Electron Diffraction and Imaging
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Lecture – 22
Atomic Scattering Factor

Welcome you all to this course on electron diffraction and imaging. In today's class we will discuss about atomic form factor what is the need for it how it is derived and as we know in the formula which is been derived for diffraction.

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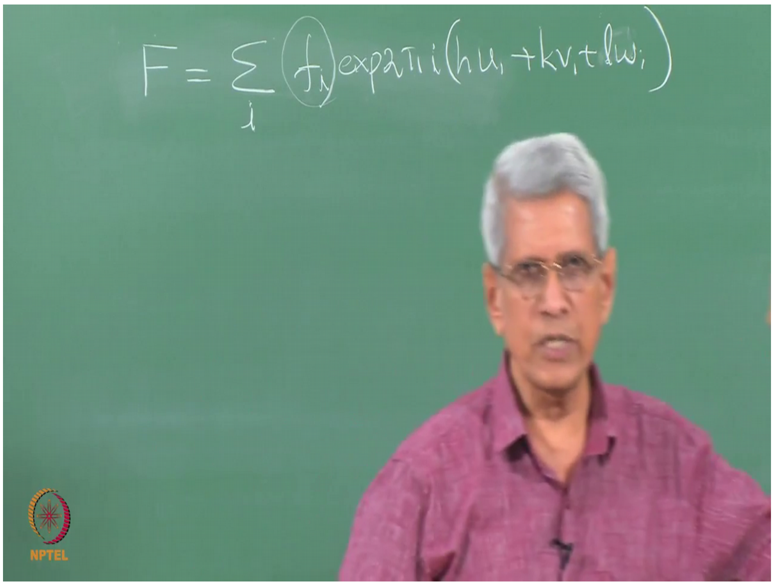

Structure factor; we write this with this expression i into exponential 2 pi i h u i plus k into v i plus w l into l i which you v l and w i this is summed over all the atoms in the unit cell here h k l represent the specific plane which is contributing to the diffraction for that plane we sum over all the atom positions what is going to be the total contribution that is what it this structure factor amplitude what it gives this is essentially a complex quantity what is essentially important is that there is a factor which comes f corresponding to each atom position each atom position what f represents is what is the contribution from each atom to the scattering that is what essentially we are trying to find out just look at a general scattering before we come to this. So, what is our aim our aim is to find out that how this structure factor the not the structure factor atomic scattering factor is derived that is what that for that we have to understand what is the way in which the beam the probe interacts with the atoms.

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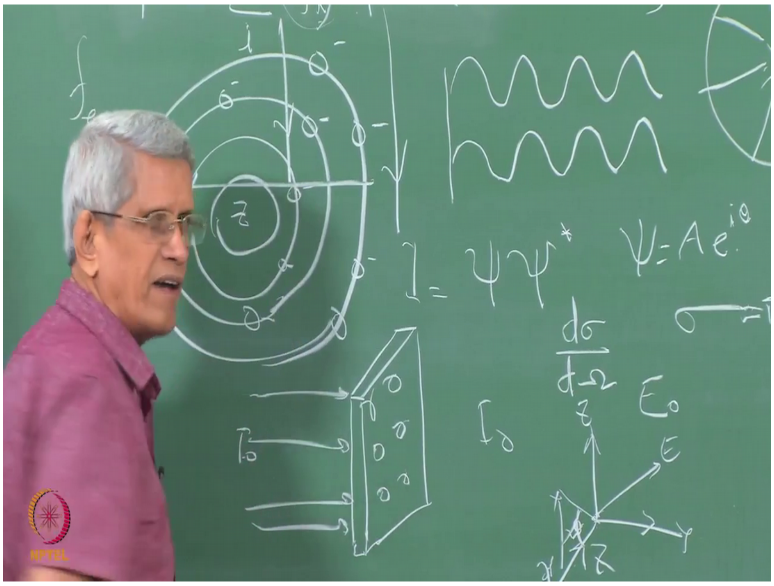

When we look at an atom how we can consider it its essentially a nuclear charge which is there some charge with this and there are many levels at which i am just putting negative to tell that electrons are at various levels electrons are revolving around the nucleus. So, this had some finite size is there how the probe is going to interact with each of the individual electrons that is what it is going to determine. Similarly how it is going to interact with the nucleus the net effect of all this interaction from each of the atom is what is going to give how much of the beam is going to be scattered by the each atom that is what we will try to look at it. So, essentially what we require is that the thing is that when a probe passes through what is the probability that the probe will be for scattered that is a information which we require the probability is a quantification of how much scattering is going to take place.

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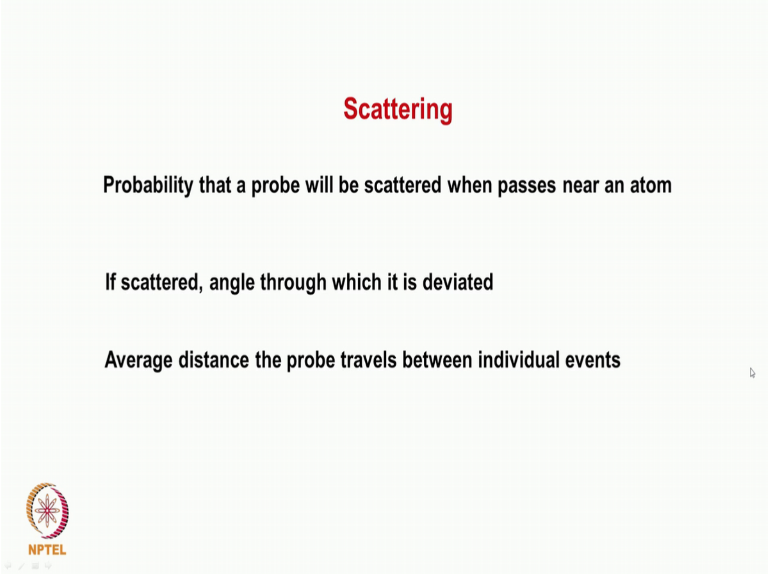

Suppose it is scattered what is the angle through which it is scattered or which the probe is deviated that is the information another; information which we require is average distance the probe travels between individual events.

