Techniques of Materials Characterization
Prof. Shibayan Roy
Materials Science Center
Indian Institute of Technology, Kharagpur

Lecture - 49
Intensity of Diffracted Beam (Continued)

Welcome everyone to the NPTEL online certification course on techniques of materials characterization, we are in module 10. That is, we are discussing X-ray diffraction and this is lecture four. We are continuing with the discussion about the intensity of the diffracted beam. And until up to now, we have seen in this module how X-ray absorption happens, what governs X-ray absorption and then we discussed X-ray filters as well.

And we then discussed the necessity of calculating this intensity of diffracted beam because we have found out that satisfying Bragg's law is not the only condition. So, it is a necessary condition of course, if the Bragg's law is not satisfied, then definitely diffraction will not happen. But that does not guarantee, we will get an intensity of this diffracted beam because that is somehow related to the position of the atom or rather the atomic arrangement within any crystalline material.

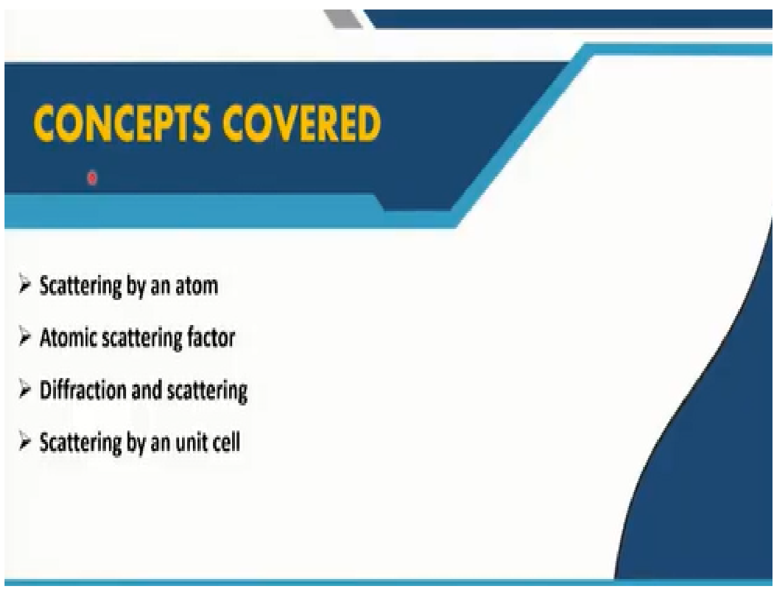
And from there, we started our calculations we understood that in order to calculate the final intensity of the diffracted beam. We should start from something like intensity from one single electron and then we have to take it all the way to one single atom and finally, all the atoms which are contained within a unit cell. So, that is what we understood and in the last class, we started discussing this.

When an x-ray beam interacts with an electron, what happens and what kind of an intensity we get out of it? So, we have seen that there are two different possibilities. One is a Thomson's effect, where it is kind of an elastic interaction and here this incoming x-ray wave is basically cause these electrons charged particles to oscillate and, in that process, continuous acceleration deceleration process.

It generates another kind of X-ray which is having same frequency and wavelength as the incident x-ray. So, it is a kind of coherent radiation is produced in the form of an X-ray, so that is a one kind of scattering of X-ray. And we have also seen another effect that is a Crompton effect, where we saw that it is when an X-ray beam hits the electrons. Then some amount of energy is transferred as a kinetic energy to this electron, which is called Crompton recoil electrons.

