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

Lecture - 48
Intensity of Diffracted Beam (Continued)

Welcome everyone to this NPTEL online certification course on techniques of materials characterization. We are in module 10 and we are discussing about x ray diffraction. So, we just started discussing about the intensity of diffracted beam in the last class. We will mostly discussing about the filter materials and just we started our discussion on intensity and how the intensity is related to atomic arrangement, what is the importance of calculating this intensity of diffracted beam so on so forth.

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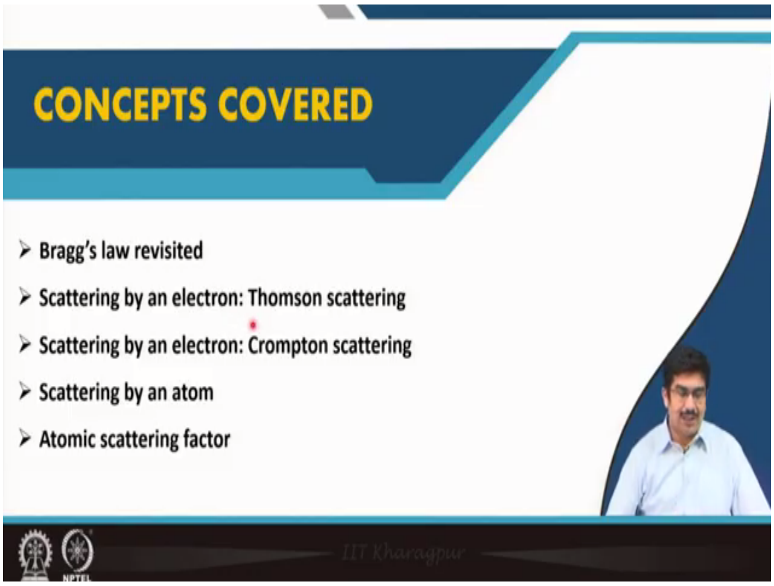

So, we will be continuing there we will keep on seeing the Bragg's law from an intensity perspective, we will be then discussing about the scattering by an electron, which is called there are two types of scattering by an electron one is the Thomson scattering and another one is Crompton scattering and then we will see that scattering X-ray scattering by an atom how it happens and we will try to discuss about the atomic scattering factor in this lecture.

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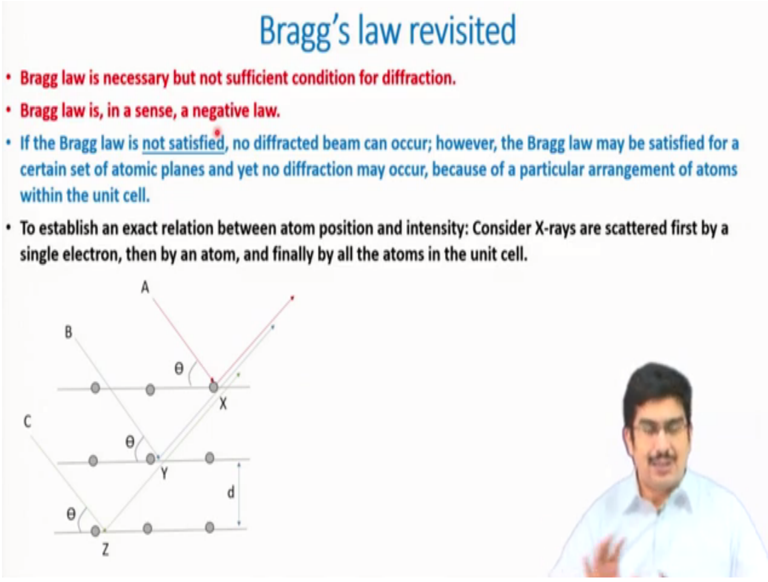

So, we have discussed enough about the Bragg's law and how that is like how the intensity of diffracted beam on an over the Bragg's law, how it is important and how it is related to atomics arrangement of it within a unit cell. So, from that perspective, what we can call or what we can say is that the Bragg's law is not necessary, but not sufficient condition for diffraction.

