Techniques of Materials Characterization
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Lecture – 51
Intensity of diffracted beam (Continued)

Welcome everyone to this NPTEL Online Certification Course on Techniques of Materials Characterization. So, we are beginning with module 11. We are almost close to the end and we are discussing with X-ray diffraction, we will be continuing with X-ray diffraction for this module and the next module which is the last one. And we were in the last module onward, we were discussing about intensity of diffracted beam and we will continue with that.

At least for this module, we will be discussing about the intensity of diffracted beam.

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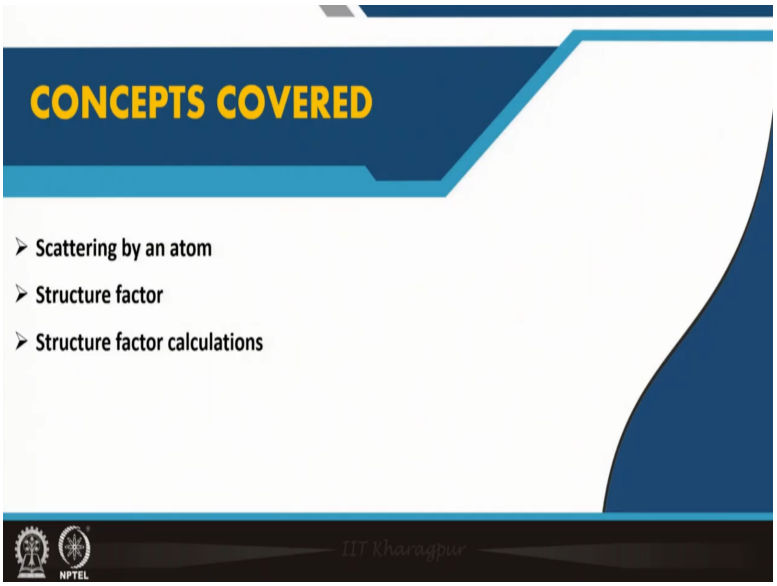

So, what we will be discussing now, is basically, in the last module, we started discussing about intensity and there we have seen the importance of arrangement of atoms in determining that what diffracted beam even after diffraction even after Bragg's Law is satisfied, whether we will be getting any intensity from that after diffraction or not. That is somehow related to the atomic arrangement within the unit cell are within a crystalline material.

So, we started from there and then we try to derive some kind of expression which will be expressing this relationship between the structure of an atom or arrangement of atoms in a crystalline materials with the diffracted beam the intensity of the diffracted beam that is coming out of the crystalline material. So, in that way we started and what we find out is that we have to start from very basic.

How the X-ray is interacting with an electrons, individual electrons in an atom. First we have to start from there. And we discuss there and we find out 2 different types of interactions. One is the Thompson Effect, one is the Compton Effect. And we just considered Thompson effect because that is what is important for calculation of diffractive intensity ultimately.

But Compton modified radiation was also important we discussed about that. That how it modifies the background and so on. And from there, after the electron what we considered is the intensity of the diffracted beam coming out of a individual atom. So, how the different electron? So, individual atoms that contains different types of lots of different electrons.

And how we can superimpose all the waves along certain direction? How we can add them up depending on their phase relationship, depending on the amplitude and so, on. And then we discussed about factor called atomic scattering factor. We define that we saw that what it depends on and how it is helpful. So, from there what we just started in the last class was the relationship establishing a relationship between the intensity of diffracted beam and atomic arrangement.

And there, we were just tried to understand the phase relationship between the diffracted intensity or diffracted beam or the waves coming out from 2 individual atoms. One is kept at the origin and another one is kept arbitrarily in somewhere in the space. So that up to there we discuss. Will continue that this week as well, this module at least this lecture, we will continue with that scattering by an atom scattering within the unit cell.

And then we will discuss about something related called the structure factor and how the structure factor is calculated.