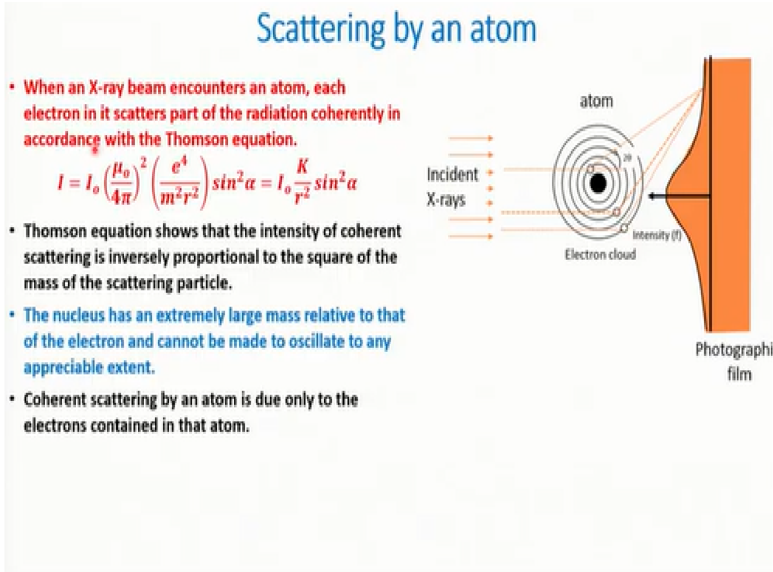
And some part of the energy will be then lost and that scattered beam will be deviated from its original path and that scattered beam will have a lower energy and correspondingly higher wavelength from the incident X-ray. So, these two types of phenomena are possible whenever an X-ray beam is interacting with electrons.

(Refer Slide Time: 03:15)



So, with that, we will be now discussing the scattering of an atom and then we will discuss the atomic scattering factor, what is the importance of this, in calculating the final intensity of diffracted beam. We will try to see a little bit relationship between diffraction and scattering and if time permits, we will also try to start our discussion about scattering by unit cells which we will continue in the next class as well.

(Refer Slide Time: 03:42)



So, let us start with this scattering by one single atom. So, what we just discussed, what we understood that whenever an incident x-ray falls on a material and that material contains various type of atoms, lots of different electrons. It has a positively charged nucleus in the middle and the electrons there are not one single electron but there are lots of electrons, various electrons are there.

And these electrons of course, each of these electrons will be interacting with this incident x-ray by either Thomson scattering or by Crompton scattering. So, these two phenomena is possible and Thomson scattering we already understood the Thomson scattering is governed by this Thomson equation and here in this equation, we can find out the intensity of the scattered x-ray beam in terms of the intensity of the incident X-ray beam plus some other factors like the scattering angle.

As well as the dielectric constant of the medium and then mass of this charged particle and the charge of discharge particle; all of these things. And we also discussed in the last class, if you remember, that for diffraction purpose only the Thomson scattering is important to consider not the Crompton scattering because Crompton scattering there is a kind of a random process and in that random process, the change in wavelength of the scattered beam is not a fixed.

It does not have a definite relationship with the incident x-ray beam. So, that is why this Crompton scattered x-rays will have a range of wavelengths and that is why this cannot be considered for a diffraction purpose because diffraction is very much needed for constructive interference. After the x-ray beams are generated from various electrons, various atoms and all you need to have a constructive interference.

That means, the waves which are generated out of this interaction, the waves should have a phase relationship between them a lot, should have a definite relationship with the incident beam and in the process, they will have a definite relationship between themselves as well. So, this does not happen for Crompton scattering and that is why we cannot consider the Crompton scattered or Crompton modified external radiation or diffraction purposes.

So, diffraction for now onwards in the diffraction purpose in this entire discussion from here onwards, when we calculate the scattering of an atom and then we take it all the way to a unit cell, all we will be considering is basically Thomson scattering, no Crompton scattering. But definitely we will come back to Crompton scattering because I told the Crompton scattering is important because it is basically forming the background in the X-ray diffraction profile.

Finally, what you get, it causes the background. So, that is also important to consider, we will come to that anyway. So, one question at this point came up and many, many times my students asked me and that may arise to you as well. That why we are considering only the electrons in this process; an atom consists of a nucleus as well which is again a charged particle. So, the way electrons act as a source of another electromagnetic wave generation.

