

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

Lecture - 50
Intensity of Diffracted Beam (Continued)

Welcome everyone to this NPTEL online certification course on techniques of materials characterization. We are in module 10 discussing about X-ray diffraction and this is lecture 5 and we will continue with the discussion about intensity of diffracted beam. So, we have until of now we have seen that how an X-ray beam interacts with an electron in an atom and how it produces the coherence scattering in form of by Thomson's effect and then a modified incoherent scattering in form of Compton scattering.

So, these are the two types of extra scattering that can happen from an individual electron within an atom. And then in the last class we were discussing about how these electrons how these scattered beams from the electrons can be added up. So, that we can finally get an expression for the intensity scattered extreme intensity for an entire atom. So, that is what we were discussing. And there we finally derived this atomic scattering factor which basically expresses the relationship between the waves scattered from individual electron;

With the final wave that is coming out of an atom which is a summation of all these waves scattered by individual electrons. And that we have derived we have seen that the atomic scattering factor depends on the direction at which this scattered beam we are adding them up. So, it depends on the phase relationship between the electrons this waves coming out of individual electron.

It depends on the phase relationship between them and depending on that in finally the direction of the scattered beam we get an expression for this calculating the entire intensity or amplitude. We calculate in terms of amplitude and then amplitude we can simply get the final intensity from

this amplitude itself. So, there we will continue that discussion today a little bit of atomic scattering factor and then we will try to derive a relationship between diffraction and scattering.

(Refer Slide Time: 02:23)

CONCEPTS COVERED

- Atomic scattering factor
- Diffraction and scattering
- Scattering by an atom

NPTEL

What now what so special about diffraction and finally we will then start with our discussion about scattering from an entire unit cell sorry, this this should be scattering from an entire unit cell.

(Refer Slide Time: 02:37)

Atomic scattering factor

$\frac{\sin \theta}{\lambda} (\text{\AA}^{-1})$	f_{Cu}
0.0	29
0.2	22
0.4	16
0.6	12
0.8	9
1.0	7

- The atomic scattering factor depends on the wavelength of the incident beam.
- At a fixed value of θ , f will be smaller the shorter the wavelength, λ since the path differences will be larger relative to the wavelength, leading to greater interference between the scattered beams.
- The actual calculation of scattering factor involves $\sin \theta$ rather than θ , so the net effect is that f decreases as the quantity $\left(\frac{\sin \theta}{\lambda}\right)$ increases.
- The scattering factor is also called the form factor, because it depends on the way in which the electrons are distributed around the nucleus.

Fig. 4-6 The atomic scattering factor of copper.

- f vs. $\left(\frac{\sin \theta}{\lambda}\right)$ curve begins at the atomic number of the element ($Z = 29$ for Cu, forward scattering) and decreases to very low values for scattering in the backward direction ($\theta \approx 90^\circ$) or for very short wavelengths.

So, atomic scattering factors the first thing again we discussed the same thing earlier also that atomic scattering factor f depends on the two things, sine theta that is the angle between incident X-ray and the scattered X-ray beam. So, it depends on that angle so as the angle increases the atomic scattering factor decreases that is one thing. And second thing it also depends on the lambda value that wavelength of the incident X-ray as the wavelength goes down then the f also is decreases.

So, these two values together these two terms together sine theta by lambda this dictates the atomic scattering factor. And atomic scattering factor is highest in the forward direction where sine theta is basically 0 and then again it decreases afterwards continuously as the sine theta is increases and lambda also together it decreases continuously. And in the backward direction where again theta equals 90 degree;

There also the atomic scattering factor is very low and it will be also very low for very short wavelength. So, this is the kind of relationship that atomic scattering factor shows with sine theta and lambda. This we saw in the last class.

(Refer Slide Time: 03:47)

- The scattering factor is applicable only to coherent, or unmodified scattering (Thomson scattering), which is the only kind capable of being diffracted.
- Incoherent or Compton modified scattering for an atom: Intensity relative to that of the unmodified/incident X-ray radiation increases as the proportion of loosely bound electrons increases.
- It thus increases as the atomic number Z decreases.
- It is difficult to obtain good diffraction photographs of organic materials, which contain light elements such as Carbon, Oxygen, and Hydrogen, since the strong Compton modified scattering darkens the background.
- Intensity of the Compton modified radiation increases as the quantity $\left(\frac{\sin\theta}{\lambda}\right)$ increases.
- The intensities of Thomson (unmodified) and Compton (modified) scattering vary in opposite ways with Z and $\left(\frac{\sin\theta}{\lambda}\right)$.
- Scattering factors apply only when the scattered radiation has a wavelength much shorter than that of an absorption edge of the scattering atom.