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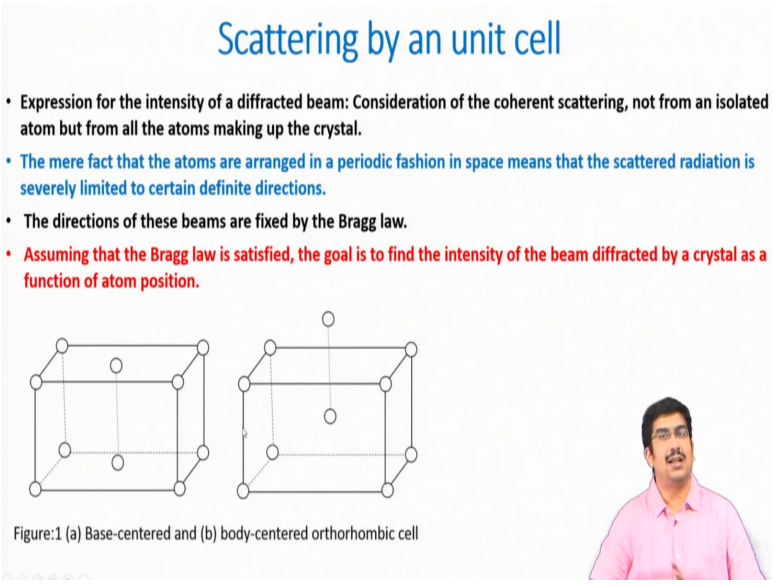

So, this part we all discussed the scattering by in itself we have seen depending on these 2 different type of unit cell. How the intensity or diffracted beam is present for one set? The one particular type of intensity diffracted beam 001 or 100 diffracted beam is present in the center and it is not present in the body centered one. So that means definitely some atomic arrangement has something to do with the diffracted beam intensity.

Do we realize from here? And even though the Braggs Law is satisfied for both conditions. In one case, we get an intensity and another case we did not get an intensity.

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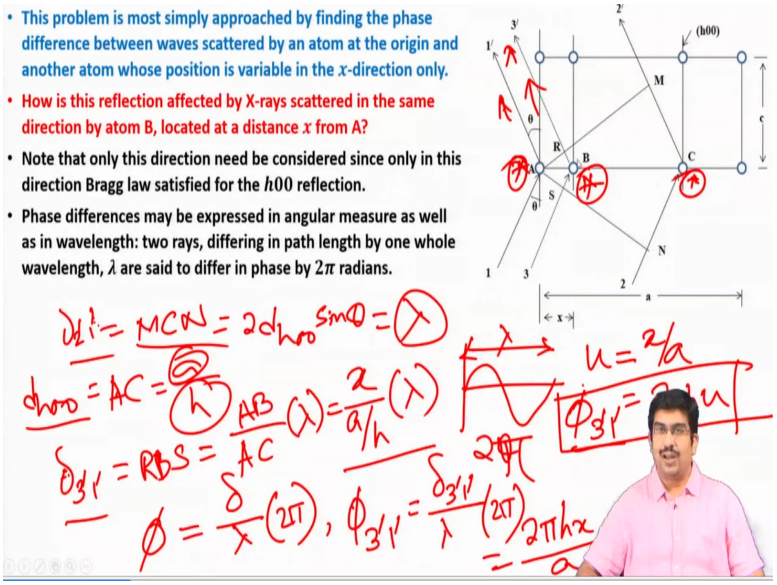

And from there in the last class we derive this relationship we did all of this I am just repeating it again. What we did is basically we imagined an atom in the origin and then we

imagine another atom somewhere in at a distance of x, somewhere in the x direction. And we imagine that Bragg's Law is satisfied for this 800 type claims here. And so, this two atoms this one and this one.

The A and C definitely they are the phase relationship is an integral multiple path difference. So that that is true, if Bragg's Law is satisfied then we imagine another type of atoms situated at a point B and then we try to find out that along this same direction that means the same for the same incident angle, were Bragg's Law is satisfied the theta angle.

How we can superimpose this to or how we can add the waves that is coming out? Extra waves that is coming out from this A atom and this B atom which is arbitrarily oriented somewhere in the space and here in this case, at an instance of x along the x direction. So, then what we find out finally is the phase relationship and that is given between 2 phase relationship of the angular phase difference between this A the wave coming out of this A atom and the wave coming out of this B atom.

The phase relationship, we finally find out first we calculated the path difference from there we calculated the phase difference and the phase difference is coming out to be 2 phi h x by a and then we take the fractional component that is A is the lattice parameter here. So, the fractional component of this position of this B atom that is given by x by a. So, finally, what we find out is the phase differences is $2 \pi h \times u$.