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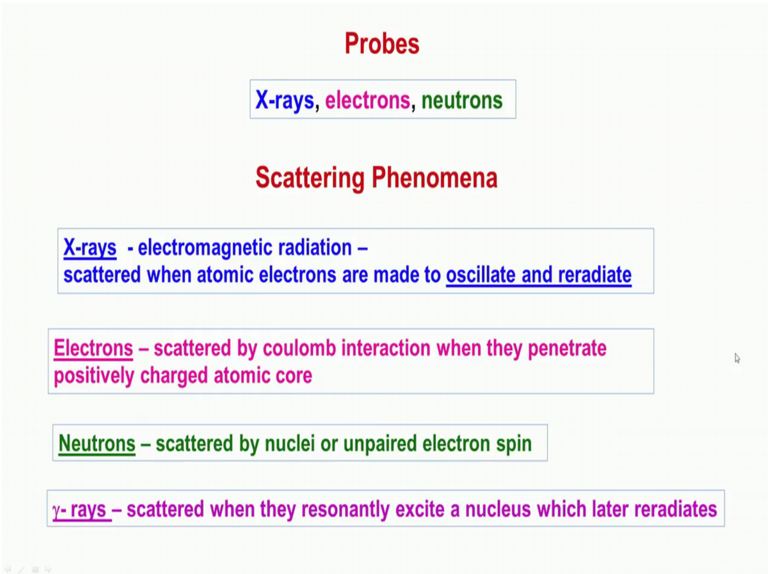

What all the types of probes which you use in diffraction X-rays electrons and neutrons what we have to find out is that how the atomic scattering factor is going to be different for this various probes for the same atom that is what we will try to find out that is for each atom depending upon the probe is it that same or what sort of interaction takes place what sort of interaction the probe has with the electrons or with the nucleus these are all the information which we in is necessary to decide what is going to be the atomic scattering factor.

Let us look at what is the scattering phenomena if you look at X-rays; X-rays are electromagnetic radiation it has an electric field and a magnetic field which is associated with it which radiation it as an electric field and a magnetic field which is associated with when it propagates and the electric field and magnetic field is fluctuating perpendicular to the propagation direction when this X-ray interacts with an electron it could be an atomic electron like I could be any electron when it comes close by what it is going to do is to make the electrons oscillate if it is an electron which is a free electron it will oscillate with the same frequency as that of that incident probe the electromagnetic radiation and then it will be re radiated because it is an essentially a electron which is oscillating.

So, electric field when electron oscillates, it is an oscillator, the electric field is continuously going to change and this is called as a hertz oscillator, so, this is the way in which electrons what is going to happen in the case of an atom there will be a restore restoring force will also come into the picture this we will talk about it a little bit later what happens in the case of an electrons if it is an electron which is interacting with an electron.

Now, it is the columbic interaction between the charge which is important whether it interacts with the nucleus or whether it is in that electron if it is with the nucleus an electron electrons it may be a attractive force if it is going to be with the electron it is going to be a electron; electron; it is a repulsive force and this depends upon how much the electron is going to come close to the nucleus that is if the incident beam is going to be here or when the incident beam is trying to enter here depending upon that this forces also columbic forces also potential will also change.

If you look at the neutrons how neutrons interact with it neutrons are essentially a neutral particle. So, it is not affected by the charged distribution its interaction is mostly with the nucleus of the atom and we know the size of the nucleus is very small and the interaction take place due to both with the nucleus that interaction is essentially it excite the nucleus and then it can come to a ground state emitting radiation and the another way which can happen is that there is a spin which is associated with the electron it can interact with the electron spin that is how it can give information about the magnetic state of the material or the magnetic structure information we can obtain similarly gamma rays also have very high energy they can also essentially excite a nucleus and which can be later re radiate radiated, but we will not be talking about these aspect because we will be considering for diffraction only these 3 aspects which will be looking at it.

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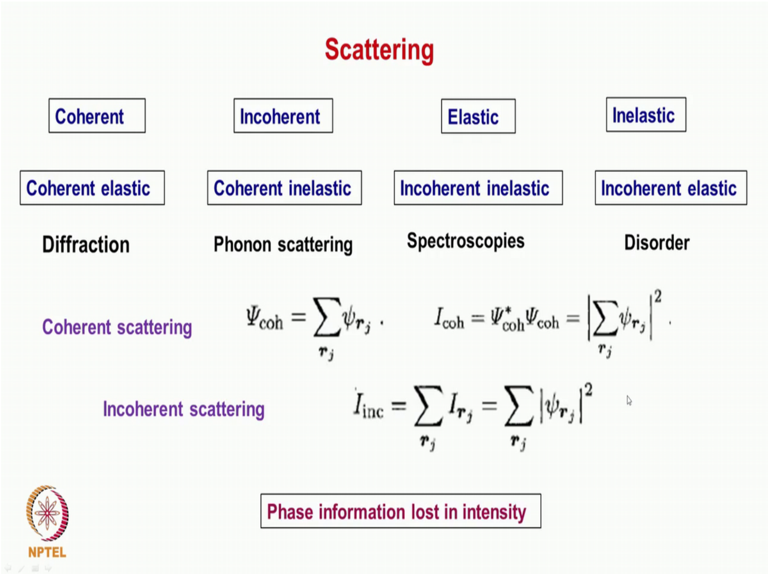

Let us look at their scattering what all the types of scattering which we know we know that the scattering can be coherent or the scattering could be incoherent when do we call a scattering a coherent scattering; scattering is coherent when if this is the way a one wave propagates another wave at another comes if there is a phase relationship between both the waves exactly at the same phase or there is a phase relationship or we can tell that phase relationship exactly what it is going to be then we can say that it is coherent if this phase relationship is random when we call that beam incoherent.

So, this is talking with respect to the type of scattering which it can take place another is the scattering itself could be either elastic or it could be a inelastic scattering elastic scattering is one in which the energy of the probe remains the same before and after scattering inelastic scattering is in which the energy of the probe is different before scattering as well as after scattering there is a difference is going to be there. So, these are all the four terms which you can see. So, in any scattering it could be a coherent scattering or an coherent scattering it could be elastic or it could be inelastic we can have combination of all this that is what. So, the scattering can be coherent elastic and that is what we considered in the case of a diffraction; diffraction is essentially nothing, but a coherent elastic scattering.

