Symmetry and Structure in the Solid State
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Lecture - 38
Calculation of Intensities 1

So, you see here now we have been discussing how this value is φ is equal to 2π. So, the value of φ now goes as 0, 2π, 4π if you look at any of the wave motion and consider the wave as a sin wave we have the trough to trough or the crest to crest distance as λ . So, if that is the wave length then we see that the change in the phase that is from here to that particular point is 180°, that 180° in the down and 180° in the up so it will become 360°.

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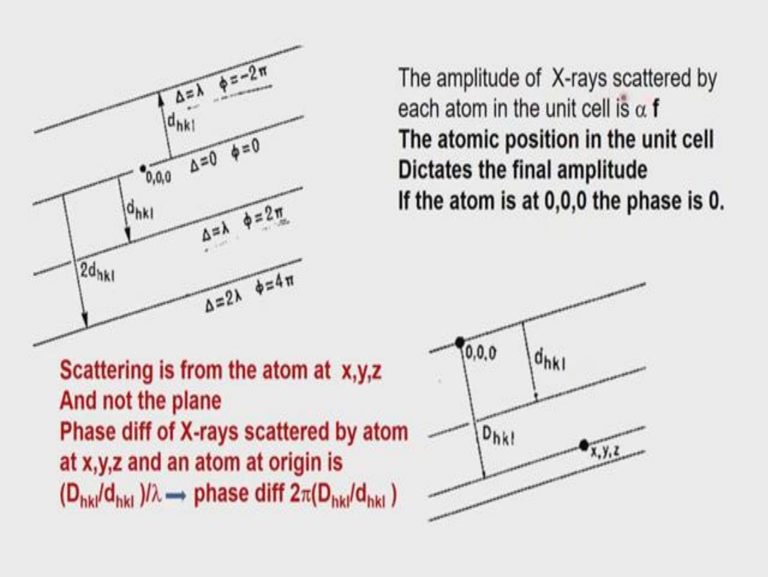

The amplitude of X-rays scattered by each atom in the unit cell is α f

The atomic position in the unit cell Dictates the final amplitude

If the atom is at 0,0,0 the phase is 0.

Scattering is from the atom at x,y,z And not the plane

Phase diff of X-rays scattered by atom at x,y,z and an atom at origin is $(D_{hkl}/d_{hkl})/\lambda \rightarrow$ phase diff $2\pi(D_{hkl}/d_{hkl})$

So, therefore, we have these kind of phases which will phases which are developing with respect to the individual planes. So, let me make it clear we have a crystal, in that particular crystal we have a plane passing through the origin 000 and this particular origin now will allow us the first diffraction to come out of this plane at a satisfaction of the path difference being λ and therefore, the phase difference is 2π.

If you go in the opposite direction the path difference is λ and phase difference is -2π and we can always develop many such parallel planes. It is also possible to have planes like that in a opposite direction, in another direction you remember the bread analogy we can cut the bread not always like this we can always cut it along 1 1 1 plane or something like that. So, you can have a sandwich kind of bread. So, we can have these cutting of the slices in various possible directions.

Now, the thing which we have to notice is that the amplitude of X ray scattered by each atom in the unit cell is proportional to f. So, each atom now the amplitude of X rays scattered is proportional to f and therefore, it depends upon the scattering angle. So, as we go to the higher and higher angles from 0 0 0 as we go to higher and higher angles of scattering the value of f falls with respect to sin θ/λ.

The atomic position in the unit cell dictates the final amplitude if the atom is at 0 0 0 the phase is 0, so, this is a point which one should remember. Now what happens if the point is not with respect to the plane and this is something which is of extreme importance and we will discuss that in a minute. Now, suppose the we have a 0,0,0 plane just like that plane here we have a 0,0,0 plane, the first diffraction will occur at a distance of d_{hkl}, now the second one will occur at $2d_{hkl}$ and so on. Suppose there is an atom x, y, z at this position in the unit cell so there is an atom here and that is in the unit cell.

So, what you do is you draw a plane which is parallel to the plane so, in two dimensions we are drawing a line. So, this line which is there 1 d_{hkl} away which is actually giving the scattering associated with it, what we do is? We draw a line parallel to that, so the *x, y, z* is an atom which is now not at a distance of d_{hkl}, but at a distance of D_{hkl}. So, D_{hkl} is the distance of the atom from the plane and we have drawn a plane which is parallel to 0,0,0 and therefore, parallel passing through x, y, z, but parallel to the first plane which is d_{hkl}. So, if that is the case then what I have written will happen scattering is from the atom and not the plane we know very very well now.