So, if the Braggs law is satisfied, that is not enough in order not enough to get a diffracted intensity in the final diffraction pattern from measurement point of view satisfying the Bragg's law is definitely a necessary condition that is not a sufficient condition for getting intensity diffracted intensity and in that sense, Bragg's law is basically negative law. So, if the Bragg's law is not satisfied in the first place, so there will not be any diffraction at all.

If the lambda value if the wavelength is not integral multiple of the path difference is not an integral multiple of wavelength of the extra beam in the first place, no constructive interference will happen. And no diffraction phenomena no possibility of any diffracted diffraction from those atomic planes for that particular direction that will not be there. That is the first thing. That is why it is a necessary condition.

But even if the Braggs law is satisfied for certain set of atomic planes, still we will not get any diffraction because of the arrangement of atoms in the in that particular atomic plane. That is that is the point that is why Bragg's law is just half satisfying the Bragg law is just half of the story, the rest half is like the other factors, which are basically determining and we will come to know about that atomic absorption factor and then most importantly, the structure factor which we just discussed.

When we were discussing about the X ray, electron diffraction, we just discussed about the structure factor and importance of it. So, we will see here that how the structure factor and the Bragg's law together they determined the entire or together they tells the entire story of X ray diffraction from a crystalline material. That is where we will be leading. So, at this point, we started with the limitations of Bragg's law and from there we slowly we will establish the importance of this atomic arrangement.

So, to establish this relationship between the Atomy position and intensity, what we have to consider is that the, we have to start from very basic the X-ray scattering from a single electron, how that is happening, then, from a single electron how, so, all the electrons how they are contributing to the overall atom, electronic scattering of an atom. And finally, the same way, all the atoms present in a unit cell, how they are contributing to the overall atomic scattering or overall X-ray scattering from one unit cell.

So, we will go by these three steps we will consider the electrons first, then we will consider the atom and finally, we will consider the unit cell and that is how the entire this derivation the relationship between diffracted beam intensity and atomic arrangement will derive in that way.

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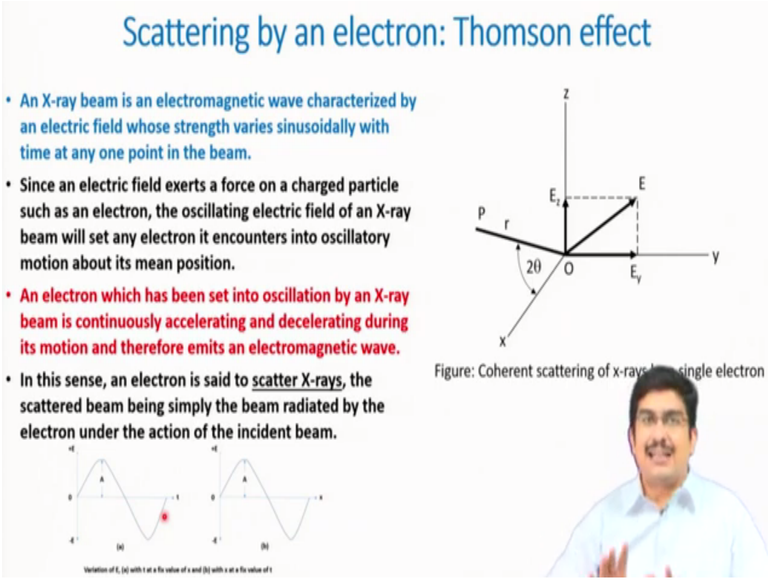

So, first thing as I said, we will be discussing about the scattering from an electron. First one is the Thomson's effect, basically so how it happens so, when we need that X-ray beam is basically an electromagnetic wave, where this electric field the strength of this electric field basically varies sinusoidally with time at any given point with distance I think at any particular distance the intensity of this electric field varies with time.