$\frac{\sin\theta}{\lambda}$	$f_{Fe^{2+}}$	f_O	f_C	f_H
0.0	25	8	5	1
0.2	20	6	4	0.8
0.4	15	4	3	0.6
0.6	10	3	2	0.5
0.8	7	2	1.5	0.4

Now the point is we have also discussed about this the scattering factor is only applicable to the coherent part of it, the coherently scattered beam that means the Thompson scattering which is only able to take part in the diffraction. We have discussed this many a times content scattering inherent or prompted modified scattering cannot take part in the diffraction process.

Because the intensity of this unmodified intensity of this Crompton scattering beam is very much random. So, it has a very random relationship its kind of an incoherent scattering and in that process the beam that is generated out of Crompton scattering process that beam does not have a definite phase relationship with the incident X-ray beam. But of course, the way the Crompton scattering generates from there we can try to bring a relationship between the Crompton scattering the atoms.

The finally the Crompton intensity of the wave X-ray wave coming out of the quantum scattering due to the quantum scattering between incident X-ray and the electrons. So, we can try to find out an expression for that also. Because as you remember I said the Crompton scattering is important because it forms the background in the diffraction process. So, when you finally basically what happens when you when you capture the intensity in a detector in an x-ray detector you capture the intensity that will capture not only the diffracted beam;

It will also capture the beam coming out of the Crompton scattering which will form the background. So, it is important to know exactly how much Crompton scattering you are going to get out of this individual atoms. So, this intensity of the Crompton scattering for an individual from one single atom, the intensity of this modified quantum scattering that is coming out of an atom this will be related to the number of vacant number of outer shell electron, a number of loosely bound electrons which are present in individual atom.

That mean because that is how the Crompton scattering is generated. Basically, in Crompton scattering what happens the incident X-ray beam comes and a loosely bound electron that is usually the outer shell electrons or valence electrons those electrons it can hit and that electron

then gets some momentum some kinetic energy and that just goes out of the atom. So, in the entire process basically it is a interaction between the incident x-ray and the loosely bound electrons.

So, if the; number of loosely bound electron or the proportion of loosely bound electron within an atom. If that increases then the modified intensity of the Compton scattering intensity of the Compton modified radiation that also will increase. So, that means the relationship between the atomic number and the Compton modified scattering is that there is not an exact relationship that exists or that relationship is a very difficult one, we are not going into this.

But basically, the intensity of the Compton scattering will increase as the atomic number decreases. Because if the atomic number decreases what happens is that higher the atomic number then higher will be the number of electrons in the outer shell as well the positively charged nucleus will not be able to bind those outer cell electrons with a strong force. If it is light element low atomic number element;

Then electrons are far more closer to the positively charged nucleus and then this energy with which or the binding force with which the positively charged nucleus is attracting this outer shell or this electrons will be much higher. So, Compton scattering basically as the number of atomic number increases, the number of electrons that increases as we are. If the atomic number is increases then the number of sorry, I am possibly telling in the other way around.

If the atomic number that increases the Compton modified the intensity of the Compton modified radiation that increases as the atomic number decreases. Because if the atomic number decreases that then this there will be more number of loosely bound electrons will be present there. When we go for a higher number higher atomic number element then the positively charged nucleus will have more energy much more positive charge will be there in the nucleus.

And then that will be able to bind all the electrons with a much stronger force. If the atomic number decreases then there will be less charge in the nucleus and this small amount of charge will not be enough to bind all the electrons which are present in the outer shell. So, those loosely bound electrons will number of loosely bound electrons proportion of loosely bound electron I should not say exactly, the number of loosely bound electron.

The proportion relative proportion of loosely bound electrons will increase as the atomic number decreases that means the relative intensity of the Compton modified material or competent modified scattering will also increases as the atomic number decreases. Basically, one thing you must understand here the inertial electrons which are tightly bound. So, inertial electrons are responsible for Thomson scattering.