So, phase difference of X ray scattered by atom *x, y, z* and an atom at the origin. So, suppose there is an atom at 0,0,0 and another atom at *x, y, z* the atom at 0,0,0 there is no problem because the phase is 0. The atom at *x, y, z* now will have a path difference of d_{hkl} this is where the atom is located, so the path difference of d_{hkl} and this is where the plane is located. So, we are actually now calculating wherever be the atom it does not matter the contribution of that atom to the plane because we are actually getting the experimental measurement in terms of the planes.

So, the diffraction spot we get is from d $_{hkl}$ which is not coming from *x, y, z* position, but the scattering is done by *x, y, z* and therefore, we have to them consider (D $_{hkl}$/d $_{hkl}$)/λ as the path difference and therefore, the phase difference will be 2π (D $_{hkl}$/d $_{hkl}$) and so we can calculate the corresponding phase difference associated with the atom being at some position *x y z* with respect to the plane.

So, now you can imagine the contribution of *x y z* to some other plane which may pass through the origin and it may go something like that, then the first plane out will be there. So, then we have to calculate that D $_{hkl}$ and the corresponding d $_{hkl}$. So, therefore, this atom now contributes to all the reflections go back to the very original idea we brought in that is when we have more than a wave coming out from a position these waves can interfere.

So, they can interfere constructively, they can interfere destructively, they can interfere with partial overlaps and so on you remember that animation I showed of a sine curve. So, that therefore, will tell us the contribution from *x y z* could be maximum to certain d $_{hkl}$ planes could be minimum to certain d $_{hkl}$ planes and so on. And therefore, the intensity that is associated with the d $_{hkl}$ in the contribution of this atom; x, y, z to that plane is very crucial and that comes out from this calculation that phase difference will be 2π (D $_{hkl}$/d $_{hkl}$).

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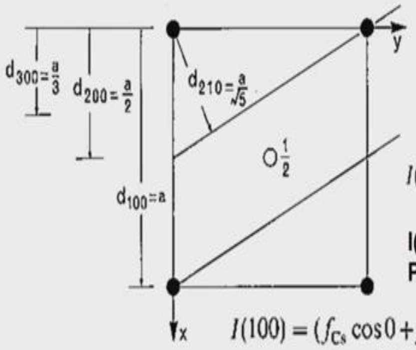

Structure of Cesium Chloride
Cubic with 2 atoms in the unit cell
Cs at 0,0,0 and Cl at 1/2,1/2,1/2

$$I(hkl)=\left(\sum_{1}^{N} f_n \cos\phi_n\right)^2+\left(\sum_{1}^{N} f_n \sin\phi_n\right)^2$$

I(100) Cl is at $\frac{1}{2}d_{100}=\frac{1}{2}a$
Path diff λ/2 so phase diff is π

$$I(100)=(f_{Cs}\cos 0+f_{Cl}\cos\pi)^2+(f_{Cs}\sin 0+f_{Cl}\sin\pi)^2$$
$$=(f_{Cs}-f_{Cl})^2.$$

$$d_{200}=\frac{1}{2}d_{100}$$
$$2\pi(\tfrac{1}{2}a/\tfrac{1}{2}a)=2\pi \rightarrow I(200)=(f_{Cs}\cos 0+f_{Cl}\cos 2\pi)^2+(f_{Cs}\sin 0+f_{Cl}\sin 2\pi)^2$$
$$=(f_{Cs}+f_{Cl})^2.$$

So, how does it help? It helps in the following way if we take an example. So, what we are therefore, going to take do is to take an example to illustrate this one and that is why I showed you this scattering factor curves of f versus sin θ/λ , corresponding to Cs + and Cl - the ions because these two ions form a compound which is Cs Cl the Cs Cl, Cs Cl is a salt we know that. So, it is exists as Cs + and Cl -.

So, the scattering factor that the atomic scattering factor that contributes to this particular structure will come from the atoms Cs + the ion the ionic species Cs + and the ionic species Cl - and that is why we drew the curve earlier on of f versus sin θ/λ .