And similarly, for any given time, the electric field also varies with its position, both of this is there, that is what characterize is basically any electromagnetic wave and X-ray is just an electromagnetic wave. Now, what happens is when an electron beam interacts with a charged particle like electrons. So, this, the electric field, which is there, which is a part of this electromagnetic radiation, like x-ray, under the effect of this electric field, now the charged particle electrons will start oscillating about their mean position.

So, you can imagine this to be like a ball is hanging with a with a string, a ball is hanging, and then you are sort of a billiard ball is hanging from a string, and you are just sort of applying a force onto it another ball, let us say another ball goes and hits it, and then it starts oscillating about its mean position. So that is what we can imagine the first kind of an interaction between an electron and which is a charged particle and an electromagnetic wave, which is an extra photon in this place.

Now, what happens is the electron when it is set with this oscillation by X-ray photons, the X-ray beam, which made the electron or charged particle to oscillate along its mean position, it continuously undergoes an acceleration and deceleration about. So, basically, when it if we just imagine that electron this is not X-ray, this is not the sinusoidal curve for X-ray, but this is the sinusoidal curve, let's imagine that for the electron beam.

Then it is going for an acceleration with certain time with time it is going through an acceleration, deceleration and maybe in the other direction, again an acceleration again deceleration. So, continuous acceleration and deceleration will happen for this charge particle under the effect of this electromagnetic wave. And already we discussed this when we were discussing about x ray generation that it charged particles which is undergoing a continuous acceleration.

And the acceleration particularly deceleration, then it is an excellent source to radiate another electromagnetic wave. So, electromagnetic waves are basically generated by a continuous by a source which is continuously oscillating or accelerating and decelerating. And in charge particle, this is exactly what is happening here. And that is exactly how we generated the continuous spectrum in the first place in the X-ray tube remember that.

So, this is basically this charged particle in this case, which is electron will in its motion, this oscillatory motion set up by this extra photon, it will generate another electromagnetic wave which is another X-ray y beam in this case. So, this way we can call it this basically this entire process is called Thomson's effect which is discovered by a famous scientist at Thomson. And in this we can call that the incident X-ray beam is being scattered basically, the electron is just working like a mediator here.

X-ray beam, comes hits this electron it generates an oscillating motion and in that rapid acceleration, deceleration process it generates another extremity. So that way basically it scatters the electron incident electron beam and this is a completely this happens in the first place.

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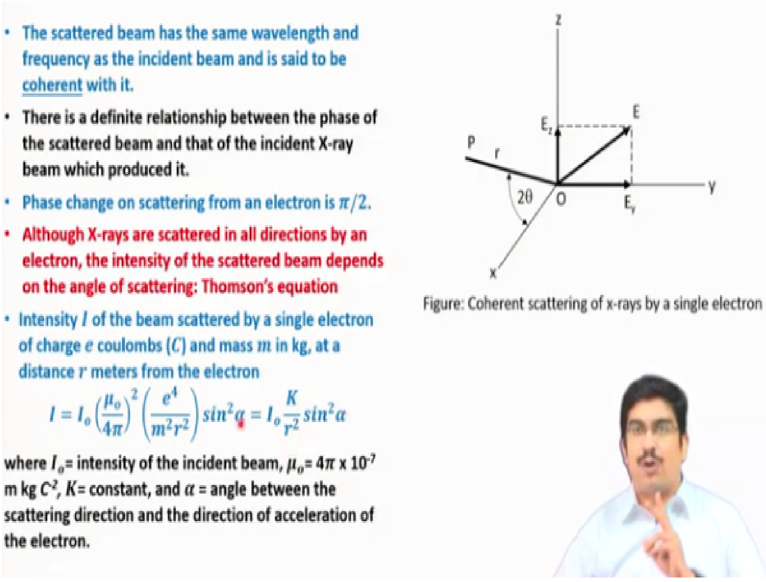

Now, the scattered beam, that scattered X-ray beam, which is generated by this Thomson's effect, that will have at the same wavelength, so, that is the relationship basically between a charged particle or rather the source which has generated an electromagnetic wave and the wave that itself generated. So, the scattered beam the wavelength and the frequency of the electromagnetic wave, which is generated from this source will have exactly the same wavelength;

And frequency with which this charge party or with which this source is basically oscillating. That means, the electrons if I imagine that this electron is there in the middle, and this electrons will generate an X-ray, that X-ray the generated the produced X-ray will have the same wavelength and frequency as that of this electron beam. Now, again, this electron, the motion that is oscillating motion this this electron has this wavelength Frequency is related to the wavelength and frequency of the incident electron incident X-ray beam.