Because if the inertial electrons are hit by the incident x-ray photon they will be since they are tightly bound by the nucleus, they will not be able to go out of this atom. They will be there and they will be oscillating about their mean position. But if the incident x-ray beam is hitting an outer shell electron that will have less amount of or that will be loosely bound with this nucleus. Because this is in the outer shell so those electrons will be able to produce a Compton radiation or Compton modified radiation scattering X-ray scattering so that is the relationship.

So, basically if the atomic number decreases this relative proportion of in shell electron and outer shell electron this will increase. So, proportion of outer shell electrons will increase if the atomic number decreases. So, the relative intensity between the Thomson scattered X-ray beam and Compton scatter x beam this will change. So, this relatively compared to the Thomson scattered, coherent scattering, incoherent scattering prompt and modified X-ray intensity that will increase for lighter elements with lower atomic number.

And this is why for low atomic number materials like for example carbon, oxygen, hydrogen for low atomic number elements it is producing more amount of Compton scattering rather than producing coherent Thomson scattering. That is why diffraction getting a diffraction pattern from

this low atomic number elements like carbon, oxygen, nitrogen basically for organic materials. If you consider the organic materials; containing mostly carbohydrate, carbon, oxygen and hydrogen.

So, this meant for these materials the Compton scattering will be much more prominent than the Thomson scattering. And that is why compared to the diffraction peaks, the background intensity will be too high. And that is what is one of the major problems of capturing a good diffraction pattern for an organic material or low atom consisting of low atomic element; low atomic number elements.

So, that is why for organic materials X-ray diffraction for polymeric materials, for organic materials X-ray diffraction is not the good process to identify their structure. For them you have to take special care in order to reduce this background in order to reduce this Compton scattering phenomena anyway. So, this intensity of the Compton scattering also increases with sine theta by lambda quantity.

So, this is exactly in the other way round as the Thomson scattering. For Thomson scattering we have seen Thomson scattering means basically atomic scattering number. So, atomic scattering number decreases as sine theta by lambda increases. So, that is the relationship between sine theta by lambda and atomic scattering factor when we consider only Thomson scattering. But when we consider something like Compton scattering, the Compton scattering has a direct relationship with sine theta by lambda.

As sine theta by lambda increases quantum scattering also increases. How it is happening we are not going into that basically wavelength of basically it means if the wavelength of the electrons is decreasing that means the electrons are now coming with a higher energy, a shorter wavelength that can able to that higher energy with for the shorter wavelength it will have a higher energy.

So, after but it will be able to transfer more amount of kinetic energy and the scattered beams. Now we have much the intensity of the scattered beam will be much more. Basically, that is what. So, if the wavelength of the incident electron decreases if we use a shorter wavelength the incident the intensity of the Compton scattering will also increases. That is that is the relationship that is why $\sin \theta$ by λ this relationship if $\sin \theta$ by λ increases the quantum scattering also increases.

And if we take if we now see that this atomic scattering factor for if we compare two elements higher atomic number elements like iron versus lower atomic number elements like hydrogen, carbon or oxygen if we see them then we will see that this for the higher atomic number elements the atomic scattering factor. Finally, the intensity, atomic scattering factor is simply the amplitude of the waves coming out or amplitude of the wave coming out of the entire atom divided by the amplitude of the wave for a single electron.

Does not matter whether it is Compton scattering or Thomson scattering, if we take it then we will see that atomic scattering factor varies very strongly with $\sin \theta$ by λ in case of higher atomic number element where only Thomson scattering is mostly contributing to atomic scattering factor. Whereas if we look at this lower atomic number elements like carbon, oxygen hydrogen will see that atomic scattering factor is not that much of a strong factor or strongly depends on $\sin \theta$ by λ .