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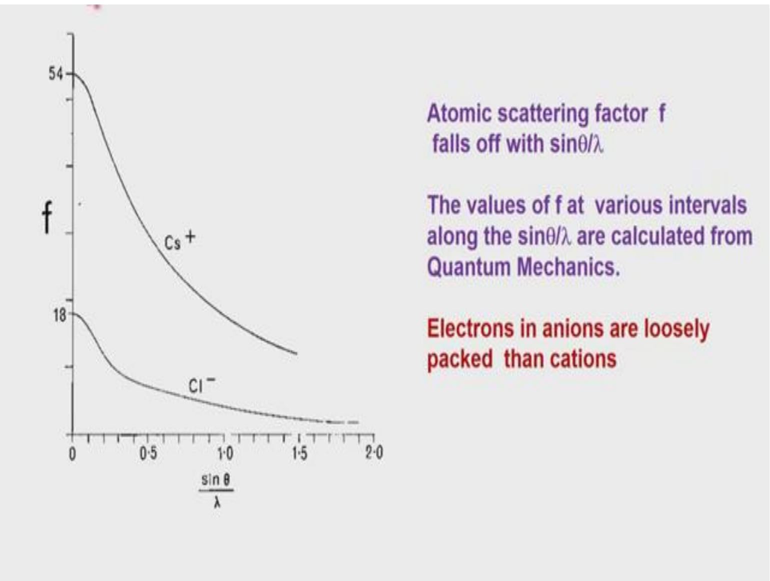

Atomic scattering factor f falls off with sinθ/λ

The values of f at various intervals along the sinθ/λ are calculated from Quantum Mechanics.

Electrons in anions are loosely packed than cations

Let me take it back to you so this is the curve which we have one for the Cs + the other for this Cl -. So, we can get the value of the atomic scattering factor at whatever be the scattering angle at which we find the diffraction spots. So, individually we can identify what is the contribution of Cs, what is the contribution of Cl -. So, if that is the case then we should be able to construct a intensity profile associated with any *hkl* plane.

See in the case of Cs Cl if the structure is known, so we are going to assume the structure this the say Cs atom is sitting at the origin and it’s a simple cubic structure. So, you will have it repeat again one unit away one unit away and one unit away. So, this is our unit cell with Cs at 0,0,0 and Cl sits at ½ ½ ½. So, this is shown as at *x* equals ½ *y* equals ½ and *z* is equal to ½ ½ is indicated next to the atom.

So, these are the positions of the two atoms there is nothing else in this unit cell. So, we want to see what are the contributions, these two atoms do or give to the individual reflections, because what we get from the diffraction experiment is the individual reflection that is associated with your *hkl* planes. So, how do we get that? So we write the I(*hkl*). So, this is a very general expression for any intensity of *hkl* we can write this expression, this is equal to I (hkl) = $(\sum_1^N f_n \cos\varphi_n)^2 + (\sum_1^N f_n \sin\varphi_n)^2$.

That is because you see have discussed earlier on the scattering factor and then eventually the structure factor. This structure factor was a complex number and the square of the structure factor gives us a value which is proportional to the intensity and it is expressed as cosine + i sine you know in the complex diagram since that is expressed as cosine + i sine and that is our structure factor when we want to square that quantity what we will get will be this expression.

So, therefore, the I (hkl) = $(\sum_1^N f_n \cos\varphi_n)^2 + (\sum_1^N f_n \sin\varphi_n)^2$. So, this is a general expression for intensities any compound intensity to any given *hkl* can be calculated based on how many atoms are there in the unit cell and what is their contribution to a given scattering angle. So, if you see in this particular case there are only two atoms in the unit cell this is summed over 1 to N all the atoms inside the unit cell, sum over 1 to N all the atoms in the unit cell.

So, if you have a 100 atoms structure; obviously, this calculation is going to be very very very difficult its; obviously, not the way to do it. So, at this moment we know what is the contribution of the intensity the contribution of the individual atoms that is present in the structure, it depends upon where it is the phase that is going to be associated will depend upon where it is sitting. So, in this particular case the Cl atom is at 0,0,0 sorry ½ ½ ½ and the Cs atom is at 0,0,0.