So, in that way the scattered X-ray beam will have the same wavelength and frequency as the incident X-ray beam that means, the scattered X-ray beam the one that is generated from this electron will be coherent to with that incident electron beam in terms of wavelength and frequency and normally, they also have a phase relationship between this incident X-ray and the scattered X-ray beam through this electron.

And this phase change is usually pi by 2 between the scattered X-ray beam and the incident extra beam the changing phase is pi by 2. Another important point is that this extra scattered extra beam of course, the electron can oscillate in any plane it is a completely random process. So, the scattered x ray beam also can generate in all possible directions, but the intensity of the scattered X-ray, scattered beams will depend.

So, since this process is completely random in this case the electron motion is completely random and this scattered beam which is generated that also can generate in any random direction, the intensity of the scattered beam will depend on the angle of scattering. The angle that the; scattered beam is making with the oscillatory motion or the motion of this electron. So, it will depend on that angle and this equation is basically given by Thomson's this equation is called Thomson's equation.

So, the intensity of the beam the X-ray beam which is scattered by a single electron, which is having a charge of e coulombs and a mass of m rest mass is m in kg at a distance r. So, this is the intensity so if you measure the intensity at certain distance from this electron the electromagnetic wave that is generated due to the oscillatory motion of this electron. If you measure the intensity of it at certain distance r that is given by this equation, I equals I 0 multiplied with mu 0 by 4 square into again multiplied by e raised to the 4 by m square r square and this sine square alpha.

So, alpha is basically here this is the scattering angle, this is the angle between the scattering direction the direction of the scattered beam and the direction of acceleration of the electron the direction at which the electron is moving and the direction at which the scattered beam is moving. So, this is the angle between that, so what you can see and of course I noticed the intensity of a incident beam the scattered beam for the scattered beam basically that is a source of intensity and mu 0 here is the dielectric constant of the medium.

Basically, this is a constant value again m is constant that is the mass of the electron and e is in charge of the electron. So, overall, what happens is this mu 0 e m square all of these are constant ultimately, we can express this equation in a simpler term that is I equals I 0 into k by r square sine square alpha. So, we have only 2 variables here that is the distance of like where we are measuring this intensity and this angle, scattering angle.

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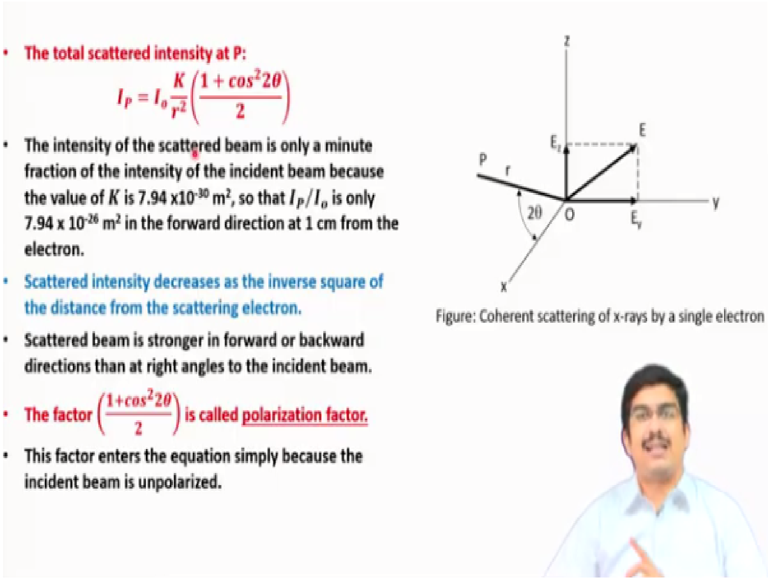