If the scattering is coherent, but it is inelastic that is what we call it as a phonon scattering where some energy is lost, but still we can get information about the lattice vibrations and all this we could get it from this the other is it could be incoherent as well as inelastic that is what we use for spectroscopy there; what happens is that the beam as such interacts with sample randomly and then it loses some energy specific amount of energy and comes out some energy in random direction there is no correlation between the which is the direction in which the scattered beam comes, but this energy which it has lost that could be used to get information about the chemical identity of the atom we can get this information these are what is used this is what is used in spectroscopy techniques another is the beam itself it can interact incoherent, but the scattering could be this one this is what it happens in the case of when we are try to look at disorder in the material it could be a positional disorder especially position disorder is there atoms are displaced from it side.

So, it need not be a coherent scattering, but the scattering will is still elastic these are all the various types of scattering which we can because why i brought in these terminologies is because we are talking with respect to diffraction where it is essentially a coherent elastic scattering for a coherent scattering what is that what we can do is if we wanted to find out finally, when we measure it is a intensity which we measure. So, the intensity is nothing, but we generally write it at in the; if the amplitude is written in terms of a complex term we write it as PSI; PSI star complex contiguity if you take.

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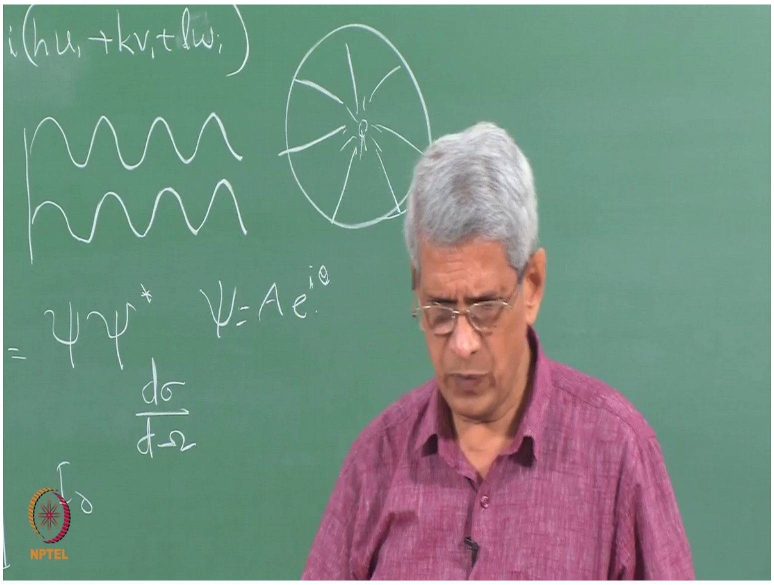

So, here what is going to happen is that in this particular case when it is coherent we first add the amplitude and find out the net resulted amplitude this can be taken in the terms of we can express each of this psi in terms of an amplitude a into E to the power of i theta or we can represent it in terms of a vector diagram and find out the resultant there are many ways in which it can be done then we once we have that total amplitude from the psi; psi star we can find out the intensity incoherence scattering is where be sent the process itself is a incoherent for each of the process we find out the psi; psi star for each individual event and add all of them together that gives rise to a total intensity which we get it for diffraction essentially it is a coherent elastic scattering which we consider a diffraction.

So, we have to add the amplitudes together and then find out the intensity, but when we take the when we finding out the intensity because that is what is measurable quantity we find that the phase information is lost because in a complex conjugate term when we take it the product the phase information cancels out.

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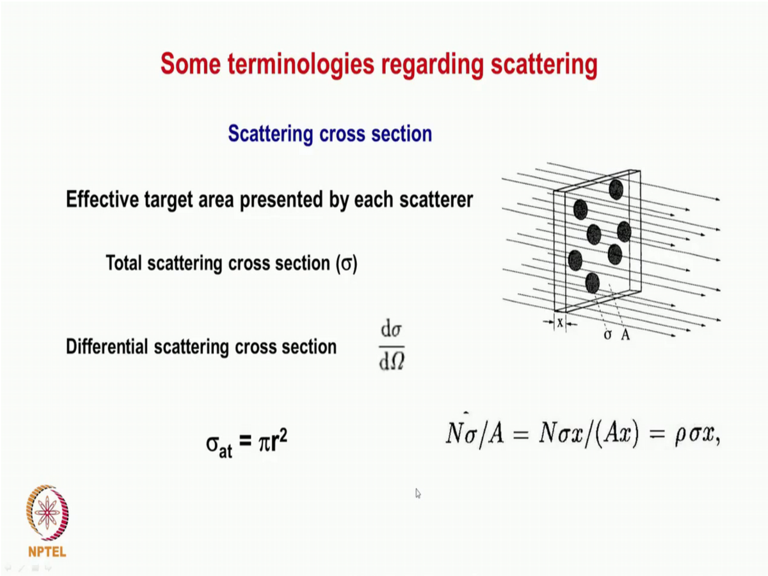

Some of the terminologies which are required regarding this scattering because this what does this f means this is essentially corresponding to some scattering cross section scattering cross section just tells how much of the incident beam is scattered in a particular direction that is what essentially that information is given essentially scattering means that effective the what the target does is that when the beam passes through the samples some area of that samples suppose we have a sample this is if the beam is entering like this if this is the incident intensity if this completely out the intensity which come out remains that it is the same as a incident intensity when they can said that it is totally transparent there is no scattering is taking place if there is a reduction in intensity then we say that some intensity is removed from the primary direction or in each direction if we look at it and that is what essentially then we say that scattering is taking place this can be expressed in terms of what is called as a scattering cross section.

There are 2 terminologies which we use one is a total scattering cross section which is does not differentiate between how the scattering varies from region to region that is what one is and another is differential scattering cross section in the case of light suppose we consider that there is a bulb which is there, kept at this center this bulb is radiating light in all these regions if we try to find out at some particular distance from if we are trying to find out what is going to be its uniformly its coming that is what the total scattering cross section we can it will not change as a function of distance anywhere here it is going to be the same, but whereas, the case of electron scattering if we can see that in forward direction it is as the angular scattering changes we find that there is a change intensity then we should know how it is changing as a function of angle then we have to use the term differential cross section and that is generally written as d sigma by d omega; omega is the solid angle which we are taking on the surface of the sphere which we consider.