H is here denoting remember this h is here denoting this planes which are satisfying the Bragg's condition. That means, the diffraction is happening from which plane. That is denoted by this h. And this u here is denoting the position of this second atom arbitrarily chosen second atom.

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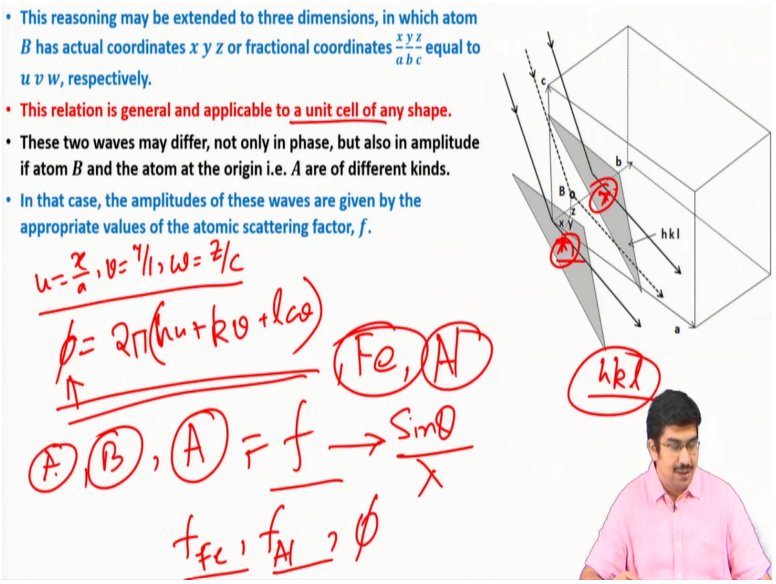

So, up to here, we discussed in the last class and today we can extend this, I am not going into a detail derivation of this entire part but what we can do is that we can check this we can this reasoning the same kind of calculation we can extend it all the way to a 3 dimensional network, where we can imagine that along the origin there is one set of plane is going. And then we can imagine another set of plane arbitrarily anywhere in the space which is making again a fractional coordinates of xa, yb and z, zc.

So, this atom instead of atom now, we are considering a complete plane here. So, in this plane which is having a coordinates of x y z and fractional coordinates, if we imagine that the lattice parameter for this unit cell is a b c. Then the fractional coordinates for this arbitrary defined plane is xa yb zc or otherwise we can write what we can write here very straightforward.

We can write something like u similarly, x by a and v is given by y by b and we can write that w equals z by c. So, this is the fractional coordinate of this arbitrary defined plane. So, for this arbitrarily defined plane now, what we can write the phase difference between the rays coming out of this plane. The phase difference come from the rays coming out of this plane and this another arbitrarily defined plane.

The phase difference between them we can extend it into 3 dimension and we can write that in this way, simply 2 π (h u + k v + l w), where h k l is basically this plane. This arbitrary, this

origin, this plane h k l. And for this h k l plane the diffraction conditions are satisfied and this h k l plane is basically diffracting in the diffracting condition that is what. So, basically this term is giving the phase difference between the origin or atoms present in the origin or the planes passing through the origin and any other arbitrarily defined plane.

So that is a phase difference between the X-rays coming out from these 2 atoms or atomic plates. Now, one thing we must understand is that this relation is very, very general and it is applicable to any kind of unit cell of any shape. There is no restriction because everything is arbitrary here, a b c lattice parameters what is their angle we did not define anything that angle can be anything that relation between a b c can be anything.

That means, this unit cell can be anyone of out of the 7 crystal systems or 14 bravais lattice anything and but for all of them this relationship will be valid that means this unit cell this relation is completely general. So, it can be valid for anything now, the point is that this relation this 2 waves, the waves that is coming out of this plane A and the wave that is coming out of this another atom B and they not only differ by on this phase difference but they can also have an amplitude difference.

And that amplitude difference will be the same, if they are same kind of atom that is okay that is fine. If it is composed of a single element let us say I am considering something like iron. So, every atom is iron and this is I mean like the amplitude of the waves coming out will be the same for all. But in case this is a multi element component, a multi element system.

Let us say, I have iron is one and aluminum is the other one. So, these 2 types of atoms are composing this entire unit cell. Then I have to consider their amplitude separately and amplitudes are normally as we already understand from individual atom, the amplitude is basically nothing but the f that atomic scattering factor appropriate values of atomic scattering factor.