So from this what we can measure the total scattered intensity at certain direction. Now this is something the derivation I am not going out is done a totally scattered intensity you basically get this electric field vector you imagine that the X-ray incident X-rays travelling in this direction this ox direction and that point or you have the electron and because of that incident X-ray beam the electrons will start having an electric field an electric field which you can then sort of vectorise you take the components into different directions.

And finally, out of that you see this x ray beam which is coming in another direction you are measuring the intensity there so I am not going into details of that. But basically, the intensity at any given point p which is situated and direction r, at a distance are r this electron charge particle which is generating this scattered X-ray beam and this angle which in this direction the scattered beam.

The direction at which the scattered beams is moving that scattered beam that the angle it makes with the incident ray. So, this final scattered intensity Ip will be I 0 K by r square into 1 plus cos square 2 theta by 2. So, this is the final expression for scattered intensity at any given direction and in that direction, the scattered beam intensity and which in that direction is making an angle to detail with the incident beam and at a distance of r.

Pretty similar in shape two this earlier Thomson's equation, but here we are measuring it at any arbitrary direction scattered direction here we are measuring at any at some fixed direction. Now a couple of things we can realize from this equation, first of all the intensity of the scattered beam that is this Ip this one the entire scattered beam intensity. So, this intensity is basically the scattered beam from one single electron X-ray beam;

Which is an electromagnetic wave hitting a charged particle which is an electron generating a scattered beam scattered x-ray beam this is the intensity of that overall scattered beam. So this intensity we can see first of all is very small compared to the intensity of the incident beam, that is simply because that is basically I am taking an ratio of this Ip and I 0 which is this intensity of the incident beam and then I am putting all these values of K and K is defined.

As you know case this is the original equation K is defined here as this mu naught square by mu 0 square into e square by m square. This is what the key value of the constant here. If we put all of these values, then we find that the constant is very small it is a very small value and this Ip by I 0, this is also has a very small value meaning that the intensity of the scattered beam is very less as compared to the intensity of the incident x-ray beam.

So that is the first thing. So, most of the intensity of the incident x-ray beam is basically goes into absorption or penetration only a very small fraction of it is basically getting scattered by at least one single electron that is all. Now the second thing you can notice is the scattered intensity, this Ip this decreases or this depends inverse has an inverse relationship with the distance from the scattered electron the scattering electron.

So, this distance so, the intensity will also decrease as the inverse square of the distance from the scattering electron if r is, if we measure the intensity at a further away from this electron which is causing the scattering then we will be getting much smaller intensity. So as the distance increases the intensity goes down. Third thing we can notice here is from this, that cos theta this entire term 1 plus cos square theta 2 theta by 2.

This term becomes unity if theta equals either in the forward direction theta equals 0 or 2 theta equals basically theta equals 0 or theta equals 180 degree, actually that means, in the forward direction the scattered beam is strongest in the forward direction either in this forward direction where we are basically in the same direction where the incident beam is moving.

If this is 0 degree this 2 theta is 0 degree or 180 degree then this entire term is becomes unity and that is the highest value for Ip. Anything in between the 0 and 180, 180 means it is basically retracing the scattered beam is retracing the incident beam that is what. Anywhere in between this will have a fractional value and the intensity will be lower than that in the forward or backward direction.

So, that these 3 things or these 3 major conclusions we can draw out of this equation the total scattered intensity for x-ray the incident X-ray of the scattered beam coming out of interaction between the incident x-ray and the electrons. This factor this 1 plus cos square theta 2 theta by 2; this factor is basically called the polarization factor and this is one of the most very important we will come to that.

