

Done.

(b) Calculate the magnitude of the wavevectors $\boldsymbol{k}$ and $\boldsymbol{k}'$ of the incident and reflected X-ray beams, and hence construct on your drawing the "scattering triangle" corresponding to the Laue condition $\Delta \boldsymbol{k} = \boldsymbol{G}$ for diffraction from the $(2,1,0)$ planes (the scatering triangle include $\boldsymbol{k}, \boldsymbol{k}'$ and $\Delta \boldsymbol{k}$).

Thinking about the system as a whole, the crystal is huge so is unlikely to take any of the energy (think about a collision with a wall). Hence, the scattering is elastic and $|\boldsymbol{k}| = |\boldsymbol{k}'|$ where
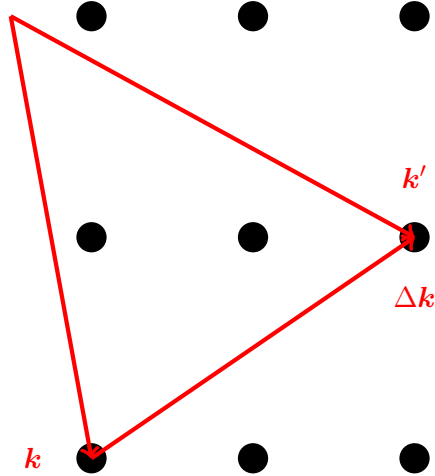$$|\boldsymbol{k}| = \frac{2\pi}{\lambda} = 37.9\text{nm}^{-1}.$$

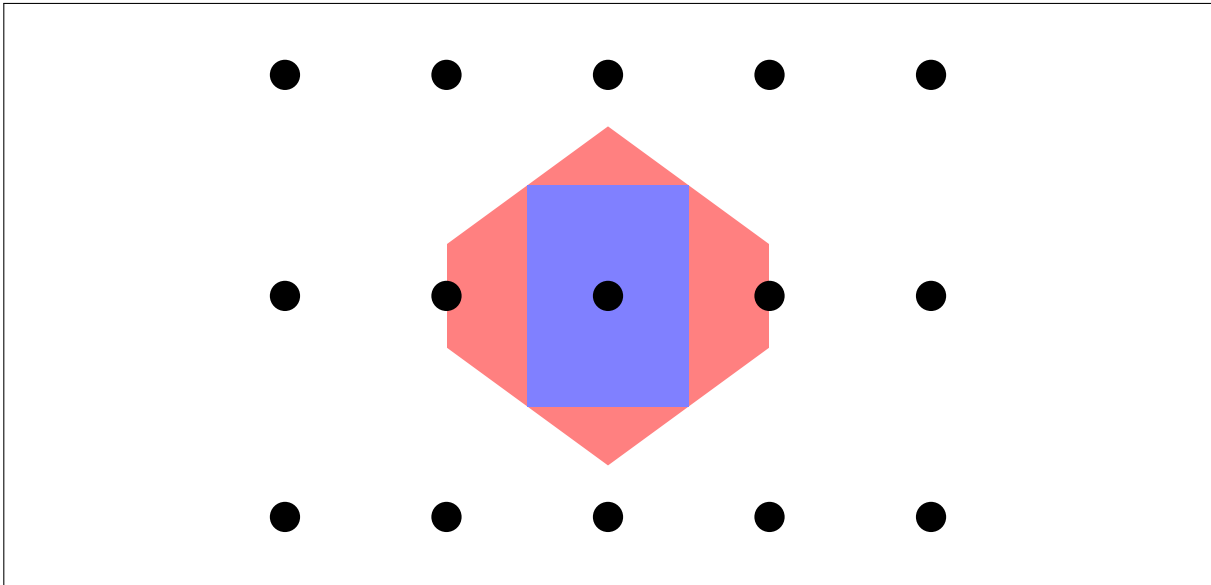Then consider that the size of the (210) reciprocal lattice vector is

$$|\Delta \boldsymbol{k}| = \sqrt{\left(\frac{2\pi}{a_1}\right)^2 + \left(\frac{2\pi}{a_1}\right)^2} = 22.8\text{nm}^{-1}.$$

The scatering triangle is therefore

or a flipped version of this.