So, let us calculate the contribution to intensity 1 0 0. So, intensity 1 0 0 will be at a distance of d_{hkl} is $d_{1\,0\,0}$. So, the d_{hkl} now is equal to a the cell dimension. So, therefore, we are considering the plane which is passing through the value of $d_{1\,0\,0}$. So, if you this is the three dimensional structure you have this line this line will now be the representation of $d_{1\,0\,0}$ therefore, 1 0 0 plane is represented by a horizontal line.

So, this is your 1 0 0 direction this is your 010 direction and therefore, if you consider this point it will be one along this and one along that. So, we therefore, consider the contribution of $d_{1\,0\,0}$ the intensity of $d_{1\,0\,0}$. The intensity of $d_{1\,0\,0}$ in this particular example where we have only 2 atoms can be very easily written that is because we can write the use this expression expand it. So, we get $(f_{Cs} \cos 0 + f_{Cl} \cos \pi)^2$. Now why did I write cos π here? You all know now by now what is phase difference which comes, if the atom is removed by the ½ the distance.

So, we say that the path difference the path length for the first plane which is out here which is now at 1 0 0 in this direction the path difference is λ and therefore, the phase difference is 2π. Whereas, the atom now is coming at ½ position so we have to take the ratio of D_{hkl} to d_{hkl}. So, what is D_{hkl} with respect to Cl you have to draw a line here parallel to 1 0 0 and that comes at ½ this position.

So, if this is the value for the path difference of λ then this will be at the point which is equal to λ/2 that is because ½ ($d_{1\,0\,0}$) is (½ a), since it is (½ a) direction we will have the path difference of λ/2 because with a full "a" the path difference is λ by definition of the Braggs law.

So, the atom now is sitting ½ way between this, since we now draw a parallel line we calculate the path difference or in fact, the phase difference as D_{hkl}/d_{hkl} and that will be equal to π, because it the path difference is λ the phase difference is π, path difference is sorry path difference is λ/2 the phase difference is π path difference is λ then the phase difference is 2π which we have already seen.

And therefore, the value of I(1 0 0) goes like this $(f_{Cs} \cos 0 + f_{Cl} \cos \pi)^2 + (f_{Cs} \sin 0 + f_{Cl} \sin \pi)^2$. So, this can be calculated we know the how the cosine behave, here takes place and how the sine function varies with respect to the angular variation and so this turns out to be $(f_{Cs} - f_{Cl})^2$. So, the intensity of 1 0 0 is the difference between this atomic scattering factor of Cs ion - the atomic scattering of Cl ion.

We have to find out where this I(1 0 0) will come see I(1 0 0) is not coming to going to come at the scattering angle θ equals 0, it will come at a certain θ value one can calculate where that θ value can come and that particular value of f should be taken from this curve. So, the it is not going to be 54 and 18 contribution it is going to be something different and that something different will come from the value of sin θ/λ we will see how it comes up.

So, what is happening here is that the $d_{1\ 0\ 0}$ represents a plane which is passing through this Cs atom, similarly $d_{2\ 0\ 0}$ which is a/2 passes through the Cs atom as the Cl atom. Now Cs atom is now removed there is no Cs atom associated with 2 0 0, but what is the contribution to the intensity this very interesting there the Cs atom is at 0,0,$\overset{o}{0}$ as you know that any atom at 0,0,0 will always contribute with a phase change of 0   that is because the path difference is 0 and the phase difference is 0.

So, we have therefore, I(2 0 0) we have the scattering factor of Cs cos 0, for Cl now it becomes cos 2π because now $d_{2\ 0\ 0}$ is the one which is the first plane out of the after 0,0,0 and therefore, it will now have a path difference of λ . So, the phase difference is 2π so we get $(f_{Cs} \cos 0 + f_{Cl} \cos 2\pi)^2$. So, when you put these values in and then you will see that this turns out to be $(f_{Cs} + f_{Cl})^2$, the only interesting point here we have to notice is that we have to see that corresponding sin θ/λ value which will come for $d_{1\ 0\ 0}$.

And the corresponding sin θ/λ which will come from 2 0 0 and read out the corresponding $f_{Cs,}$ f_{Cl} values; that means, if you go back here the 1 0 0 may come corresponding to these two points 2 0 0 may come corresponding to those two points. So, the value of f will not be now 54 and 18 it will be much lower. So, as you go to the higher angles from 1 0 0 to 2 0 0 the value of f_{Cs} and f_{Cl} will reduce; however, you see that the contribution to the intensity 2 0 0 comes out as $(f_{Cs} + f_{Cl})^2$.