Why appropriate values of this? Because we know atomic scattering factor depends on sin theta by lambda this term. So, an appropriate value of atomic scattering factor will define this amplitude of this 2 waves. So, not only the phase difference we have to consider, we also

have to consider their amplitude and that amplitude is given by the atomic scattering factor. So, if it is composed of 2 iron and aluminum then these 2 X-rays will contain 2 different waves.

And one of these waves will have amplitude of this f F e and another one will have f A l with a phase difference of phi between them.

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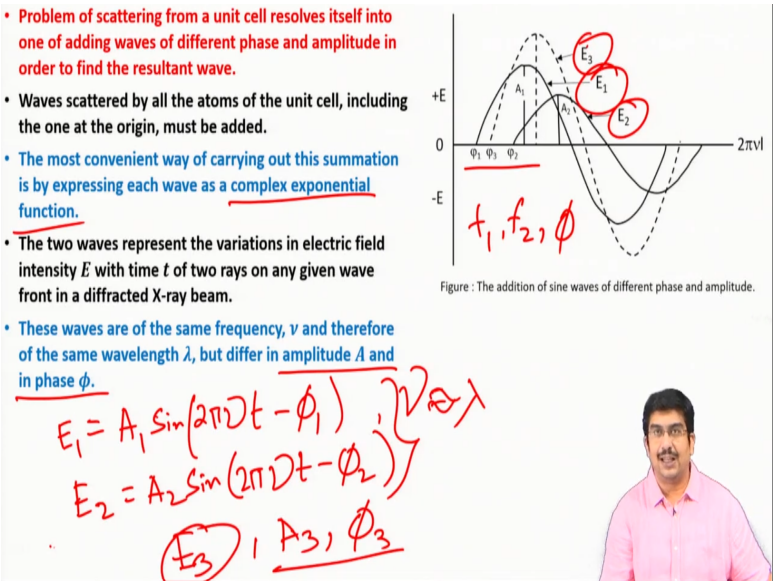

So now, simply we can imagine that the problem has become the center problem of scattering from unit cell is now, comes down to a problem where we have to just add up these 2 waves. As I already said, 2 waves we have let us imagine that we have one way with f 1 wave with f 2 and a phase difference with phi. So, this we have to just add them, this is the entire problem for the entire unit cell.

This is what will be telling us or this is what we will be giving us the diffracted wave, the intensity of the diffracted waves, the amplitude phase everything. If we just add up these 2 waves. And these are completely arbitrary 2 different arbitrarily defined atoms for any kind of unit cell, so, this is completely general. So that means basically, we have to add up this wave scattered by the atoms in the unit cell one in the origin and another one somewhere else.

This summation, the best way of doing the summation is by expressing this 2 waves in terms of a complex exponential function. So, we will see what basically means by complex

exponential function and all. What we can do is that we can represent first of all we can represent these 2 waves, let us imagine one of the waves is coming out of the origin, one of the waves is coming out from this arbitrarily defined plane any atom from this arbitrarily defined plane.

We can represent this, 2 waves by the variation in the electric wave, electric field vector, electric field intensity. Because, if you remember, we already said that every wave these are electromagnetic waves. So, they can be represented by the electric field vector and that electric field vector continuously, sinusoidally varies with respect to the time for a fixed position and with respect to position for a fix time.

So, we can imagine these 2 waves as these 2 sin waves basically. Where there electric field vectors is varying with time and then we can add them up and get the resultant width. So, the way we can possibly express these 2 we can express one of these is like this, where we have this A 1 into sin these are both we are expressing basically these 2, 1 is this u 1 both of them are sin waves.

One is this and one is this. Both of them are sin waves. So, we are just writing their expressions. So, what we can write here is 2 φ ν. This is not μ actually this becomes almost like a gamma. It is just not gamma and this is basically we have to write mu. $E1 = A1 \sin(2\pi\nu t - \varphi 1)$ and the second wave we can write it in this way $E2 = A2 \sin (2\pi\nu t - \varphi 2)$. So, these 2 waves has exactly the same frequency that means same frequency or for that matter, they have the same wavelength.s

Both of them have the same wavelength, these 2 waves and they have to have same wavelength because then only they will be able to they can be add up. These 2 waves, they can be added up. This but they differ in the amplitude and in their phases. One is having φ1, one is having φ2 and ultimately, if we add them up, we will get this third one, E3. Third wave E 3 which is again a sinusoidal wave.