This polarization factor when we take the complete intensity or from an unit cell this again this polarization factor will come there and as I just now I discussed this polarization factor is basically one issue which reduces, other than the forward or backward direction. It generally causes a reduction in the intensity of the scattered beam from the electrons and this factor comes in this equation simply.

Because the incident extra beam is unpolarized. If the incident beam is polarized, we have discussed what is a polarized one, basically in a polarized beam this electric field vector has a particular plane and particular relationship with the magnetic motion of this x-ray photon, so that is the polarized beam. I am not going into that so if it is a polarized beam then this polarization factor does not come into play.

And intensity will be pretty high it is scattered beam intensity is comparatively high. That is why we want to have a polarized beam in order to reduce the polarization factor we want to have a polarized X-ray beam in the first place. So not only monochromatic X-ray beam, we also need to have a plain polarized X-ray beam in order to get the intensity considerable intensity from the diffracted in the diffracted beam. So that is the Thomson's effect.

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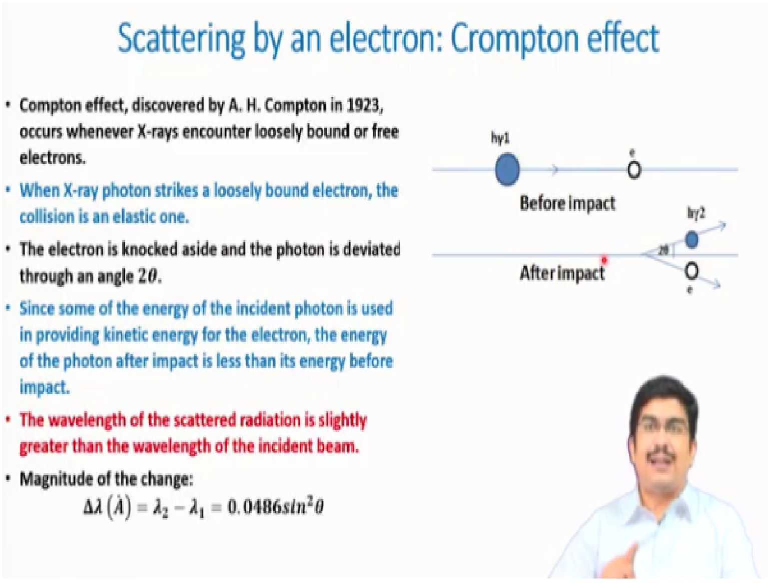

Now there is another perfect another way of in which the X-ray beam will be interacting with the electrons. But for this one, we will have to imagine the X-ray to be having the particle, I mean like we in the quantum mechanics we know that every electromagnetic wave we can imagine them either as a particle or as a wave. So, in this case, we have to imagine this X-ray beam as a particle and then we can very easily understand this effect which is known as the Compton effect.

And this Compton effect just like Thomson effect was discovered and proposed by JJ Thomson, Crompton effect was discovered by A H Compton and other famous scientists in 1923. So, this happens between the X-ray beam or X-ray photons in this case with the loosely bound of free electrons with the atom. If the atom has certain amount of free electrons then the X-ray beam will interact with them.

And the way this interaction happens we can imagine that it is like a bigger ball heavier ball is hitting a smaller board and so this is the heavier ball that is the x ray photon and this is the electrons charged particles which is a smaller ball and this after the collision this X-ray will be deviated from its original direction original path it will be going in some other direction, but in the process the electron the smaller ball will also gain certain amount of kinetic energy.

So, here it is a static now, it gained certain amount of kinetic energy from this impacting ball from this bigger ball and it will also be moving in another direction. So, this in this process I will get 2 things I will get an electron which is generally called the recoil Compton and recoil electrons and scatter the X-ray beam or an this incident beam which is modified its energy gets modified due to this impact. So, these 2 things will be generated in a Compton scattering.

So, obviously, one thing we can immediately understand that some amount of energy will be lost in this impact process. So, because here this incident ball will have certain amount of energy now, some part of the energy is transferred as a kinetic energy for this recoiling electronic electrons and only a part of the energy will be retained by this deviated X-ray beam. So, obviously, the energy of the incident X-ray beam is much higher or it is higher at least considerably higher than this scattered electron beam.