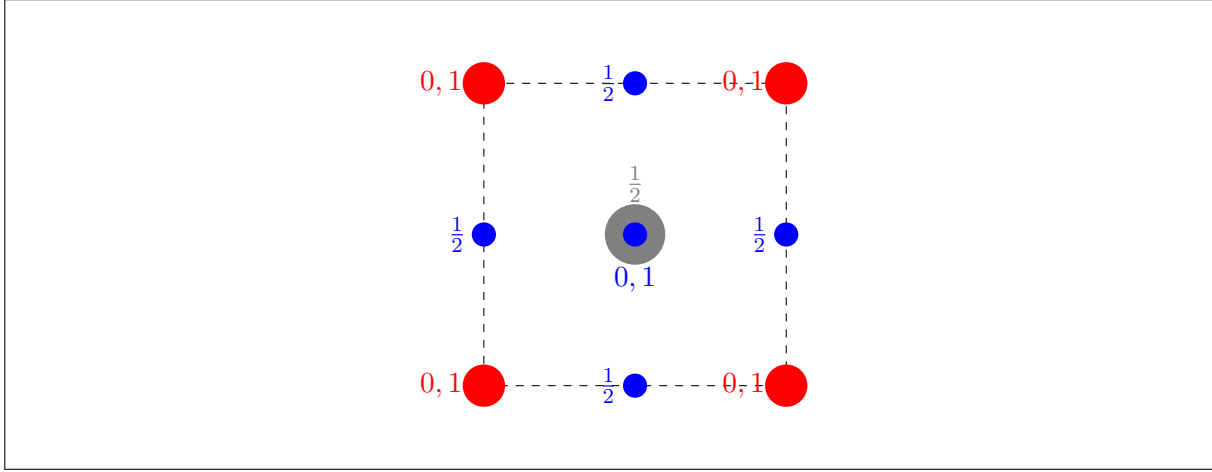(c) Draw the first and second Brillouin zones using the Wigner-Seitz construction.

5 X-Ray Scattering II

$BaTiO_3$ has a primitive cubic lattice and a basis with atoms having fractional coordinates

$$
\begin{aligned}
&\text{Ba} \quad [0,0,0] \\
&\text{Ti} \quad \left[\frac{1}{2},\frac{1}{2},\frac{1}{2}\right] \\
&\text{O} \quad \left[\frac{1}{2},\frac{1}{2},0\right], \quad \left[\frac{1}{2},0,\frac{1}{2}\right], \quad \left[0,\frac{1}{2},\frac{1}{2}\right].
\end{aligned}
$$

Sketch the unit cell.

Show that the X-ray structure factor for the $(0,0,l)$ Bragg reflections is given by

$$
S_{hkl} = f_{\text{Ba}} + (-1)^l f_{\text{Ti}} + [1 + 2(-1)^l] f_{\text{O}}
$$

where f_{Ba} is the atomic form factor for Ba, etc.

The form factor is

$$
S_{hkl} = \sum_{\text{unit cell}} f_{\text{atom}} e^{i\boldsymbol{G}_{hkl} \cdot \boldsymbol{r}_{\text{atom}}}
$$

where $\boldsymbol{G}_{hkl}$ is the reciprocal lattice vector with Miller indices h, k and l. Thus,

$$
\begin{aligned}
S_{001} &= f_{\text{Ba}} + f_{\text{Ti}} \exp\left(2\pi i l \times \frac{1}{2}\right) + f_{\text{O}}\left(e^{2\pi i l \times 0} + e^{2\pi i l \times \frac{1}{2}} + e^{2\pi i l \times \frac{1}{2}}\right) \\
&= f_{\text{Ba}} + f_{\text{Ti}}(-1)^l + f_{\text{O}}\left(1 + 2(-1)^l\right).
\end{aligned}
$$

Calculate the ratio $\frac{I_{002}}{I_{001}}$, where I_{hkl} is the intensity of the X-ray diffraction from the (h,k,l) planes. You may assume that the atomic form factor is proportional to the atomic number Z and neglect its dependence on the scattering vector. $[Z_{\text{Ba}} = 56, Z_{\text{Ti}} = 22, Z_{\text{O}} = 8]$.