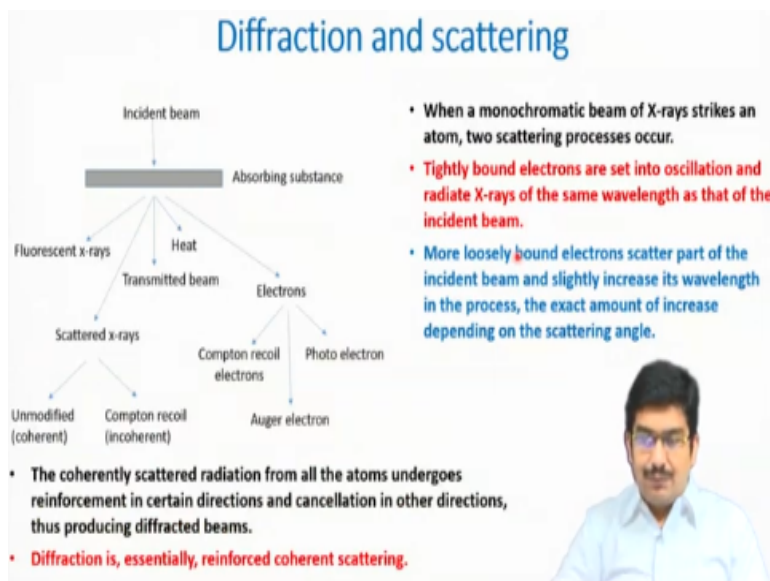
Because what happens is the Thomson scattering factor if we only consider the Thomson scattering then that will decrease the atomic scattering factor that part will decrease with $\sin \theta$ by λ . But the Compton scattering will increase with $\sin \theta$ by λ and together these two will go into other two different directions. And all together then the atomic scattering factor the decrease in the overall intensity of the scattered beam from one single atom will be not that sharp.

It will not decrease that sharply will sine theta, these two affect Thomson's and Compton scattering. The way they varies with sine theta by lambda this will be possibly some way mitigate each other or some way they will be balancing each other. So, that is the importance of considering the Compton scattering as well in addition to Thomson scattering in the atomic absorption atomic scattering factor.

So, the point is atomic scattering factor does not know whether it is a Thomson scattering or Compton scattering. All it knows is that expression that is the power of that expression it only knows the amplitude of the wave or intensity of the wave coming out from an entire atom divided by the intensity of the wave coming out from one single electron that is what. So, that is how we can explain for at least for lighter elements;

Where the λ variation is not as strong as the higher atomic number elements in order to explain this kind of variation. We have to also consider the Compton scattering that is the point.

(Refer Slide Time: 16:08)



Anyway, now if we look at the diffraction and scattering the entire phenomena and that entire x-ray electron interaction this entire phenomena is shown in this chart this will help us to understand what basically is the diffraction. So, when an x-ray beam incident on a material some

part of this extra beam will definitely be absorbed by the material. The rest of the X-ray beam which is coming out of this specimen this will be 95% of it will be transferred to heat first of all.

Then we will have a transmitted beam as well. No diffraction, only in the forward direction will have a transmitted no scattering nothing forward scattering. If we takes forward scattering fine it will be only in the forward direction. So, we will get a transmitted beam or forward scatter beam whatever. Then we will be having a fluorescent X-ray. Fluorescent X-ray definitely we have discussed the fluorescent X-rays because of the absorption X-ray absorption incomes.

Due to the X-ray absorption will have a fluorescent texture which is basically the characteristic X-ray for this one. Then we will have a scattered X-ray beam here and we will have different type of electrons here. So, let us discuss first electron then we will come to scatter x ray. Electrons we will have photoelectron which is a part of this X-ray absorption process. So, true absorption in the true X-ray absorption process will be getting a fluorescent X-ray and will be getting a photoelectron this one.

Then we can have auger electron as well in the same process fluorescent x-ray or photoelectron instead of that we can have a auger electron particularly for lighter elements. The same process the true absorption process and we can now have in the scattering process we can have two types of scattering. One is the unmodified or coherent scattering that is Thomson scattering and we will have a modified or incoherent scattering that is the Crompton scattering.

And in the Crompton scattering as we discussed we were also getting a recoiling electron, the electron which basically gets the kinetic energy and knocked out of the of the atom. So, that is also there and that is another kind of electron that is generated in the process. So, this basically summarizes all different processes that can happen when an X-ray beam is incident on any crystalline materials.

So, out of now if we consider only these scattered beams we know two types of scattering, modified scattering and unmodified scattering. And only on the modified scattering part, the unmodified scattering part, coherent scattered path, Thomson scattered part that is taking part in the diffraction that is making the diffracted beam. So, ultimately what we can say is that diffraction is a reinforced coherent scattering.

So, out of the entire scattering process X-ray scattering process diffraction is a special type of scattering which is happening due to the coherent electron or coherent X-ray beam, coherently scattered X-ray beam. So, this is the relationship between the diffraction process and the scattering process in terms of the intensity of the diffracted beam. Earlier we have derived this relationship and there we have seen that diffraction is basically diffraction is a special scattering. Because it happens in a particular direction but the Bragg's law is satisfied.