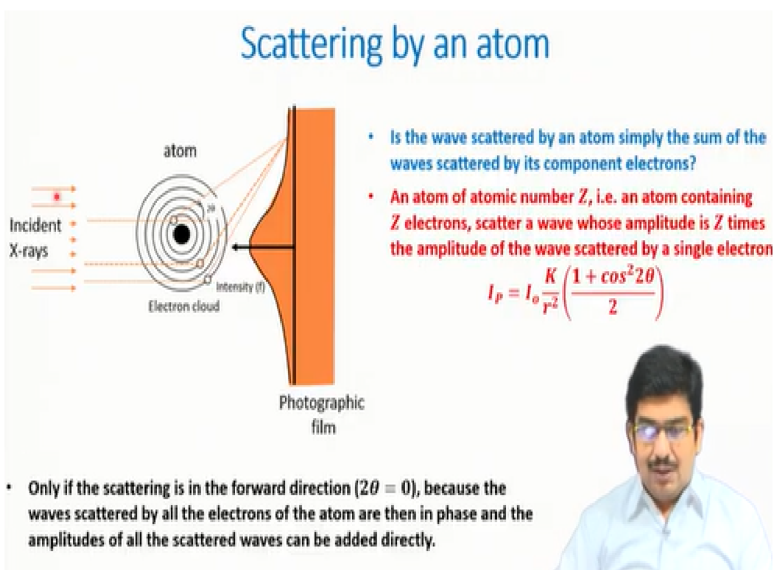
The nucleus can do the same thing, they are also positively charged and they are set in an oscillatory motion, they can also produce another set of electromagnetic waves true. Point is the nucleus is heavily charged and also its mass is much higher than the electrons. So, that is why the incident extra photon, it is not possible for them. They are not energetic enough to cause or to put the positive for most of the materials.

For most of the metals except for very small very light elements I would say, except for them for most of the general type of materials that we put for X-ray diffraction for them the charge, the positively charged nucleus is heavy enough and that is why they cannot be put into oscillating motion, so easily by the incident X-ray. So, we can safely neglect the interaction between a nucleus and the incident X-ray and then the resulting effect on the diffraction.

So, we can safely neglect this and that we can also check from this equation, Thomson equation because here if you look at here. This intensity of this electromagnetic wave or the X-ray that is scattered, that intensity of that X-ray beam is inversely related to the mass of this charged particle which is acting as a source of this electromagnetic wave. So, the nucleus is heavy and that is why the wave even if we consider that it generates some wave, the intensity of the wave will be very, very small.

So, we can safely neglect that. So, that is why the nucleus does not come into play and all we will be considering here Thomson scattering, coherent Thomson scattering from an atom is only due to the electrons contained in the atom. So, we just need to consider the Thomson scattering from electrons in order to calculate the final scattered intensity from one complete atom.

(Refer Slide Time: 08:51)



That is the first condition or not. Now, the question comes already. We said that there are many electrons here within the atom within one single atom here you can see there are three electrons I have seen. But we know that many electrons are there and the number of electrons is, of course, related to the atomic numbers Z. So, now if we; want to calculate the total intensity of this entire atom.

The question is should we measure that intensity, wave that is coming out of the incident X-ray interacting with all the electrons and finally, the scattered wave that is coming out of this atomic cell. That intensity of that wave is it simply the sum of the waves scattered by all the electrons that it contains or we can put it another way, if an atom contains an atomic number is Z and that means the atom contains Z number of electrons.

Then the scattered wave from this entire atom is the amplitude of the scattered wave; it is simply Z times the amplitude of the wave scattered by a single electron. And that means, we have already seen that this is the intensity from a single electron measured at a point P which is at a distance of r. So, this is the intensity of that Thomson scattering and expressed in terms of again at the angle, this scattered beam and the incident beam is making and of course, with respect to distance.

So, is it simply Z time multiplied by this I P is that the total intensity of the scattered X-ray beam coming out of an atom? That is a question. Point is, if you put up a photographic plane here, what you will see is that depending on the direction? So, if you put a two dimensional photographic film here and you will see that only in the forward direction the intensity is highest and then in any other direction the intensity goes down.

So, that means, this intensity that we have collected here definitely has a relationship with the angle that the scattered beam makes with the incident X-ray which is this relationship is anyway there definitely, this also says the same thing. But the intensity will be highest if we are checking only in the forward direction. We have discussed that I P the intensity coming out of, Thompson's intensity coming out of an electron will be the highest.