As an example if we consider it this is what I have done in this suppose we say that some regions are essentially opaque then what it can happen is that the total intensity of the transmitted beam is going to come down and if it is an opaque object and beyond which there is no interaction with the matter if we consider it then what is going to happen is that the total area of this itself will decide how much of the intensity is going to be cut down per unit the scatter if we consider it that will turn out to be some factor of r square it is an area that is essentially what it is written generally for a steady circular one this can be written as pi r square. So, this is how it is and r is called as a scattering length.

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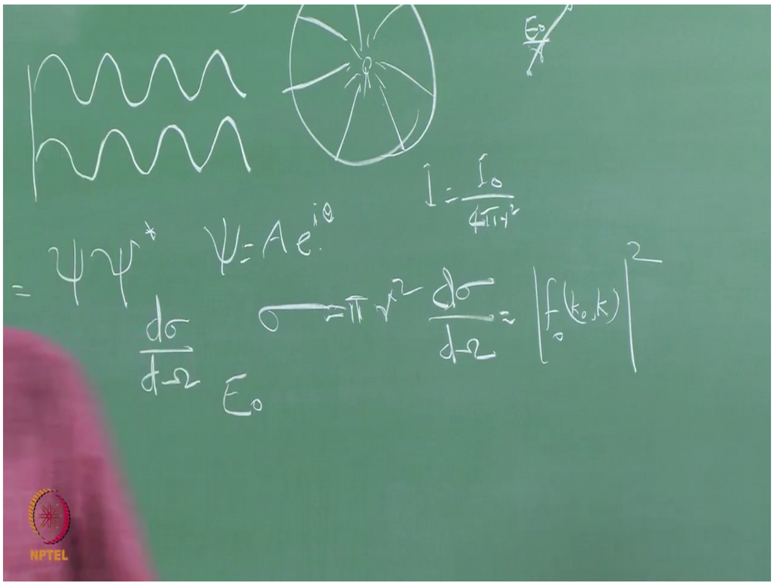

So, what is essentially important here we have to remember is that the scattering is essentially over a surface when we consider it whether it is a sphere or if we consider effectively from the sample how it is going to change as a function of distance that is what we are trying to find out and what is the effective area over which it is scattering the beam away from that is what is defined the scattering cross section when example which we can take for differential scattering cross section is given here.

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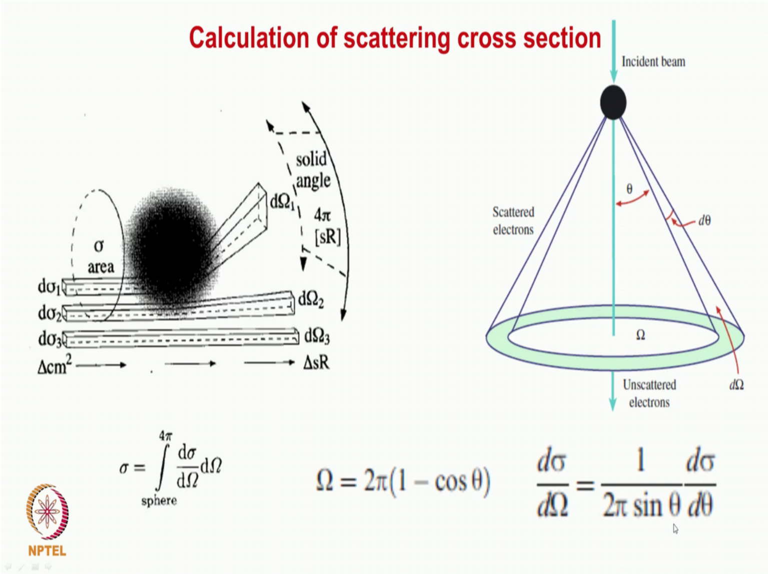

There is this is an effective area which we are considered sigma and if you look at this region the beam which is entering it is scattered quite a bit may be an electron goes to a nucleus and from here if you look at it its less and here there is no scattering. So, if we look here the total scattering cross section for we have integrate over the full area, but it has to be considered at each point and then its added together and that is equivalent to integrating over the full area of this sphere the same way you can consider suppose electron is getting scattered into a small region we wanted to find out what is going to be the scattering and this is the sort of formula which we can write it is a quiet simple derivation.

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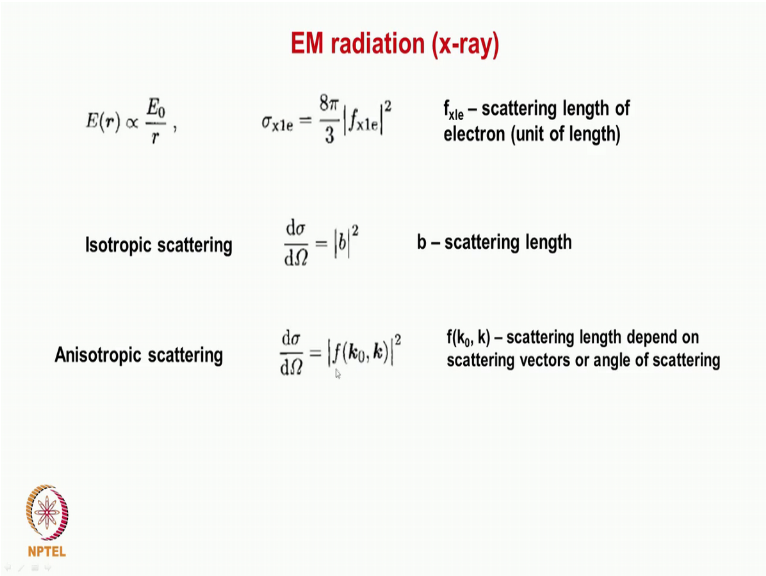

And now you can see that the d sigma d by d omega here if you look at it this depends upon the angle of scattering also and as I mentioned if we consider an electron which is being scattered and its with an amplitude each row because electric field is E 0 from a point its getting scattered at some distance like from here its getting scattered at a distance if you are trying to find out how it is going to.

The amplitude turns out to be E 0 by r at that point this is because the intensity if we consider i equals i 0 by four pi r square any point on the surface of that sphere. So, from this the amplitude is square root of that that is how we are taking. So, essentially the electric field at the any point under surface of sphere if we consider this is proportional to what that proportionality constant that is what is going to is the atomic scattering factor.