But this time with a completely different amplitude and different phase in itself. This will be a resultant wave of out of these 2 wave, if you sum them up at any given position any given

point, if we sum them up, we will be getting this third one with its own phase and amplitude which is of course related to the phase and amplitude of this 2 waves that we define. So, we have to now, basically find out this third wave.

This E 3 that will be the resultant final diffracted intensity coming out of this unit cell, complete unit cell.

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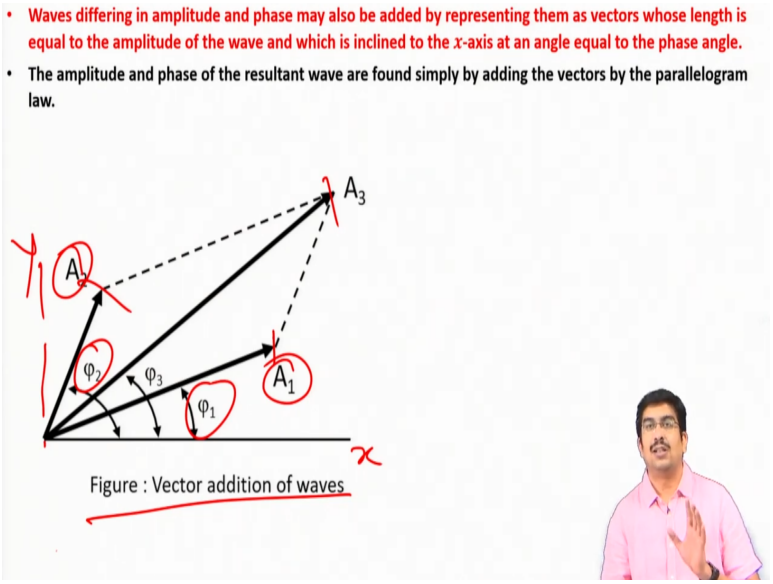

So, one way we can do that is basically by expressing these 2 waves as vectors. So, this vectors basically what we can do is that we express the vectors in the plane in this vector. This vector addition waves which is I think everyone knows the way we can express one of these waves, we can think about the length as their amplitude and the angle is related to the angle the mix with the x axis this here.

This is basically the angle is the phase angle here. This is your phase angle, this is another wave, this is the amplitude and this is the phase and then the third wave or the resultant wave is basically this with an angle phi 3 phase angle phi 3 and we can just find out this resultant wave from simply adding this to vectors by following the parallelogram law. So, this is one way we can very easily find out the resultant wave out of this.

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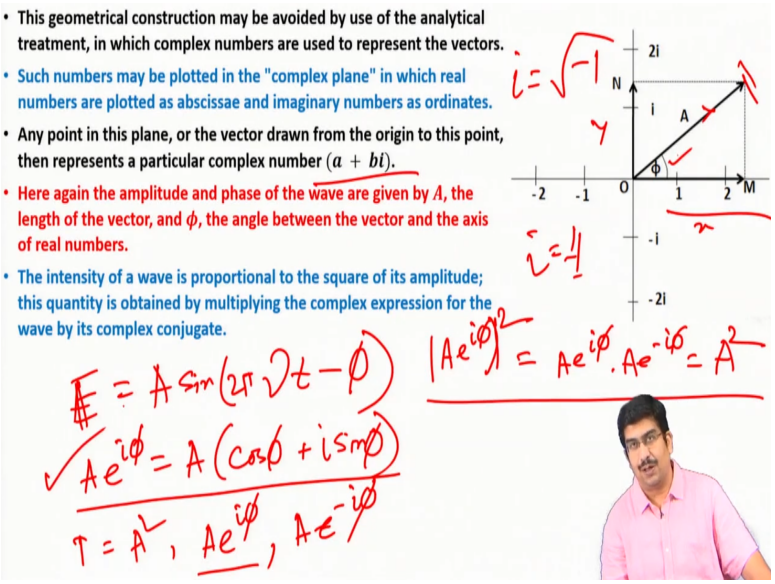

This is a little tricky to do it and we cannot find out the general expression so easily. So, we will do it we will solve this problem in some different way altogether. Basically, this geometrical construction, this vector construction, we can avoid it by some analytical treatment by using complex numbers. So, we can bring this complex geometry here, the complex numbers we can bring it here.