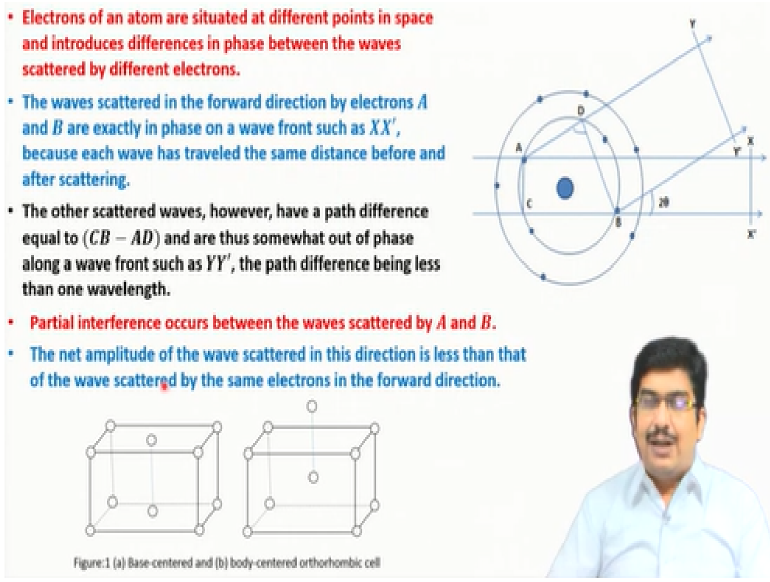
That intensity will be highest if we are in the forward direction. In any other direction this entire term will be less than unity and correspondingly I P will also be lesser than the forward direction or extreme backward direction. These two are the directions where the intensity will be highest. Point is this is valid that we can simply calculate the intensity of the X-ray beam coming out of the atom is Z times I P.

This is only valid in the forward direction where all the atoms or all the waves coming out of the Thomson's scattered waves coming out of each of these electrons all of them will be in phase. So, when we sum up the waves coming out from the electrons, we cannot simply add up their amplitude, because this is a wave and they have a phase as well. So, we have to take care of that phase relationship between various electrons.

Only in the forward direction simply we can call that it is an amplitude, we can just sum up their amplitudes and we can just because here only in the forward direction all of them will be having the same face. All of these electrons through waves coming out of this electron wave coming out of this electron wave coming out of this electron all of them will have intensity simply expressed in terms of their amplitude phase will not be important there.

This will be the phase relationship; this term will come as one, simple unit. So, because all of these beams are in the forward direction, they are all in phase, only in the forward direction we can simply add their amplitude and that will be giving finally their intensity only in the forward direction.

(Refer Slide Time: 13:21)



What happens of other direction? That is what we have to define or we have to derive or rather what happens in any arbitrary direction? Other than this forward direction in any arbitrary direction if we want to calculate or if you want to know the intensity of the diffracted beam what will be the relationship, that is the point. Now, of course electrons of an atom are situated at different points in space, here like this fine.

So, we are considering this atom and this atom has this nucleus and it also has electrons, many numbers of electrons in different places. We just put 4 4 4, schematic purpose just to understand this, we have put them in different places. Now, we imagine and all of these electrons just now, we understand that all of these electrons will have differences in phases, only in the forward direction, all of them will have the same phase.

Any other direction they will have a phase relationship and this we can check it also. Let us imagine that we are considering two electrons, one is A and one is B here and if we check the intensity, this A is producing one wave, so this incident x-ray beam is causing one type of wave scattered wave and this B when it interacts with B it generates another x-ray beam another scattered beam. So, if we consider in the forward direction, if we take measure the intensity here.

That means, if we just sum up these two waves. Basically, they will be on the same face because they travel, these waves now travel the same distance, before and after the scattering. So, if we check this, if you take it from the source let us imagine that this is a source. So, these waves basically have travelled the same distance, the entire distance whether before and after. So, this wave in here has travelled less before scattering and more after scattering.

This one here more before scattering less after scattering but overall, the entire distance is the same in the forward direction. So, that is why they are in phase. We know that phase relation, phase related to the path difference basically. So, here that there is no path difference and the phase is the same, we will be getting intensity if we add them up, they will simply be added because their amplitudes will be simply added, that is it.

Now, if we imagine other than this forward direction, if we imagine any other scattered beam in the same direction, let us imagine. So, let us think that from electron A, I am getting another scattered electron beam instead of forward scattering, I am getting a scattered beam which is going in this direction and making an angle 2 theta with the incident beam here. This angle; let us imagine that this is 2 theta.