Consequently, the wavelength of the scatter X-ray beam will be slightly greater than the wavelength of the incident beam. Whatever be the difference between them the energy difference between them is basically this energy of this electron. So, in some sense, this process is pretty similar to the fluorescence radiation and photo electron emission if you remember.

So, there also the incident X-ray electron incident X-ray beam X-ray photon whatever it brings the energy it brings, that energy goes in generating fluorescence radiation and the photo electron. Same thing here in a different way the incident whatever energy this incident like X-ray photon was bringing part of it is going as this recoiling electron kinetic energy of the electron recoiling electron and part of it is going there is the energy of the scattered beam.

So, this magnitude of this change in wavelength and this wavelength of this scattered beam is slightly greater energy that means, energy is slightly lower than this incident electron incident X-ray beam. So, this magnitude of this change if we if we take that as lambda delta that is basically delta 2 minus delta 1, delta 2 is the wavelength of this scatter beam minus delta 1 is the wavelength of the incident beam.

And from there we can again I am not going into derivation we can find out this relationship which is coming out to be around 0.05 around sine square theta 0.05 sine square theta. So, what is theta here? Basically, theta again is the scattering direction, the direction or the angle that the scattered beam is making with the incident beam, here just like Thomson's effect, where this is the incident beam and this is a scattered beam and 2 theta was the angle between them.

Here also in the compton scattering 2 theta is defining the angle between the incident electron beam and the scattered electron beam. So, in that sense theta has pretty much the same meaning between these 2 things, but only differences is, we will come to the difference of all of this. Only difference is the Thomson’s effect is basically an elastic interaction whereas the Compton Effect is an inelastic interaction.

Because in the Compton Effect as you can understand there is some amount of energy which is lost whereas, in Thomson's effect the energy was not lost.

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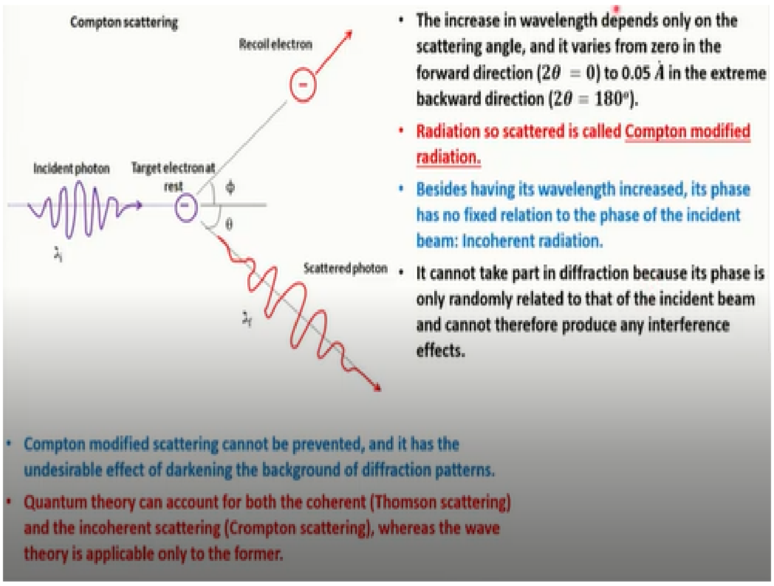

Now, the increase in energy as we understand obviously depends on the increase in wavelength obviously, depends on the scattering angle only on the scattering angle. So this increase in energy or increase in wavelength rather the decrease in energy increase in wavelength, this varies with direction with this 2 theta angle and it is this lowest in the or lowest or 0 in the forward direction that is 2 theta equals 0 degree in the forward direction.

So, if I forward direction means there is no scattering at all basically or if I imagine that this is the incident photon and this is the electron, if the scattered beam is again off even after the interaction it is moving in the same direction, then obviously there is no change in the wavelength. So, it is another way of thinking that there is no change of energy as well and it will be, minimum in the extreme backward direction.