Suppose it is isotropic scattering then d sigma by d omega it will be a constant it will not be varying as a function of angle otherwise we will be writing it as here if you see it we are writing it as d sigma by d omega is equal to k 0 and k are essentially the incident beam direction and k is the scattered direction. So, it will be varying a that has to be the average we have to take it that magnitude is given if you have to find out for a full atom then what we have do it is for each individual electron each one of them where they are present we find out the scattering then add all of them together the whole question which comes is that if I take it for one electron and each of the electron I find out the contribution add them together is it going to be the total sum z into the scattering contribution each of them that is the what the question is for coherence scattering.

This we will look at it. So, this is what I have just calling this is as length scale.

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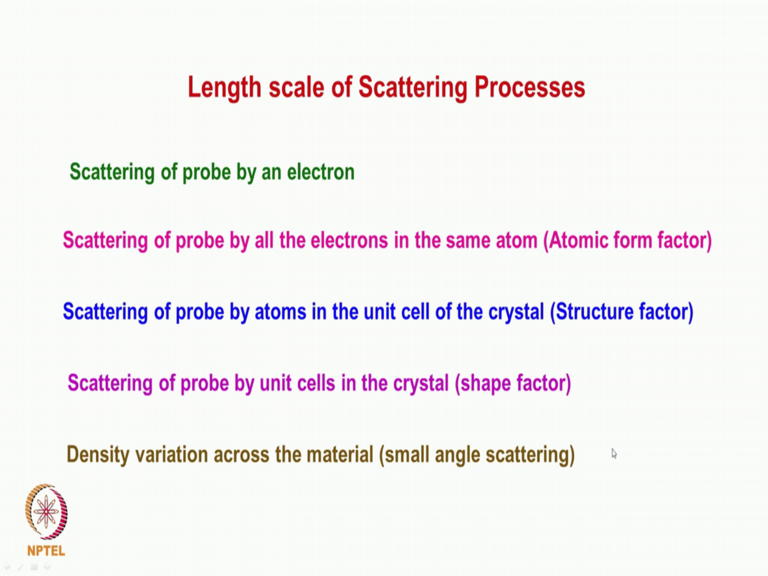

So, essentially like one electron if you consider it is like a point from which a scattering is taking place because scattering of probe by an electron another is the sum total that is a if a atom is there from here at this particular point we wanted to find out if it is plane wave which is coming it is getting scattered from this as a spherical wavelength in all this direction.

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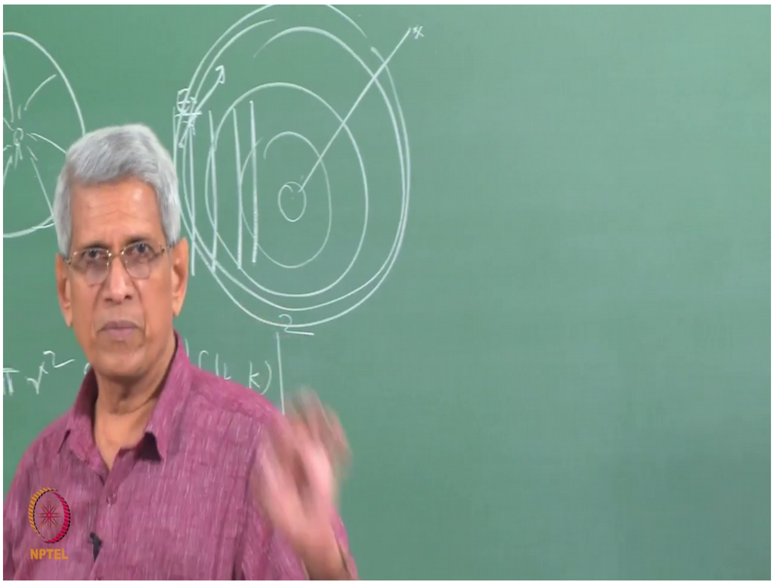

This wave also will be coming this will also be coming meeting at this point then from each electron that scattering which is going to take place all some total what it is going to be that is what we call it as the atomic form factor then the next information which we require that ones that we have then using this formula we can find out what is going to be the scattering of probe by atoms in the unit cell all the atom together what is going to be the scattering contribution that is what essentially f represents that part of it we have already looked at it. So, what we have to look at is only by the electron and by all the atoms in the all the electrons in the atom how they contribute to the scattering.

Then another is that from the sample when we have to get that information then we have to look at what is the volume over which the beam is falling and the number of unit cells are there take that contribution also then we can tell that when a beam is falling onto a sample what is going o be the intensity of the scattered radiation we can quantitatively determine or what were we have experimentally measured theoretically we can derive a formula which will quantify this is the value which has to come another is some material density variation can occur this gives rise to some small scattering.

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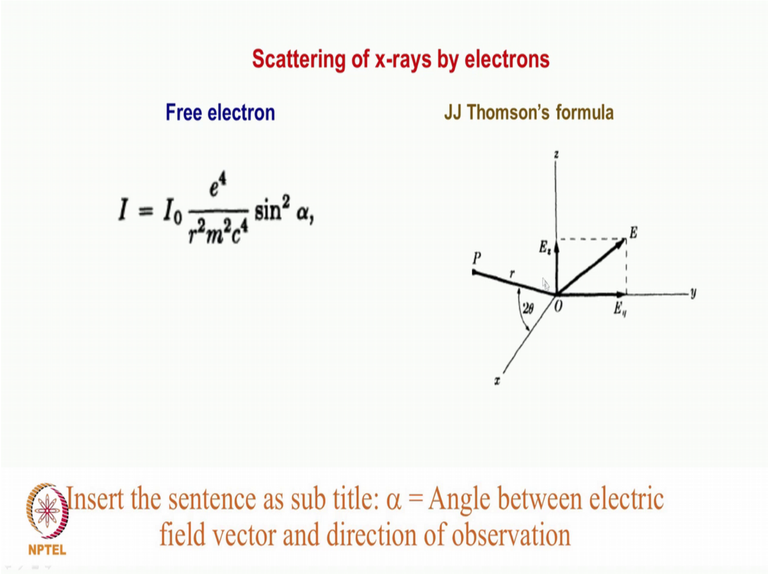

This is very much important for the scope of this lecture. So, I will not go into detail. So, this probe we could consider generally 2 types of probes which we use neutron 3 types of probe which are being used X-rays electrons and neutrons, but in any laboratory X-ray and microscope are common facility. So, that can be used in a lab, but neutron requires some special facility only at few places it can be done. So, I will spend more time and X-ray is the most common one. So, I will start with the X-rays first.