And from atom B also there is another scattered beam that is generated and making the same angle 2 theta. So, finally, we are trying to calculate the intensity of this scattered beam from this entire atom in this plane in this direction Y, Y dash meaning, on this plane in this direction, I am trying to add up these two waves here. I am trying to find, this is completely arbitrary, because 2 theta can be any value.

So, I have to find an expression for this in any arbitrary direction and as we already immediately understand that this path difference is now not the same for the atom which is or for the wave which is scattered from point electron A and the atom which is scattered from point or electron B. This two has completely different path, they have travelled different distance before and after the scattering.

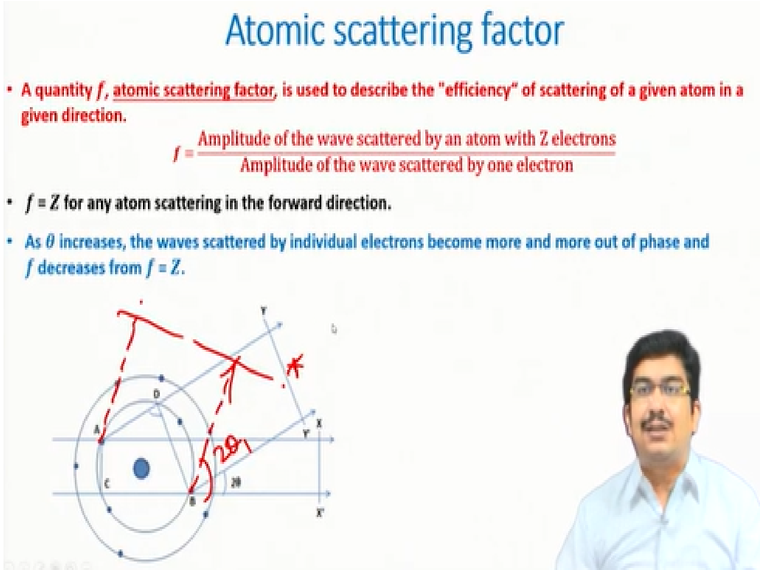
That is why they will be having a path difference between them which will translate into their phase difference and we will have something like a partial interference, it will not have a complete interference or complete constructive interference if you put it in this way. We will have a partial interference there and that will modify the resultant wave that we will be getting somewhere over here will have its amplitude and intensity modified.

That will not be a direct summation of these two, so the net amplitude in this direction will be less than that of the wave scattered by the same electrons in the forward direction. So, here, if we calculate the intensity in any other direction other than forward direction, it will have comparatively lesser intensity, and that is what we have shown here that only in the forward direction and that is now this is not only because of this.

This is because of now electrons or waves coming out from two different electrons all together. So, in the forward direction only we will get maximum intensity and the more we are going further away from this forward direction meaning, the 2 theta as the 2 theta is increasing, we will be getting a lesser and lesser intensity. And that is how the entire relationship of this diffracted beam intensity or x-ray, we are now not in diffraction we can call that this is a scattering.

So, the intensity of the scattered beam from one single atom, this is how it is related to the intensity of scattered beams from different electrons that it contains. So, this is how it varies depending on which direction I am looking at or what is the relationship or difference phase relationship between the scattered beams from various electrons.

(Refer Slide Time: 18:54)



So, the best way we can understand this summation or best way we can calculate the intensity of the scattered beam coming out of one single atom here. Let us say in any arbitrary direction, the best way to express this one is by a term called atomic scattering factor. So, the atomic scattering factor simply expresses the efficiency of scattering of a given atom at a given direction. So, in any given direction anywhere here or even including the forward direction.

Any direction what is the efficiency or what is the scattered beam intensity how the scattered beam intensity is related to the scattered beam intensity from single electrons individual electrons. The entire the intensity of the scattered beam from the overall atom, how it is related to the intensity of the scattered beam from individual electrons that it consists that is in any given direction. So, that is expressed by this atomic scattering factor.

And the way we can put this atomic scattering factor is simply an ratio of amplitude of the wave scattered by an atom with Z electrons that means the atomic number is Z and divided by the amplitude of the wave scattered by one single electron. So, one single electron whatever the amplitude of the wave and that is it divides to the amplitude of the wave scattered by the entire atom. That is the atomic scattering factor.