Now we are saying diffraction is a special process or a special type of scattering where we have only coherent scattering. Diffraction all others are incoherent scattering, Compton scattering, a part of that only a part of that which is coherently scattered due to the Thomson effect that will form finally the diffracted beam in terms of intensity.

(Refer Slide Time: 19:51)

Scattering by an unit cell

- Expression for the intensity of a diffracted beam: Consideration of the coherent scattering, not from an isolated atom but from all the atoms making up the crystal.
- The mere fact that the atoms are arranged in a periodic fashion in space means that the scattered radiation is severely limited to certain definite directions.
- The directions of these beams are fixed by the Bragg law.
- Assuming that the Bragg law is satisfied, the goal is to find the intensity of the beam diffracted by a crystal as a function of atom position.

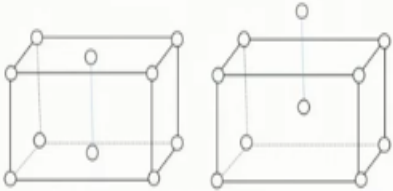



Figure:1 (a) Base-centered and (b) body-centered orthorhombic cell



So, from there now we will be considering the scattering by an unit cell. So, what is this? Now the expression for the intensity of a diffracted beam considering the coherent scattering it only considered coherent scattering now. And we will not be considering any incoherent scattering, the first thing. So, what we will be considering now is this coherent scattering not from one single atom, but from all the atoms which makes up a crystal.

So, we have to now add it up. Earlier we have and we will come to this. Earlier we have seen how the electrons how we are adding up the waves coming out of individual electrons in order to find the final diffracted beam from an atom. Now we will consider individual atoms, the diffracted beams coming out of individual atoms how it will make the final diffracted beam from a complete crystal.

And this also we have seen that the atoms are arranged in a periodic manner in the space. And that is why the scattered radiation finally the scattered radiation is limited in certain definite direction. So, we have seen that even the Bragg's law is satisfied we were not getting intensity due to the crystal structure. Due to the atomic arrangement we have seen this base center the difference between base centered and body centered.

Orthorhombic cell in one case from $0\ 0\ 1$ plane one case base centered case we were getting an intensity and in body centered the case $0\ 0\ 1$ intensity was not there just simply because of the atomic arrangement. So, that is why when we calculate when we consider the atomic arrangement, atomic positions and we have to consider where exactly this atoms are located that also is important.

When we consider or when we try to calculate the intensity of the x-ray diffracted or intensity of the diffracted beam coming out of this entire unit cell. So, the goal here when we calculate this scattering by an unit cell the goal here is to find out the intensity of the beam diffracted by a crystal as a function of its atomic position. So, the final expression will contain the diffracted beam intensity with respect to the atomic position.

If we can derive such an expression then that will help us to understand what will be the diffraction or what will be the intensity of the diffracted beam from any unit cell in terms of the atomic position that is what we will try to derive here.

(Refer Slide Time: 22:26)

- Qualitatively, the effect is similar to the scattering from an atom: Phase differences occur in the waves scattered by the individual electrons, for any direction of scattering except the extreme forward direction.
- Similarly, the waves scattered by the individual atoms of a unit cell are not necessarily in phase except in the forward direction.
- **Final aim: To determine how the phase difference depends on the arrangement of the atoms.**
- Since the crystal is merely a repetition of the fundamental unit cell, it is enough to consider the way in which the arrangement of atoms within a single unit cell affects the diffracted intensity.

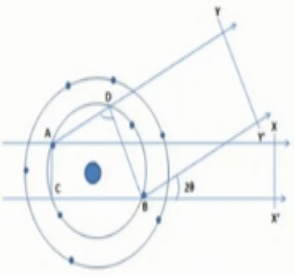
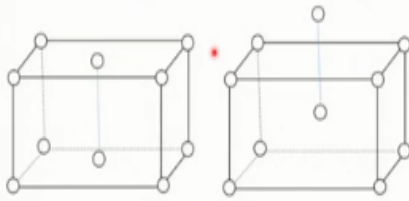




Figure:1 (a) Base-centered and (b) body-centered orthorhombic cell



And as I already said that to calculate this that final diffracted beam coming out of a unit cell. This is basically what we have to consider here is the phase difference that happens between these different atoms which are located at different positions. And this problem is very much similar to the way we have calculated the final. We have find out the final diffracted intensity from an individual atom.