So, it may be that even though $f_{Cs,}$ f_{Cl} individual values are lower the contribution to the I(2 0 0) will be much higher because they are adding up whereas, in this particular case the contribution is subtracted. So, the individual values of the scattering powers of Cs and Cl may be higher for 1 0 0 case because of this position in the sin θ/λ where we have to read out the corresponding f value. On the other hand the 2 0 0 will be further away in sin θ/λ , but since there is an addition here this value may be much higher than that value we will see what are those values which will come as in a few minutes.

So, how does this happen? This happens because $d_{2\ 0\ 0}$ is ½ of $d_{1\ 0\ 0}$ and that is therefore, 2π times (½ a) this is D_{hkl}/d_{hkl}, the D_{hkl} is (½ a) the small d_{hkl} is also (½ a) because we are now considering the reflection 2 0 0 which is ½ way between 1 0 0 and the origin. And therefore, we have a 2π value corresponding to the phase difference and that is what has appeared here. So, if you now study this carefully once more this particular slide you will see that it is very very easy to identify how these contributions are coming.

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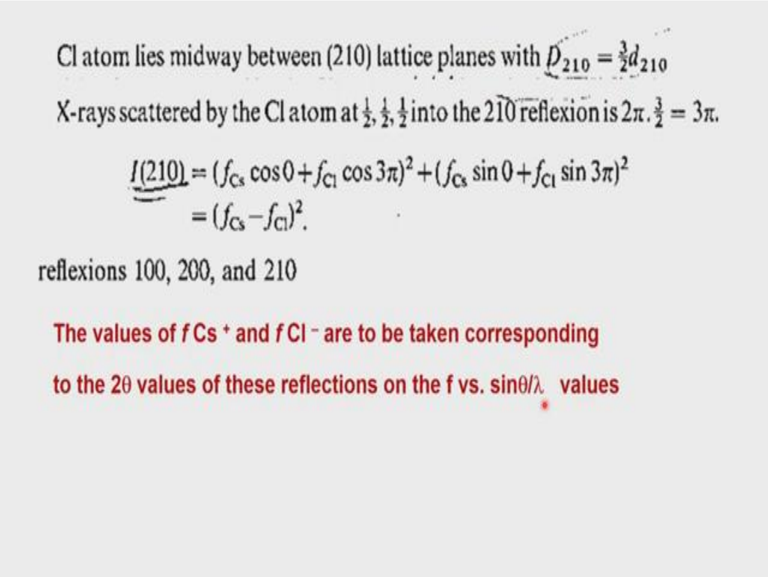

Cl atom lies midway between (210) lattice planes with $D_{210} = \frac{3}{2}d_{210}$

X-rays scattered by the Cl atom at $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ into the $2\bar{1}\bar{0}$ reflexion is $2\pi . \frac{3}{2} = 3\pi$.

$$\begin{aligned} I(210) &= (f_{Cs} \cos 0 + f_{Cl} \cos 3\pi)^2 + (f_{Cs} \sin 0 + f_{Cl} \sin 3\pi)^2 \\ &= (f_{Cs} - f_{Cl})^2. \end{aligned}$$

reflexions 100, 200, and 210

The values of *f* Cs$^+$ and *f* Cl$^-$ are to be taken corresponding to the 2θ values of these reflections on the f vs. sinθ/λ values

So, when we consider the 2 1 0 plane Cl atom will lie midway between the lattice planes to $D_{2\,1\,0}$. So, it will get 3/2 ($d_{2\,1\,0}$) let me indicate where 2 1 0 is it's here. So, this is the $d_{2\,1\,0}$ we are now calculating the contribution from Cs as well as from Cl, we do not have to worry about contribution from Cs because it's sitting at the origin. So, it contributes equally to all the reflections because the atom is at the origin.

So, since the atom is at the origin it contributes to all the reflections equally there is no difference in path, there is no difference in phase. So, whether the plane is here parallel like that $d_{1\,0\,0}$ $d_{2\,0\,0}$ $d_{3\,0\,0}$ or a plane which is going now like this is now 1 unit along y and (½ a) unit along x. So, therefore, this is the $d_{2\,1\,0}$ plane corresponding to $d_{2\,1\,0}$ this is the plane 2 1 0 and you see that the plane 2 1 0 is how the Cl atom now sits ½way between these two and so if you calculate that value it turns out that it is at 3/2 ($d_{2\,1\,0}$).