So, of course, in this relationship, we are taking the direction as well, how? Now, the point is how we are taking the direction; it is simply taking the ratio of this amplitude. So, how the direction thing comes out here, basically, if you now consider as we already said that, if you are considering the forward direction only the forward scattering direction. There has this amplitude and we said that simply you have to multiply.

You have to just sum up all the waves their amplitude summed up because they have no phase difference among them. So, there what will happen the atomic scattering factor will be simply atomic number, $f = Z$ for any along the forward direction, for any atom scattering along the forward direction. So, if we consider the intensity, if we measured the intensity here, so this intensity will simply be some of the amplitude of the atomic number of it.

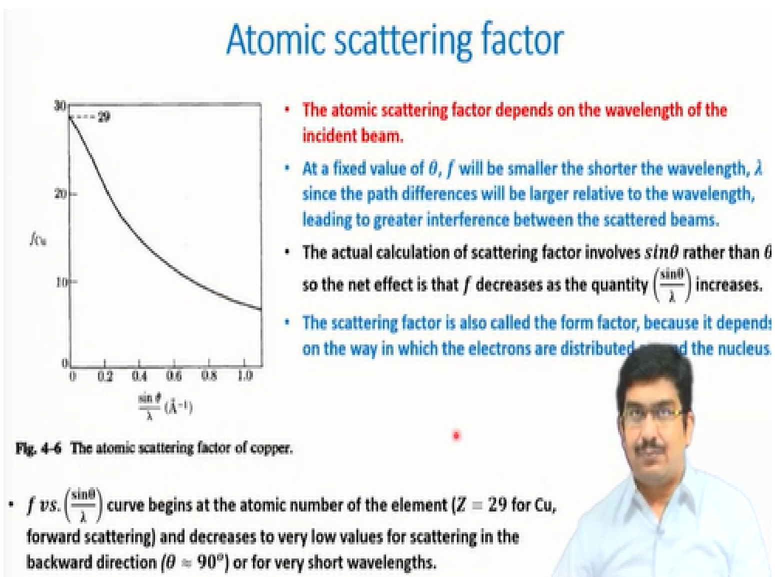
So, that means, if we measure it here, so in the forward direction exactly in the forward direction this intensity will be some multiplied it will relate it to the proportional to the atomic number of that element. Simply atomic number, nothing else will come, no phase nothing, no other expression will come. Now, as the theta increases, we already saw that as theta increases here the angle 2 theta, basically these 2 thetas the angle that scattered beam makes with the incident beam as this angle increases.

Then the wave scattered by individual electrons will be more and more out of phase. So, if you increase this angle, if this angle increases, electrons will be going more and more out of phase. So, if this angle increases, if we consider another ray which is something like this direction, which is possible if I can draw this here, if I consider this may change it to a pen. So, if we consider let us say another direction here something like this direction, where I have this angle to be some other 2 theta 1.

Then what we can get is that basically what we are getting here is, if this 2 theta is increasing to this direction, if we are taking and then some other direction. So, here the two theta is increasing and then we will be having f more of these beams here, if we measure it here somewhere over here, they will be more and more out of phase compared to something like here. So, that means the atomic scattering factor will decrease.

As the theta will increase from the forward direction, as the theta will increase the atomic scattering factor will also be increasing the atomic scattering factor will basically decrease from the f = Z, that is the forward direction. So, if we are moving to any other direction from the forward direction continuously, the atomic scattering factor f will decrease from a value f = Z, simply like this.

(Refer Slide Time: 23:36)



So, atomic scattering factor the first thing it depends on is basically the angle that the incident ray makes with the scattered beam makes with the incident and that is precisely because you can prove this geometrically as well, why this will go more and more out of phase? Because as it is moving in this direction and this path difference will be sort of the lambda, the wavelength of this lambda will be path difference will be larger relative to the wavelength.

So, that is the only point which will happen and therefore, the theta will be reduced. So, this we can also see from another perspective as well. So, the atomic scattering factor will also depend on the wavelength of the X-ray beam. So, number one it will depend on the angle 2 theta that this incident beam and scattered beam is making with the incident beam. That is the first thing atomic scattering factor depends on.