Let us consider the case of an X-ray beam which is travelling in a this is x y z X-ray beam is assume that travelling in that direction at the point at the origin it is seeing an electron and you know X-ray is an electromagnetic radiation it is got an electric field and the magnetic field associated with it under electric filed if you consider it will be in these 2 it will be essentially assume it is in these direction it could be randomly any orientation which can have perpendicular to it then we say that it is an un-polarized one if it is polarized the electric field is in a specific direction in this particular case we wanted to find out at any particular point with respect to this electron which is there it take let us take in this plane itself x z plane as an angle 2 theta how it is going to the intensity is going to vary this was calculated by a classic formula which has derived by classical theory classical electro dynamic by J J Thomson essentially the answer turns out to be i equals i 0 E is the charge of the electron r is the distance where it is going to be m is the mass of the electron c is the velocity this one is essentially giving with respect to a propagation direction at what point we are trying to measure it.

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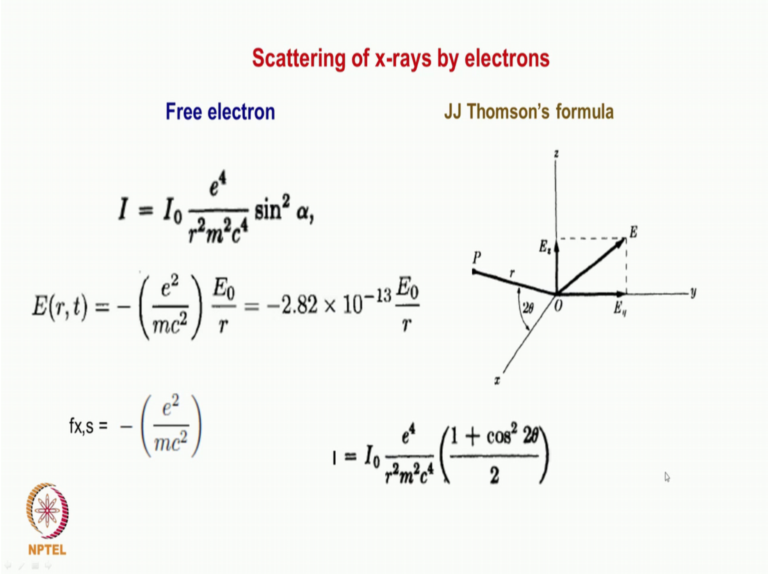

So, if we try to calculate and in this specific case which we are considering it this angle is going to be ninety degree. So, this will turn out to be one and from this if we know it we can calculate what is going to be the amplitude its function of time if we take it this value if you consider it this turns to be E square by m c square here what we assume is that it is a very high energy X-ray which is falling on to the sample surface and one has one can see that that is a negative one comes; that means, that if you look at the amplitude one is negative of the other that is very important because when we look at the intensity we do not see these effect and another important is that this factor is could by m c square.

This is what in the case of an electron scattering factor I will call it is an f E that is scattering factor like an atomic scattering factor this has scattering factor when individual electron this value turns out to be f E if you look at it this is a small value. So, the intensity of the radiation is going to change considerably and the unit if we look at it this has to be since it is here its electric field this also an electric field this has to be inverse of r is what this f has to be is it clear that is what I have written from single point; single electron.

And in this particular case if we are looking at a scattering from this electron this angle is continuously changing then that brings about a variation in the intensity. So, essentially what is going to happen is that the total intensity if we calculate that is a term due to because this electric field can be split into one in this E y and another is in E z the effect of both of them onto this beam we can effect of both of them on the amplitude at this point p can be and this is the sort of a formula which will turn out to be which depends upon this angle cos theta this is what we call it as a polarization formula in X-ray diffraction.

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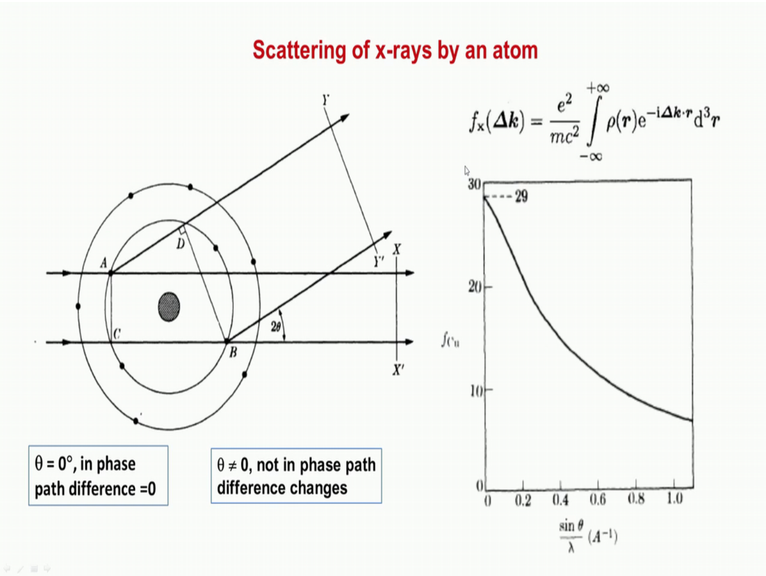

Now, what is going to happen is that in that formula if the beam is travelling in this forward direction itself if we consider it the same direction then what is going to happen this theta value it become 0. So, this becomes the same as the; that means, that irrespective of whatever be the electron in the forward direction intensity to maintain that same its the same; that means, that it is going to be in phase they add together from. So, that is essentially what is being shown here is that if you look an electron which is a which is gear scattering in the forward direction the path phase difference if you see its going to be 0 for all. So, all the intensities add together.

So, it will be the same as that of the primary beam for any other angle a path difference which is going to come which depends upon the angle theta and also it depends upon the theta essentially depends upon the delta k value if this is the k 0 and this is k direction this is what the theta comes into the picture and also the wavelength of the radiation which comes then what is going to happen is that a phase which is being introduced depending upon the phase of. So, from here as well as here if an electron is this electron or this electron which scatters when we find out the amplitude at some specific point add them together with the phase we have to see it.