So, the X ray scattered by Cl atom at ½ ½ ½ into this reflection will be 2π times (3/2) that happens to be 3π. So, 2 1 0 therefore, you can calculate you have f_{Cs} cos 0 that does not change, but f_{Cl} cos 3π now square of that and the sine part also go become square. So, the value can be calculated as $(f_{Cs} - f_{Cl})^2$.

So, the reflections 1 0 0, 2 0 0 and 2 1 0 they do not appear as we again discussed earlier on with a figures the values of f Cs+ and f Cl- are to be taken corresponding to the 2θ values of these reflections in the f versus sin θ/λ curve these values. So, we have to pick up those values of the f. So, if we do that then we will be able to contribute calculate what should be the contribution of Cs Cl to these individual reflections.

Now, imagine a structure which has 100 atoms you have a unit cell let us say 8 * 10 * 12 an orthorhombic unit cell. So, you can actually generate how many possible planes can be created because we now know how to generate the planes, the planes need not be along a or b or c direction this is our bread analogy we can cut this loaf of bread in any orientation we want and each loaf each slice will now represent a plane.

So, the plane the bread can be cut like this bread can be cut like that bread can be cut along the diagonal and so on. So, if you cut the bread along the diagonal the first plane out at the middle at the a = 1, b = 1, c = 1 will be the 1 1 1 plane. So, all planes which are parallel to 1 1 1 can come if we keep slicing the loaf in that particular direction.

So, therefore, we now know how to calculate the contributions for the individual reflection. So, suppose there are 100 atoms each and every atom wherever it is sitting will contribute to this. So, it is not going to be a very easy task here we have taken 2 atoms we have taken a Cs at origin and Cl at ½ ½ ½, very easy to see how these are all coming, but when we have 100 atoms in a x_n, y_n, z_n positions randomly distributed, but covered remember it is in the crystal, so it is always covered by symmetry rules.

So, we have our symmetry rules validated, so keeping the symmetry rules in mind we will have these atoms, but still it’s a large number of atoms and this is not the way which we should be calculating. However, if you want to see how the Cs Cl behaves, this is a chart which I am giving you this chart tells me tells you the following this is a simple cubic as we said.

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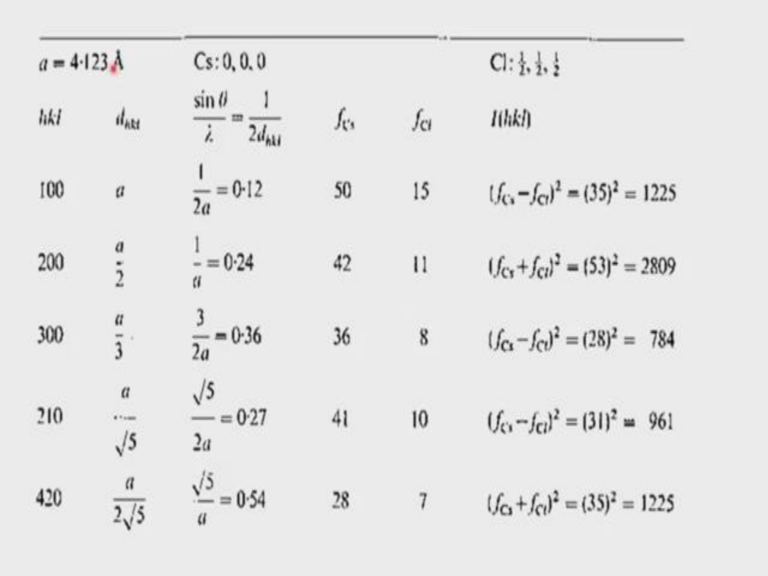