And then we can do this adding the same summation we can do it in a much simpler way. So, how we can do that? That is what we will be seeing now. So, complex numbers as we know that this numbers complex numbers are plotted in same way as the vectors we can plot them in this complex plane where again the amplitude is represented by the amplitude. So, amplitude is represented by this length of this and this is the given this and this angle that it makes with this real axis.

The real axis is this one this is the real axis here. And x axis is the real axis this one and this is the imaginary axis, this y axis is basically the imaginary axis. Complex numbers, you know, they are expressed by this way a + b i that is i is root over – 1. So, i is basically having a value of root over –1 which is the imaginary part of this entire expression so, in this complex plane, if we express any of these waves here.

Now, the amplitude is again just like vectors amplitude is represented by this length and this angle with upsizer this x axis, this angle is the phase axis that is it. So, here now, what we can

do is that this vector, we represent this one vector in this complex plane and then we can try to sum them up. And that we can do it in this way. Basically, here, we represent the waves in by this amplitude that same wave, if we imagine that E equals A into the way we have expressed them earlier.

E equals $\sin(2\pi\nu t - \varphi)$. This is the general expression that we earlier wrote for this complex this waves that is coming out from each of these planes or each of these setup atoms. So, we can represent them in this complex plane here itself. And similarly now, we can add them up using this complex number. So, what we can do here is that by each of these waves, we can express them in this way.

That is we can express them by a power series expansion, where we can write this as basically equals $A (\cos \varphi + i \sin \varphi)$. So, this is how we can express any of this waves, any wave in the complex plane, we can express them in this term. Here it has a power series expansion where we have this cost phi and sin phi basically $\cos \varphi$ and $\sin \varphi$, if this one is the wave in the complex plane then $\cos \varphi$ and $\sin \varphi$ are the 2 components along the x axis and y axis.

That is how we basically express them here in the complex plane. Any way we can express them here in the complex plane and simply we can the intensity of the of this waves, we know the intensity is basically its square of the amplitude. So, what we can get the intensity of any wave just by multiplying this wave this one, this wave by its complex conjugate.

So, what do you mean by complex conjugate? Basically, if any of this any wave is expressed by this then it is complex conjugate will be $A e^{(-i \varphi)}$. So, this is the complex conjugate of this wave and if I multiply this 2 that means, what I can do is that I can write $A e^{(i \varphi)}$ just the modulus of it means the absolute value of it, we can multiply it. We can imagine it in this way into $A e - (i \varphi)$ and this equals to A square.

Because i square we know i square equals 1 basically. This is i and if you square it, this will be –1 sorry this will be –1, i square will be –1. So, this basically finally comes out – i square which is again the 1. And finally, this is how we can get the intensity of this wave simply

from this by multiplying it with its complex conjugate. So, what we now basically the way this part.

The importance of this part is to make you understand that any wave in the complex plane same with this the waves that we were talking about in the earlier cases here. So, one wave coming out of this origin and one wave coming out of this arbitrarily defined plane anywhere from this plane. So, these 2 waves we can just represent them either as a vector here or we can represent them in this way as a sinusoidal waves.

And then find out the third one, we can represent them in a vector as a vector here and then we can find out this using the parallelogram law, we can find out the third one the resultant vector or the simplest way of doing it is by imagining them as a complex number in the complex plane and then try to see how they sum up.