The intensity is the modulus squared of the scattering amplitude (which is proportional to the structure factor). Thus,

$$\frac{I_{002}}{I_{001}} = \left| \frac{Z_{\mathrm{Ba}} + Z_{\mathrm{Ti}} + 3Z_{\mathrm{O}}}{Z_{\mathrm{Ba}} - Z_{\mathrm{Ti}} - Z_{\mathrm{O}}} \right|^2 = \left| \frac{102}{26} \right|^2 = 15.4.$$

6 | X-Ray Scattering and Systematic Absences

(a) Explain what is meant by "lattice constant" for a cubic crystal structure.

> For simple cubic crystals the lattice constant is the distance between any two lattice points. For FCC and BCC however, this is the distance along the side of the cube which denotes the conventional unit cell.

(b) Explain why X-ray diffraction may be observed in first order from the (110) planes of a crystal with a body-centered cubic (BCC) lattice, but not from the (110) planes of a crystal with a face-centered cubic (FCC) lattice.

> Recall the structure factor's form.
>
> $$S_{hkl} = \sum_{\text{unit cell}} f_{\text{atom}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{\text{atom}}}.$$
>
> This is a sum over the whole unit cell, so $\boldsymbol{r}_{\text{atom}} = \boldsymbol{r}_{\text{lattice}} + \boldsymbol{r}_{\text{basis}}$. This is a crucial point! We can then take out the lattice component of this sum from all atoms in the unit cell to find
>
> $$S_{hkl} = S_{hkl}^{(\text{lattice})} \times S_{hkl}^{(\text{basis})}.$$
>
> So consider the form factor for the basis in each of the cases given. A BCC has a basis of $[0,0,0]$ and $\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$ so
> $$S_{110}^{(\text{BCC})} = e^{2\pi i(0+0)} + e^{2\pi i\left(\frac{1}{2}+\frac{1}{2}\right)} = 2.$$
> FCC lattices have a basis of $[0,0,0], \left[\frac{1}{2}, \frac{1}{2}, 0\right], \left[\frac{1}{2}, 0, \frac{1}{2}\right]$ and $\left[0, \frac{1}{2}, \frac{1}{2}\right]$ so
>
> $$S_{110}^{(\text{FCC})} = e^{2\pi i(0+0)} + e^{2\pi i\left(\frac{1}{2}+\frac{1}{2}\right)} + e^{2\pi i\left(\frac{1}{2}+0\right)} + e^{2\pi i\left(0+\frac{1}{2}\right)} = 2 - 2 = 0.$$
>
> So, indeed, an FCC lattice does not show a (110) peak.

Derive the general selection rules for which planes are observed in BCC and FCC lattices.

> Generalising what we just saw,
>
> $$S_{110}^{(\text{BCC})} = 1 + e^{\pi i(h+k+l)}.$$
>
> Therefore, $h + k + l$ must be even.
> For FCC,
> $$S_{110}^{(\text{FCC})} = 1 + e^{\pi i(h+k)} + e^{\pi i(h+l)} + e^{\pi i(k+l)}.$$
>
> Therefore, iff all h, k and l are odd this is non-zero. If they're all even this is non-zero. If any one is odd (even) and the other two are even (odd) then this is zero. So h, k and l are all odd or even.

(c) Show that these selection rules hold independently of what atoms are in the primitive unit cell, so long as the lattice is BCC or FCC respectively.