$a = 4{\cdot}123$ Å		Cs: 0, 0, 0			Cl: $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
hkl	d_{hkl}	$\frac{\sin\theta}{\lambda} = \frac{1}{2d_{hkl}}$	f_{Cs}	f_{Cl}	$I(hkl)$
100	a	$\frac{1}{2a} = 0{\cdot}12$	50	15	$(f_{Cs} - f_{Cl})^2 = (35)^2 = 1225$
200	$\frac{a}{2}$	$\frac{1}{a} = 0{\cdot}24$	42	11	$(f_{Cs} + f_{Cl})^2 = (53)^2 = 2809$
300	$\frac{a}{3}$	$\frac{3}{2a} = 0{\cdot}36$	36	8	$(f_{Cs} - f_{Cl})^2 = (28)^2 = 784$
210	$\frac{a}{\sqrt{5}}$	$\frac{\sqrt{5}}{2a} = 0{\cdot}27$	41	10	$(f_{Cs} - f_{Cl})^2 = (31)^2 = 961$
420	$\frac{a}{2\sqrt{5}}$	$\frac{\sqrt{5}}{a} = 0{\cdot}54$	28	7	$(f_{Cs} + f_{Cl})^2 = (35)^2 = 1225$

So, a is equal to 4.123 it so happens the unit cell dimensions are all 1234 is by chance, so a is 4.123Å, Cs is 0 and Cl at ½ ½ ½. So, we can calculate the *hkl* 1 0 0 what should be the intensity for that. So, we get the d $_{hkl}$ which is equal to a in this particular case because 1 0 0 is the reflection we are considering. So, if we calculate the sin θ/λ using the formula 1/2d $_{hkl}$ we will get 1/2a = 0.12, so this is the value of sin θ/λ . So, corresponding to 0.12 you have to read out the Cs and the Cl scattering factors. So, let us go back and see how to do that.

So, here you take the value of 0.12 somewhere here, so you will have to now read the Cl contribution and read the Cs contribution at 0.12. Now the 0.12 values are in fact, given in this table, the table gives you the values to be coming in such a way that the difference in these two the value of f_{Cs} is 50 for f_{Cl} it is 15. So, there is a reduction in the contribution of the individual atom.

So, the even though we have a Cs+ and a Cl- in this structure the contribution from Cs and Cl is coming as though the atoms have only 50 electrons and 15 electrons in these two cases the ions have only 50 electrons and 15 electron. So, the this is something which you must remember when you do the calculation and so we therefore, all have already seen what is 1 0 0 in the previous view graph that is $(f_{Cs} - f_{Cl})^2$. So, the difference 50 - 15 is 35 square. So, we get an intensity of 1225; we get an intensity of 1225.

So, similarly we can do for 2 0 0, 3 0 0, 2 1 0, 4 2 0 depending upon the value of d we substitute this value of d up here we get the sin θ/λ value you see that the sin θ/λ value keeps on increasing and correspondingly the value of Cs and Cl keeps on decreasing and depending upon where the f_{Cs} f_{Cl} values are for example, 3 0 0 is a reflection which comes after 2 1 0.

And therefore, you see the contribution is 41 and 10 here and 36 and 8 there, but what is more important is the way in which the phase addition takes place and therefore, here you have $f_{Cs} + f_{Cl}$ giving you 2809 as the intensity. This intensity is an absolute value because we do not have anything else other than these electrons. So, these are therefore, showing the absolute value and the absolute values are now 1225, 2809 you see that even though this is f_{Cs} - f_{Cl} square even though the values are 28 and 7 the contribution of 4 2 0 is very large, so you get a value of 1225.

So, what does it all mean what it means is now you take Cs Cl crystal put it in the path of the X ray beam and do a diffraction pattern what I will show you instead of showing these parts which will appear for these individual reflections I will show you a powder diffraction diagram which is simulated.

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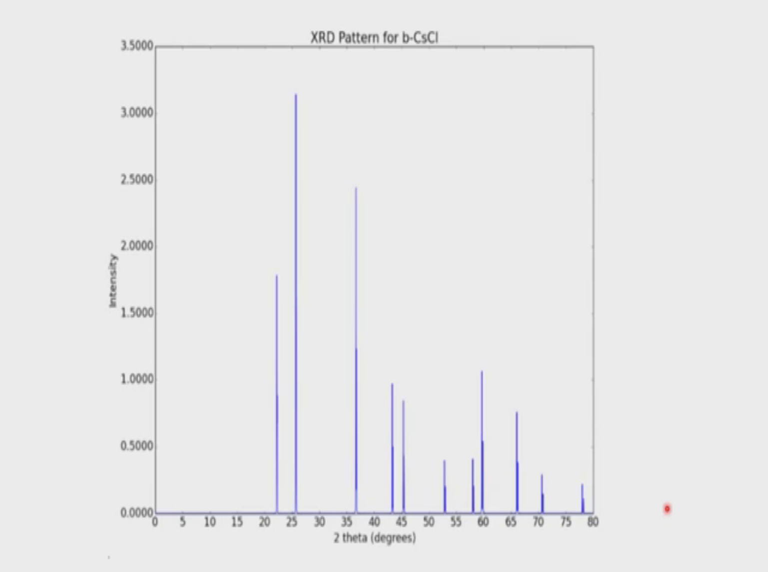