Here also what we did is that we have calculated we have taken or we have considered the waves coming out from different electrons. And then we have considered the phase difference between these waves between different electrons and then we try to derive an expression for any arbitrary directions. We have seen that in the forward direction the intensity is highest because in that direction all the waves are in phase.

And if we move on from any other direction the intensity will decrease because the phase difference now there will be a partial interference because the phases are different from this. So, here also we can do the same thing the waves we are instead of these electrons we will be considering the atoms. And what we will do is that the waves that is scattered by individual atoms here in unit cell, these atoms will have of course will have certain phase difference between them due to the different atomic position.

For example, if you consider this body center orthorhombic cell the atomic position of this corners you corner atoms and the atomic position of this body centered atom this position is not exactly the same. So, that is why the atoms if we consider the x-ray beam that is coming out of this corner atoms and the x-ray that is coming out of this position, this atom they will be at different phases.

If we measure in some direction some individual arbitrary direction if we try to see that or certain direction which is Bragg's defined direction if we consider that Bragg's law is satisfied for certain direction if you try to capture the diffraction or try to calculate the intensity of the diffracted beam. We will see that the atoms or the waves coming out from this corner atoms and the wave coming out from body centered atom they will have a different phase maybe around that.

And we have to basically this finally we have to calculate. In order to calculate the intensity of the diffracted beam in terms of the atomic position we have to determine the phase difference basically, how this phase different depends on the arrangement of the atoms. So, if we do that if we are able to do that then we can find out an expression basically in terms of atomic position how the final intensity of the diffracted beam will vary.

Basically, as you understand each of these waves you can consider them to have amplitude and the phase. So, amplitude of this waves coming out if they are consisting of same type of atoms the amplitude will be the same for all of them. But they will be differing in phase if they are

different type of atoms that is a different situation. We will come to that. When we calculate the diffracted intensity ϕ first, we will try to calculate a general expression and then we will see the special kind of expressions.

There were different types of atoms so their amplitude will also differ and so on. But basically, what we will be trying to calculate now is the phase difference between the waves coming out from this atom and the wave coming out of this some other atomic position. And also, we know that this entire crystalline material is basically composed of this unit cell that is what we discussed in the last class that is the entire crystal is composed of this unit cells.

So, if we can calculate or if you can find out an expression for one single unit cell that will be enough for the entire crystal. So, the atomic arrangement basically unit cells are represented by the atomic arrangement. The atomic arrangement of atoms whatever is there in one unit cell it just gets repeated for next all other unit cells. So, finally if we; can derive one such expression for one in itself because of the symmetry itself that will be repeated for the entire crystal in the bulk.

(Refer Slide Time: 26:47)

- This problem is most simply approached by finding the phase difference between waves scattered by an atom at the origin and another atom whose position is variable in the x -direction only.
- How is this reflection affected by X-rays scattered in the same direction by atom B, located at a distance x from A?
- Note that only this direction need be considered since only in this direction Bragg law is satisfied for the $h00$ reflection.
- Phase differences may be expressed in angular measure as well as in wavelength: two rays, differing in path length by one whole wavelength, λ are said to differ in phase by 2π radians.

Handwritten notes and equations:

$$d_{h00} = \frac{a}{h}$$

$$d_{h00} = AC = \frac{AB}{h} = \frac{a}{h}$$

$$\delta_{31} = RS = AC$$

$$\phi = \frac{\delta}{\lambda} (2\pi), \quad \phi_{31} = \frac{\delta_{31}}{\lambda} (2\pi) = \frac{2\pi h x}{a}$$

Wave diagram showing λ and $u = \frac{2}{a}$. Phase difference $\phi_{31} = 2\pi h x$.

So, that is what we need to do? Now the point is how we can approach this problem. Basically, best way of approaching the problem is by finding out the phase difference between waves scattered by certain electrons. So, in this schematic you can imagine that I have an electron or I have an atom sorry I have an atom in the position a which is a origin basically and then I put another set of atom or this atom or this atomic plane whatever.

We consider we consider that along through this origin there is an atomic plane that is going and like that I have continuous planes I have one set of plane here, one set of planes here these are we can express them some arbitrary $h00$ type of plane. And then with respect to this plane if I put an another atom which is again arbitrarily put a atom somewhere. Then the X-ray beam which is coming scattered by this atom and extra beam scattered by this atom what is the phase relationship between them.