We've already dealt with this but let's make it 100% clear.

$$S_{hkl} = \sum_{\text{unit cell}} f_{\text{atom}} e^{i\mathbf{k}\cdot(\mathbf{r}_{\text{lattice}}+\mathbf{r}_{\text{basis}})}.$$

The sum over the unit cell can also be broken up into a lattice+basis and so

$$S_{hkl} = \sum_{\text{lattice}} e^{i\mathbf{k}\cdot\mathbf{r}_{\text{lattice}}} \sum_{\text{basis}} f_{\text{atom}} e^{i\mathbf{k}\cdot\mathbf{r}_{\text{basis}}}.$$
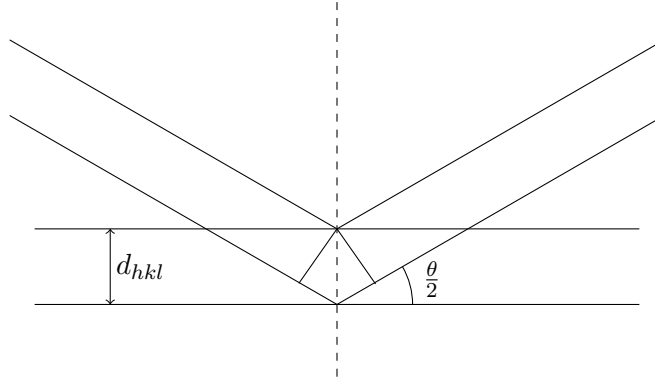
Thus,

$$S_{hkl} = S_{hkl}^{(\text{lattice})} \times S_{hkl}^{(\text{basis})}$$

so if $S_{hkl}^{(\text{lattice})} = 0$ then the basis in unimportant.

(d) A collimated beam of monochromatic X-rays of wavelength 0.162nm is incident upon a powdered sample of the cubic metal palladium. Peaks in the scattered X-ray pattern are observed at angles of $42.3°, 49.2°, 72.2°, 87.4°$ and $92.3°$ from the direction of the incident beam. Identify the lattice type.

Here we treat the planes as Bragg planes from which the X-rays reflect. The extra distance travelled by reflecting off any one plane must then be a whole number of wavelengths different than if we reflect off some other plane. So

Where θ is the total deflection angle then the extra distance travelled by the second ray is

$$d = 2d_{hkl} \sin\frac{\theta}{2}$$

where d_{hkl} is the distance between planes. Thus, setting $d = \lambda$ in each of these cases (as that is constructive interferance), we know $d_{hkl} = \frac{\lambda}{2\sin\frac{\theta}{2}}$. We then use that $d_{hkl} = \frac{a}{\sqrt{h^2+k^2+l^2}}$ to guess h, k and l and then a.

θ	d_{hkl}	$3 \times \left(\frac{d_{\min}}{d_{hkl}}\right)^2$	(h,k,l)
42.3°	0.224	3.00	(1,1,1)
49.2°	0.195	3.96	(2,0,0)
72.2°	0.137	8.02	(2,2,0)
87.4°	0.117	11.00	(3,1,1)
92.3°	0.112	12.00	(2,2,2)

Therefore, this is FCC as h, k and l are all even or all odd.

Calculate the lattice constant.

Proposing that the $42.3°$ peak comes from $(1, 1, 1)$ tells us that

$$0.224\text{nm} = \frac{a}{\sqrt{3}} \qquad \Longrightarrow \qquad a = 0.388\text{nm}.$$

If you assume there is only a single atom in the basis, how well does this lattice constant agree with the known data that the density of palladium is 12023kgm^{-3} [atomic mass of palladium $= 106.4$].

In FCC there are 4 atoms per unit cell if only one atom is in the basis. This would suggest the density is
$$\rho = \frac{4M_{\text{Pd}}}{a^3} = 12100\text{kgm}^{-3}.$$
This agrees very well.

(e) How could you improve the precision with which the lattice constant is determined?

To improve our measurements we need to improve the accuracy with which we measure the angle of reflection so one should first make sure this measuring device is as accurate as possible. If we increase the intensity of the source for example (using a synchotron perhaps) then there is less noise and the measurement is more accurate. It is also important that the beam is sufficiently well collimated. We might also want to change the temperature of the sample as thermal expansion will change the lattice constant. Finally, it turns out that we're most accurate near scattering angles of 90 degrees so analysing these peaks in the most detail will give us the best results.