So, it is not that the amplitude should directly add together. So, the net amplitude is not going to be a direct some of the amplitude of each individual one. So, that is what is essentially given by this formula and this is a how we define the structure factor and this can be looked at it one way in an atom if you consider its a nucleus and surrounded by electrons which are there at different distances from the nucleus electrons are situated. So, the electron density we can see it and if we wanted to average out not take individual electrons we can use that density variation instead of individual that is what essentially is being done E to the power of delta k that r that is what essentially it is going to determine how much is this variation which is going to be if we try to plot this for a specific value of lambda which we take it.

Now, we can see that this is been take for copper k alpha copper. So, when the angle of scattering is 0 the it is maximum as the scattering angle increases one can see that the f scattering contribution from atom is going to get reduced correct. So, this is what it has been all added together. So, this what this value which we call it. So, this is essentially is in an another way in which it is defined in the book is that if all the electrons which are there taking the phase factor if all of them are put at to the center what is going to be the contribution which is going to be the phase factor that is what essentially what we are doing it to one individual electron.

So, you can see that as a function of. So, how we can write it sin theta is one and another is this path difference depends upon lambda also no not the path difference depend on lambda the phase difference if we consider it path difference also is there that angle also has to come into a picture that is why we write sin theta by lambda which we take it normalized one and now you can make out that this is how it is varying so; that means, that when h k l reflection is we are going to particular specific SQL reflection we are looking at the diffraction which is taking place depending upon that angle at which we are getting the diffraction peak the atomic scattering factor which we have to use we cannot just use the atomic number it has to be calculated for each of the electron.

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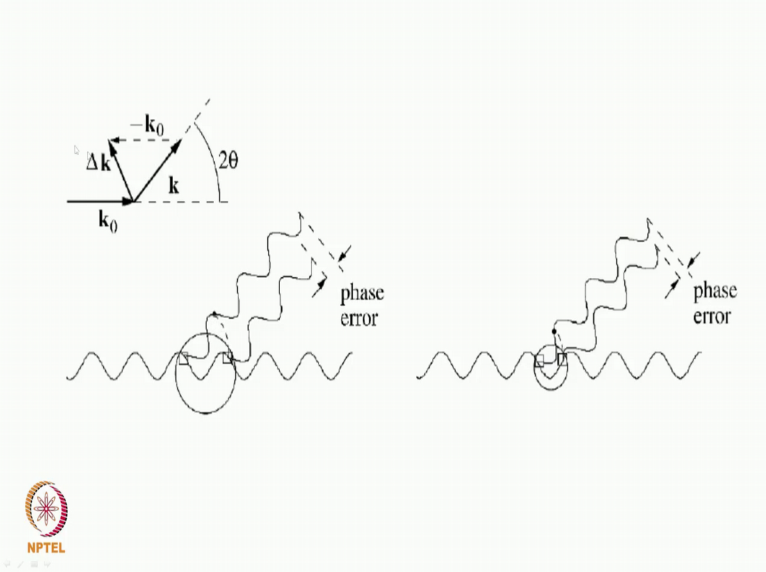

And we have to use that value that is what it is being shown here in all other way this is k 0 this is k the values are fixed and at some particular direction k delta k if we take it this is corresponding to a this determines what the 2 theta angle is going to be if for the same wavelength if it is a small size of the atom then what is essentially going to happen is that the path difference which atoms from here as well as here it will introduce is going to be very small if the size of the atom is large then for the same radiation the path difference is relative phase error is going to change depending upon that the value of atomic structure in factor also change.

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Atomic scattering factor for high energy x- rays

s	0.0	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.5	0.6	0.7	0.8	0.9
Ti^{+4}	18.00	17.81	17.26	16.42	15.36	14.20	13.01	11.88	10.85	9.20	8.05	7.26	6.69	6.22
Ti	22.00	21.17	19.41	17.64	16.05	14.58	13.21	11.96	10.86	9.16	8.02	7.25	6.68	6.21
V^{+5}	18.00	17.84	17.37	16.63	15.70	14.65	13.54	12.46	11.43	9.70	8.44	7.55	6.92	6.43
V	23.00	22.21	20.48	18.66	17.00	15.47	14.03	12.71	11.54	9.67	8.38	7.51	6.90	6.41
Cr^{+4}	20.00	19.80	19.23	18.34	17.23	15.98	14.68	13.42	12.25	10.27	8.83	7.84	7.14	6.62
Cr	24.00	23.33	21.79	20.02	18.25	16.56	14.97	13.52	12.24	10.19	8.77	7.80	7.12	6.61
Mn^{+2}	23.00	22.71	21.87	20.63	19.13	17.52	15.92	14.42	13.06	10.84	9.24	8.14	7.37	6.81
Mn	25.00	24.28	22.61	20.76	19.01	17.36	15.81	14.36	13.04	10.85	9.25	8.15	7.38	6.81
Fe^{+2}	24.00	23.71	22.89	21.65	20.14	18.51	16.87	15.32	13.89	11.50	9.75	8.51	7.65	7.03
Fe	26.00	25.30	23.68	21.83	20.05	18.35	16.75	15.24	13.85	11.51	9.76	8.52	7.65	7.03
Co^{+2}	25.00	24.72	23.90	22.67	21.17	19.52	17.85	16.24	14.75	12.22	10.30	8.93	7.96	7.26
Co	27.00	26.33	24.75	22.90	21.10	19.37	17.71	16.15	14.70	12.22	10.32	8.94	7.96	7.27
Ni^{+2}	26.00	25.72	24.92	23.70	22.20	20.54	18.85	17.20	15.65	12.97	10.91	9.39	8.30	7.52
Ni	28.00	27.36	25.81	23.98	22.16	20.40	18.70	17.09	15.59	12.97	10.92	9.40	8.31	7.53
Cu^{+2}	27.00	26.73	25.94	24.74	23.24	21.58	19.86	18.17	16.57	13.77	11.56	9.90	8.69	7.81
Cu	29.00	28.38	26.87	25.05	23.22	21.44	19.71	18.06	16.50	13.76	11.57	9.91	8.70	7.82

Atomic scattering factor as a function of Bragg angle is shown for different elements and ions ($s=(\sin\theta/\lambda)$). Tabulated values of $f_x(s)$ are in electron units. Multiply by classical electron radius to convert to units of cm. ($e^2m^{-1}c^{-2} = 2.81794\times10^{-13}$cm) $f_x = z + f' + if''$ (f_x in unit of length)

Atoms and ions

This has been calculated and I had just taken from the many of the books where the values are standard tables which are given.