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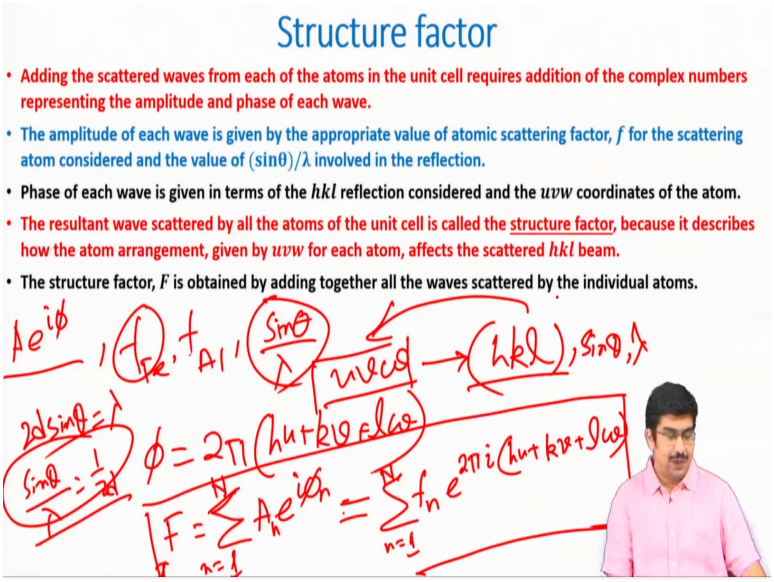

So that is exactly what we are trying to do here. So, when we do this addition, adding the scattered wave from each of the atoms in the unit cell, this when we do is basically requires the addition of this complex numbers representing this amplitude and phase of each of this waves that is what. So, one of these waves as we understand this waves are represented by this.

This expression for each of the wave and then one wave coming from the origin, one wave coming from any other atom any atom situating anywhere else and we just add them up. As, we said the amplitude and we have to just add their amplitude and phase. So, amplitude is given by the appropriate value of atomic scattering factor, we have already seen that atomic scattering factor, if we have 2 different one.

Then we can write 2 different atomic shattering factor, if we have one single type of element, we can write one single atomic scattering factor. And we have to find out the appropriate value of this atomic scattering factor considering the sin θ by λ. That means, if we know, understand this 2d sin θ = λ. That means, basically, so, what we can write here is sin theta by lambda is basically 1 by 2 d.

So, this we can find out exactly for which sin θ by λ this atomic scattering factor is valid. So, we have already seen the relationship from there we can calculate this atomic scattering factor of any particular sin θ by λ ∑means any condition particularly Bragg's condition where the diffraction condition is satisfied, for that what should be the atomic scattering factor.

So, these 2 we can find out for a single element the F will be the same and phase we have already seen that the phase difference is given by this expression 2 π (h u + k v + l w). So, this is the phase relationship between them. So, the resultant waves that is scattered out of this entire unit cell. This we can the final one we can write it in this way that is F which is the final resultant wave that is coming out the entire unit cell.

We can write down that as a summation of basically, if we imagine that there are n number of such atoms. If we imagine n number of such atoms we can calculate this n equals to 1 to capital N, ∑ A e^(i φ). So, this is individual or rather what we should write it here this we can write make it special and write it as A_n e i φ_n. So, this one is the general wave and we are just summing it over all the atoms present in that unit cell.

And that is giving me the final expression for ultimate expression for this diffracted beam coming out of this unit cell. So, this we can write it as again summation of n equals from 1, if it contains capital N number of atom then we can write it, if we imagine that it is one type of

element then we can write it as e into 2 phi and for phi we can write this expression is k v + l w. This is the final expression.

So, this expression is the final expression for the diffracted beam intensity coming out of the unit cell and this is called this is the resultant wave basically this is the result and wave from coming out of all the atoms in the unit cell. This one, this F is called the structure factor because it describes how the atomic arrangements which is given the atomic arrangement for in the unit cell which is given in terms of u v w.

How this atomic arrangement is basically affects the intensity of the scattered beam for a h k l diffraction. So, h k l diffraction is happening, diffraction is happening for h k l planes which is for have a fixed sinθ for a fixed λ. How this diffracted beam intensity is getting affected by the atomic position u v w? So that is given by this structure factors and we calculate the structure factor by adding up all the waves coming out from individual atoms in a unit cell. So, this is the final structure factor expression that can we can calculate.