7 | Neutron Scattering

(a) X-ray diffraction from sodium hydride (NaH) established that the Na atoms are arranged on a face-centered cubic lattice.
Why is it difficult to locate the positions of the H atoms using X-rays?

> As alluded to in an earlier question, the X-rays scatter predominantly off electrons. Therefore, given that the number of electrons around the Hydrogen atom is 1, as compared to 11 around the sodium, the intensity of scattering from H is small.

The H atoms were thought to be displaced from the Na atoms either by $\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$ or by $\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$, to form the ZnS (zincblende) structure of NaCl (sodium chloride) structure, respectively. To distinguish these models a neutron powder diffraction measurement was performed. The intensity of the Bragg peak indexed as $(1, 1, 1)$ was found to be much larger than the intensity of the peak indexed as $(2, 0, 0)$.
Write down expressions for the structure factors for neutron diffraction assuming NaH has
(i) the sodium chloride (NaCl) structure,
(ii) the zinc blende (ZnS) structure.

> The lattice is FCC so we must include this is the overall form factor. The first basis then has
> $$\text{(i)} \qquad S_{hkl}^{(\text{basis})} = b_{\text{Na}} + b_{\text{H}}(-1)^{h+k+l}.$$
> The second has
> $$\text{(ii)} \qquad S_{hkl}^{(\text{basis})} = b_{\text{Na}} + b_{\text{H}} i^{h+k+l}.$$
> In each case these are multiplied by
> $$S_{hkl}^{(\text{lattice})} = 1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l}$$
> to find the total S_{hkl}.

Hence deduce which of the two structure models is correct for NaH [nuclear scattering length of Na $= 0.363 \times 10^{-5}$nm; nuclear scattering length of H $= -0.374 \times 10^{-5}$nm].

> For both $(1, 1, 1)$ and $(2, 0, 0)$ the lattice structure factor gives 4. For the ZnS structure
> $$S_{111} \sim b_{\text{Na}} - i b_{\text{H}}, \qquad S_{200} \sim b_{\text{Na}} - b_{\text{H}}.$$
> For the NaCl structure
> $$S_{111} \sim b_{\text{Na}} - b_{\text{H}}, \qquad S_{200} \sim b_{\text{Na}} + b_{\text{H}}.$$
> We should then worry about multiplicities.
> $$M_{111} = 2^3 = 8, \qquad M_{200} = 6.$$
> Therefore,
> $$I_{111}^{(\text{i})} \sim 4.35, \qquad I_{200}^{(\text{i})} \sim 0.001,$$
> $$I_{111}^{(\text{ii})} \sim 2.17, \qquad I_{200}^{(\text{ii})} \sim 3.26,$$
> in totally arbitrary units. Thus, we must be in case (i), the NaCl structure.

(b) How does one produce monochromatic neutrons for use in neutron diffraction experiments?

Ablation is a good method. You accelerate atoms and slam them into a target with a lot of neutrons in the hope that some are produced/kicked out. You can then make them monochromatic using, for example, time of flight methods.

What are the main differences between neutrons and X-rays?

The key difference between the two is that X-rays scatter from the electrons, with the number of electrons on the atom being proportional to the individual atom's form factor. This process has a reasonably large cross-section and so the intensity of this process is strong. Neutrons have a much smaller cross-section as they scatter either from the nuclei (via strong/weak forces) or magnetically from moments in the sample. This latter fact can be useful if one wishes to probe the magnetic structure of a system (for example, antiferro-magnetism is easy to see despite the lack of a total magnetic moment).

Explain why (inelastic) neutron scattering is well suited for observing phonons, but X-rays are not.

X-rays have really large momenta compared to the momenta of phonons. Therefore, one can imagine that the deflection of an X-ray must be very small to conserve momentum. However, we must also think about energy conservation, and taking the energy (and hence momentum) away from the photon to excite a phonon whilst still conserving momentum is really difficult. The number of ways to do it are vanishingly small and hence, the amplitude for such processes to occur is small.
Neutrons, on the other hand, find it far easier to keep everything conserved, effectively there are vastly more processes which could conserve energy and momentum available, and so the amplitude for these processes is far greater.