And then I can take a summation of them I can find out an expression and I can sum them up along certain direction which is again related to the Bragg's condition. I can find out certain direction I can find out an expression related to one set fixed atom in origin and one arbitrary atom anywhere in this two dimensional space that is what we are considering. We will first calculate in two dimensional space and then we will extend this in three dimensional.

Three-dimensional will not extend this we will just simply derive the simply write the expression because it is much more difficult. So, that is how we can we are going to do this and this basically x-ray scattered by this what we said in this this atom the extreme coming out of this atom how it is affected by any arbitrary one which is again sitting at x direction and at a distance x from this a atom that is what we have to consider.

And if we write this then we can find out something of this sort an expression with which we will start with here and we will possibly continue this in the next class. So, what we can write is basically like this that we take this atom a here this one and this another atom. We take atomic

plane here somewhere here as you understand both of them are from this 000 family of planes.

So, from the blank slope from this geometric consideration you know already we can write the path difference between them. Let us say imagine that Bragg's condition is satisfied for them. We can write down the path difference between them that is this $\Delta_2 - \Delta_1$ this we can write from this geometric consideration we can write as MCN . So, basically this construction we are now considering this construction MCN this is the path difference between the rays 111 here this one and 222 .

This is basically just the way we prove the X-ray Bragg's law here. So, this we can write it as $2d \sin \theta$ and since this is from a 000 plane and $\sin \theta$, θ is basically this incident angle and this should be an integral multiple of λ . Because Bragg's law is satisfying that is what I imagine the Bragg's law is satisfying for this $h00$ type of plane. So this kind of an expression I can very safely write here and also I can see that this d that is the distance between this atomic planes or inter planar spacing this d_{h00} .

This from this construction I can very I can write it as AC which is again $a \sin \theta$. So, a is the complete this if we imagine that a is some lattice parameter or some lattice parameter then that is what I can write as a in terms of lattice parameter. And h is basically the distance between this a to c . So, finally that is what I can write for the interplanetary spacing in terms of something like lattice parameter and the final intercept that it makes on this lattice parameter.

So, now we are calculating for an arbitrary this plane we already placed an atom here which is again arbitrarily placed at a distance x from this a origin this atom x from here. And if we imagine if we consider this ray 333 ray this one here in this direction if we consider the same direction where the Bragg law is satisfied. If we consider this direction; then what we can get the path difference between these two rays 111 and 333 , this rays.

So, the path difference between this one and path difference between this one this will come out to be from the same kind of consideration this come out to be this RBS. So, this RBS is basically RBS this one from this construction again we can use it the same geometric consideration. And what we can find out is basically the path difference is $AB - AC$ into λ and AB is basically this distance which is x and AC already we have seen AC is something like this and this is the λ value here.

This is coming out to be same from the same construction same way we are considering the path difference between or the phase difference here. This is the phase difference in terms of the path difference. We have finally find out the phase difference in terms of path difference and same way now we are finding out the phase difference between these two wave in terms of the path difference here.

Now the phase difference can be expressed in terms of angular in a way. So, phase difference can either be expressed in terms of path difference, a phase difference can be expressed in terms of angular difference as well. And angular differences we know that for an angular difference if we draw it in this way then we know for a complete wavelength λ we have a phase difference of 2π .

So, if we bring that and we put this as the phase difference in angular means we can get this to be this value λ by 2π . And if we write a specific one that is phase difference between this $\frac{3}{3}$ bar and $\frac{1}{1}$ bar a this will come out to be this, $\frac{\Delta \frac{3}{3} - \frac{1}{1}}{\lambda} \times 2\pi$. So, finally this expression will be coming out to be of this value $2\pi \frac{hx}{a}$. We are just putting all the variables here;

And if we express the fractional coordinates so this b value if we express in the fractional in terms of fractional coordinate at this x by a then finally what we can get is an expression of this sort. The phase difference between these two will be expressed as $2\pi \frac{hu}{a}$. So, this is the final

relation phase difference between these two rays. One coming out from origin and one coming out from any other place, any arbitrarily placed atom, any other atomic plane.

One is the atomic plane because of which for which the Bragg's condition is getting satisfied. And another one is an arbitrary plane placed arbitrary set of atoms placed anywhere in this entire drawing. So, the phase difference between them we can find out from this expression. So, we will stop it here and we will continue in the next class. We will continue more with this phase difference, determination of phase difference for various ways, thank you.