The second thing it depends on is the wavelength of the incident beam. So, for a fixed value of theta, if we imagine that we are still considering this direction, if the wavelength decreases, so if the wavelength decreases, then what will happen is this path difference will be larger compared to the wavelength. So, the wavelength is much less here, theta remains the same. So, we are talking again, we are calculating, we are summing these two waves in this direction.

Theta remains the same, if the wavelength is reducing then the path difference will be larger compared to the wavelength itself. And that means, the two waves which are generated from these two points will be now, more and more out of phase from there. So, path difference depends on the wavelength that we have seen, please recall if you are not able to understand yet, please recall. The way we have geometrically we derive Bragg's Law.

The similar type of derivations now, we can do and we can find out that the path difference, if the lambda decreases, we will have path difference more and more out of phase. So, the path difference will not be an integral multiple, the chances of path difference to be an integral multiple of lambda will be lesser if the lambda goes down. And the same thing the path difference will be an integral multiple of lambda this possibility will go down if we increase the theta.

And geometrically can be proved I am not going here, if you like you can try this. But what we are saying here is now, is that for both this atomic scattering factor will depend on the theta as well as on lambda and actually this atomic scattering factor will involve not the theta, actually depends on sin theta. So, ultimately the atomic scattering factor will decrease as sin theta by lambda. So, it is inversely proportional to the lambda.

And it is directly proportional to the sine theta, as the lambda decreases f increases, I mean, the smaller the shorter the wavelength the greater the interference, so this lambda f will be smaller. So, f will decrease as lambda is becoming smaller and smaller and it will also depend on the sin theta, sin theta increases lambda f will also decrease. So, basically ultimately f will decrease as the quantity sin theta by lambda increases this one.

So, these two, this is the final relationship that we can get about atomic scattering factor. If f is inversely related to lambda and f is directly related to sin theta. So, finally this is the relationship, I said in the other way around basically if f is inversely related to sin theta and directly related to the lambda. If lambda decreases f will decrease, if sin theta increases f will decrease. So, ultimately this entire term is sine theta by lambda if this time increases then overall f will decrease.

And remember one thing if this sin theta and lambda cannot be varied independently, sin theta and lambda vary together from Bragg's Law. So, if you vary the lambda sin theta will automatically vary, if you vary the sin theta lambda will automatically vary. So, that is why this entire term sin theta by lambda is considered as one single entity. And we plot, what we plot here is basically the variation in atomic scattering factor with respect to the term sin theta by lambda.

Which is expressed normally in angstrom inverts; so, distance inverse unit. So, what we now see is the atomic scattering factor here, so as an atomic scattering factor, one important term is that the atomic scattering factor is also called the form factor sometimes. Because it depends on the way in which the electrons are distributed around the nuclear. So, the atomic scattering factor also depends on where exactly these electrons are, from which electron.

So, the position of the electrons is also important in determining the f value, amplitude value, but we are not considering it here we are not going into that anyway. So, now, if we see this variation of atomic scattering factor with respect to the sin theta by lambda this term, obviously in the forward direction when they are at 0, so 0 means sine theta is basically 0. So, that is the forward direction, so in the forward direction here the atomic scattering factor is equal to Z.

And this is we are seeing it for copper is Z = 29, that is that is for copper. So, in the forward direction when scientists equals 0, we are seeing that the atomic scattering factor is equal to the atomic number and then as this term increases sin theta by lambda as we are going away, both sine theta is increasing and lambda is decreasing. So, as we are going away from the forward direction, as well as the wavelength of the incident X-ray is decreasing.

The atomic scattering factor is continuously decreases and finally, it decreases to a very low value in the backward direction, that is when 2 theta = 180 degree, that means theta = 90 degree. In that case when 2 theta = 180 degrees, again this is sin theta equals this lambda value. Now the theta = 90 degrees, so sin theta is 1, they are also this value is very, very less or otherwise very short wavelength that will also make this atomic scattering factor to be of very small value.

So, this atomic scattering factor, the importance of this graph is this is basically telling you if you just consider one single atom. How the intensity of that X-ray beam scattered from one single atom, how it is varying with the angle that this scattered beam is making the incident beam and the X-ray intensity. How the intensity of the scattered X-ray beam is varying in case of a single atom. So, that is what is shown by this graph here. That is the importance of this graph.

So, we will stop here, and we will continue with a few of the other issues in the next lesson. Thank you.