So, we know where Cs is sitting and where Cl is sitting so I took it out from the web and this is the XRD pattern of Cs Cl. So, you see now that this is the intensity and this is the

2θ, you see here the intensity values are given some numbers here. So, what why is that given like that, it depends upon the instrument you are using.

So this is therefore, what we can call as the relative intensity it is not the absolute intensity, but you see that the first reflection and the second reflection is 1 0 0 and 2 0 0 and you see the values were 1225 and 2800. So, you see the relative variations of the intensities in the powder pattern. So, the powder pattern or the single crystal pattern suppose this was single crystal.

In fact, the simulated pattern is very useful because you draw a single line in case of the single crystal you get a spot here corresponding to this intensity a spot there corresponding to that intensity and so on. So, this is therefore, the plot of the Cs Cl X ray diffraction pattern. So, now, you see a one to one correspondence for the first time, you see the diffraction occurring the diffraction therefore, as I made you believe and now you know very well very thoroughly that it is now associated only with the planes atoms are sitting at 0 0 0 and ½ ½ ½, but the X ray diffraction pattern is produced from the planes and you have calculated yourself the contribution to each of these planes in case of Cs Cl.

And you see that behaviour is shown in the X ray diffraction pattern and what you have calculated of course, is a little more sacred than this in the sense that you have calculated the absolute intensities. So, what you have to therefore, do is to convert the relative intensity you have got in the X ray experiment to the absolute intensity there are so many other factors which are involved to do that operation, we will see how we do it at a later date when we actually determine these structures.

But at this particular point we see that the intensities can be calculated if you have a very simple structure like Cs Cl where we know already the structure Cs is at 0 0 0 and Cl is at ½ ½ ½ then it is very straight forward as we have done now and we also now know how the pattern arises because of the positions of these atoms, but what is more important is to take a case where we do not know where the atoms are.

Suppose we had a Cs Cl structure where we had not solved the structure then there is no way I would have done this calculation. So, there is no way I would have got these relative intensities; however, if I had recorded a powder pattern I would have got this powder pattern this is for reality. So, we have the Cs Cl sample and you record powder the Cs Cl crystal and recorded the powder pattern.

Of course, this is a simulated pattern, so it does not give you any widths, in a typical powder pattern there is a certain width associated with it this we will all discuss when we go to powder diffraction methodology, which is very crucial particularly for the pharma industry people to remember that there will be a certain width with each of these peak positions and that is very crucial.

So, effectively this is the intensity we will get when we put the Cs and Cl in known positions and calculate the corresponding contributions to individual reflections. So, X ray diffraction pattern therefore, is coming from the planes and the atoms are sitting need not sit in any plane they can sit wherever they want, but their contribution to the plane can be calculated best as we have done in the case of Cs Cl.

I think this kind of brings us to a stage where we can stop at this juncture, because what we are going to do next will be a situation where we can get to the general expression to calculate the intensities, see we cannot all the time calculate the intensities this way which we did. For example, in this case we have the intensity expression which is a general expression, but then we cannot get the every time where the atoms are sitting and with respect to them calculate this. This is a very simple calculation where we had only 2 atom in the unit cell, but if there are more atoms in the unit cell and they are distributed all over the unit cell how do we get to that position, how do we calculate the intensity?

So, we have to have a general formula. So, the next job would be to generate a general formula by means of which we can calculate the intensity given the atom positions we still given the atom positions, if the atom positions have to be determined that is a next step which is our structure determination we do not know where the atoms are, but we do have the experimental data now which gives us the I versus 2θ plot whether it is a powder diffraction or if it is a single crystal we get the individual reciprocal lattice points which can be indexed and the intensities can be measured.

So, we have reached a stage of let us say it’s a mid level stage of this particular course where we have more or less covered all the aspects of symmetry, all the aspects that are associated with space groups and so on, how we generate the equivalent points? Now we have also found a situation how the atoms sitting in different positions contribute to the intensities of individual reflections.