That means, when 2 theta equals 180 degrees that means, this scattered electrons are scattered X-ray photon is just tracing back the incident electron that is what and that value will be obviously 0.05 angstrom because in that case sine theta will be 1, if it is theta equals to detect called 180 degree then sine theta will definitely be 1. So, that is the 2 extremes for this scattered the change in wavelength of this scattered electron beam.

So, the radiation of this scattered electron beam is called Compton modified radiation and this electron is called recoiling electrons. And, besides, one more important point is that, that other than changing by blank, the Compton modified radiation, this process is pretty much a random process, because it is not certain how much of energy will be transferred to this electron and how much of energy it depends on a lot of things.

So, even if you think that in a small bigger ball hitting a smaller ball, it is a complete random process, how much energy will be transferred to the smaller ball and what will be the direction the bigger ball will move. So, the scattered photons, this process is pretty much again very much random process. So, the way it affects is that, the wavelength definitely in the process of this energy transfer the wavelength modifies other than that the phase of this Compton modified radiation;

The scattered photon X-ray photon that generic that does not have any typical phase relationship with this incident electron a because of this randomness in the process. That means, the scattered beam jazz is generated here is an incoherent to this incident photon that is another difference between the Thomson's effect and the Compton Effect. Thomson's effect the scattered beam was completely coherent with the incident X-ray beam.

Whereas the Compton modified radiation this x scattered X-ray beam from Compton radiation it is having no particular phase relationship or wavelength, phase relationship means wavelength frequency etcetera. So, wavelength frequency of this one is not at all related to the wavelength of this or frequency of this incident electron. So, in that sense these are in coherent discounted scattering always generate an incoherent X-ray beam.

So, this definitely the Crompton scattering, So, this part of the scattering electron or scattered X-ray beam this cannot take in a diffraction process in the first place itself because for taking part in a diffraction it should have the scattered beam should have a particular phase relationship with the incident exhibit then only that Bragg’s law will be satisfied in the first place.

If it does not have any phase relationship, phase relationship means lambda has to be or path difference has to be an integral multiple of lambda then only constructive indifference will happen, if that path difference is not certain if the lambda of the scattered beam is not is completely changed with respect to the lambda of the incident beam, then this relationship this constructive interference possibility of the constructive interference will also not be satisfied at all.

So, this will have the scattered beam will have a completely random phase relationship with the incident beam and in the process, they will not be able to generate any kind of diffraction phenomena in the first place. So, Crompton scattering is not important to be considered for diffraction purpose, we will be only considering the Thomson’s effect Thomson's beam because that is what is a coherent that has exactly the same wavelength as the incident beam.

And this difference obviously now it should be clear that this difference is the way these two effects are happening, one is happening through an elastic interaction mostly another one is happening by an inelastic interaction mostly. Other than this of course there is some the Crompton scattering is also some having some importance because it basically it generates the background in the diffraction pattern and basically darkens the background in the diffraction pattern.

We will come to that in a little later, how the quantum scattering is important for mostly for lighter elements into cause the background or to cause the noise in the signal. Finally, but one more important difference between Thomson scattering is and quantum scattering is that the quantum theory can account for both the coherent and the incoherent scattering that means, both the Thomson and Crompton scattering can be explained using the quantum theory where we are dealing with extra photons.

Whereas, the; wave theory is applicable only to the Thomson scattering. Thomson scattering can be explained both by considering we have seen how it is how we can explain the Thomson scattering just by imagining the X-ray to be an electromagnetic wave and that is interacting with electrically charged particle and generating this another electromagnetic wave.

So, from classical wave theory we can explain Thomson's effect, but from classical wave theory we cannot explain the Crompton Effect. Crompton effect can only be explained if we imagine like stress to be a photons that is another big difference between these two. So, we will be continuing our discussion of scattering by an atom in the next class and then we will be discussing about atomic scattering factor as well. Thank you, Goodbye.