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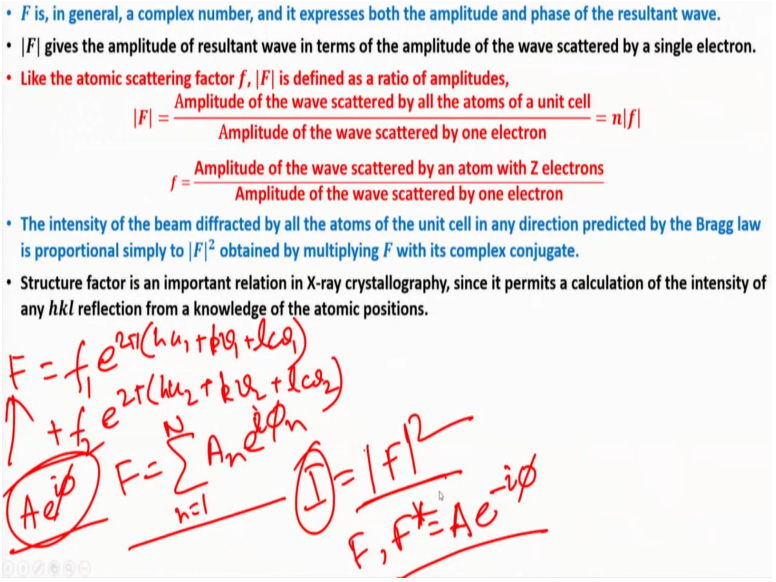

So, this is basically the structure factor is a complex number and it expresses both the amplitude and phase of the resultant wave. So, what we can write is that, if we have let us say 2 different types of atoms in the unit cell, we can write first one is having an amplitude that is atomic scattering factor f 1 and if it has the fraction of like u 1 v 1 w 1 then what we can write from this expression.

From this expression basically what we can write is e raised to the power 2π and we are satisfying something like h k l a diffraction is happening. So, h u 1 + k v 1 + l w 1 for the second atom we can write like this, if that has a fraction this fractional coordinates at u 2, v 2 and w 2 we can write this. So, by adding these 2 we will be getting the final structure factor.

So, structure factor in general it is a complex number just like any way can be expressed by this term. Structure factor also can be expressed by this one, we have already seen structure factor is basically expressed as a complex number which is a summation of this all n number of waves which are present from individual atoms which are coming with different amplitude and different phases.

So, structure factor can be expressed in terms of a complex number like this. And the mode that is the absolute value of the structure factor basically gives the amplitude of the waves scattered by this entire unit cell. So, this the mode of this that means, this structure factor we can go back to the laser point again. So, the structure factor is given like, just like the atomic scattering factor, structure factor can also be given or can be defined as the ratio of the amplitudes and structure factor.

The way we define it is basically the waves scattered by all the atoms in a unit cell divided by the amplitude of the wave scattered by one single electron. So, in that respect structure factor is basically n times the absolute value of atomic scattering factor. Atomic scattering factor you know the way we define it is basically the amplitude of the wave scattered by one single atom divided by the amplitude of the wave scattered by one single electron.

Whereas structure factor is the amplitude of the wave scattered by all the atoms, if the unit cell contents n number of atoms. So, simply we multiply the atomic searching factor by n and we get the absolute value of structure factor provided the unit cell containing only one type of atom. So, this is how the structure factor and atomic factor basically are related and this is how we can also define the structure factor or the amplitude.

The absolute not basically the structure factor but the absolute value of structure factor we can because here this is the amplitude of this complex this wave of that is defining the structure factor. The amplitude of the wave coming out of the unit cell that amplitude we can define that amplitude in terms of amplitude of waves scattered by one single electron.

And the intensity of the beam diffracted by all the atoms is predicted by Bragg's Law. And the intensity is simply proportional to F square which is the intensity that as I said that can go back to the pen. So, the final intensity is simply the square of the modulus of this amplitude of the beam. Amplitude is basically this as we just now, discuss the amplitude is given by mod F and mod F square this is what the amplitude.

And this mod of F square we get by multiplying again F with its complex conjugate which is represented like this and which we can say is again it is expressed as – i φ. So, if we multiply F with its complex conjugate, what we get is this intensity of the diffracted beam coming out of the entire unit cell. So, the structure factor the dependence or the importance of the structure factor is calculation is that.

This is a very important relation and it permits a calculation of the intensity, final intensity of the diffracted beam coming out of a unit cell of any shape, unit cell of any kind, any kind of crystal system. The intensity of the diffracted beam for a particular h k l deflection means for a particular h k l set a plane, if they are satisfying the diffraction condition, what will be the intensity of the final diffracted beam irrespective of any kind of crystal system?

We can calculate simply by calculating its structure factor. So, this is what is the importance substructure factor and this is where we will stop for this and we will continue with structure factor calculation for some specific crystal systems in the next class. Thank you.