Here you can make out that what s represents is nothing, but sin theta by lambda for various values when it is going to be 0 when the theta is 0 this is what the value which is its almost correspond to a atomic the number of electrons which are going to be there in the atom suppose the atom is ionized then what is essentially is going to happen is that the number if electrons going to be less. So, essentially the atomic scattering factor us going to be different for atom and then ion, but one should remember that since the electrons it is an electron with the photon interaction which is taking place the number of electrons it only determine we can assume take the nucleus the same electric field that photon it come very close to nucleus then what is it going to happen it can make the nucleus also move, but the size of the nucleus is so large that the vibration the amplitude is going to be very small. So, we may not see the radiation if we look at it so, weak that we can ignore that part of it. So, essentially what we have to consider in the case of an X-ray is only the electrons surrounding the nucleus is what is contributing to atomic scattering factor.

So, now here if we see this as the atomic number increases the f also increases and as the it gets ionized suppose atom is ionized the number of electrons in the atom in the ion is going to be small depending upon that there is going to be a variation now if we can see that as far as the this is the contain, but as we go away from at different angles then there are some subtle differences which we will be seeing it, but this also could be used to get some information about what is the state in which that element is, but the effect is not that drastic here, but between atoms and ions also there is going to be difference in the so, depending upon that we have to choose that specific value of atomic scattering factor.

Now, what is essentially important is that. So, far we have considered with respect to very high energy X-rays is falling the atom and how do we say that energy is high it is like suppose we look at that atom that k alpha electrons are occupying the k level if that electron is removed what is the energy which it which it will be coming out that is where the X-ray energy which it can come that is a frequency with which that vibration can continue and that is going to be very small binding energy of the k k electron is much small compared to that of the energy of the incident X-ray, but what is going to happen is that different type of atoms contains electrons at various energy levels at each atom and their binding energy going to be different; that means, that we have to consider cases where as a function energy of the incident radiation is the atomic scatter factor is going to be the same or its it can change or not that is something which we have to consider for X-rays.

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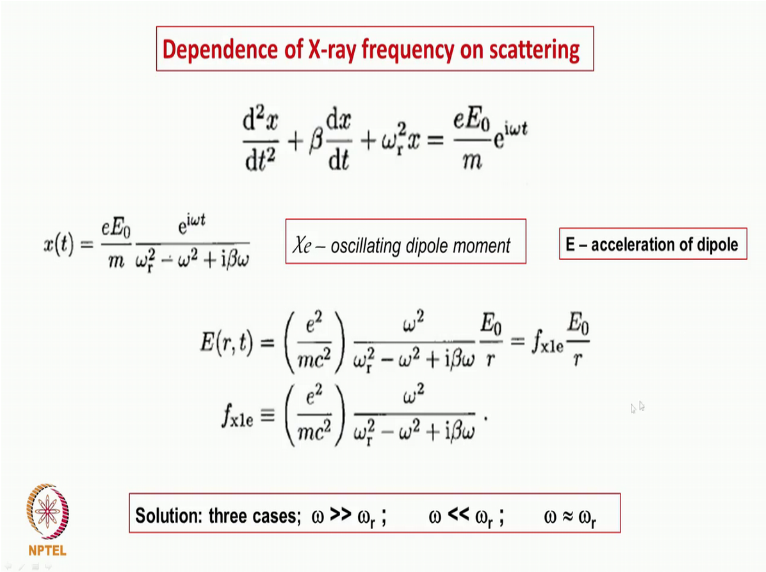

That is what we are trying to look at it that how we can do it is that electron is bound to an atom the k electron is bound very closely strongly compared to an electron which is outside. So, when that incident X-ray beam comes and if it is trying to make this electron ion oscillate there is a restoring force also will be coming from this. So, then if you write a differential equation of that incident wave with respect to this is the sort of a differential equation which will be writing this is the restoring force the solution to this gives what sort displacement which it will be time it with which it will be changing this is what essentially. So, here one is a resonance frequency of the electron is going to come in to the picture which is dictated by the type of the atom and another is the incident frequency.

So, if you look at the electric field also similar expressions will come here 3 cases which we can consider one which is very high another case which is the incident energy is very small compared to that of this one the third case is when the incident energy is very close to each other incident energy and the natural frequency of that electron is becoming almost near to each other this particular case.

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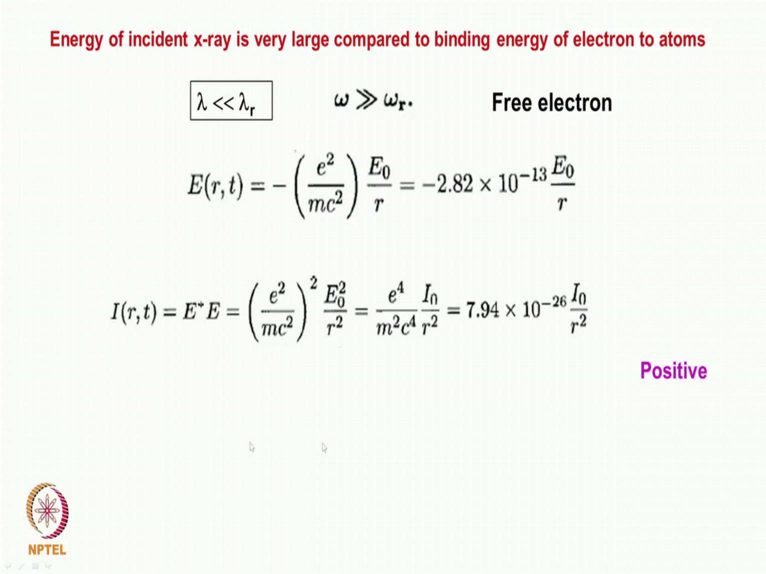

Where this concerned that is the case which we when the energy incident energy is very large compared to that then it is similar to that of a free electron the restoring force then this factor we have already taken into consideration.

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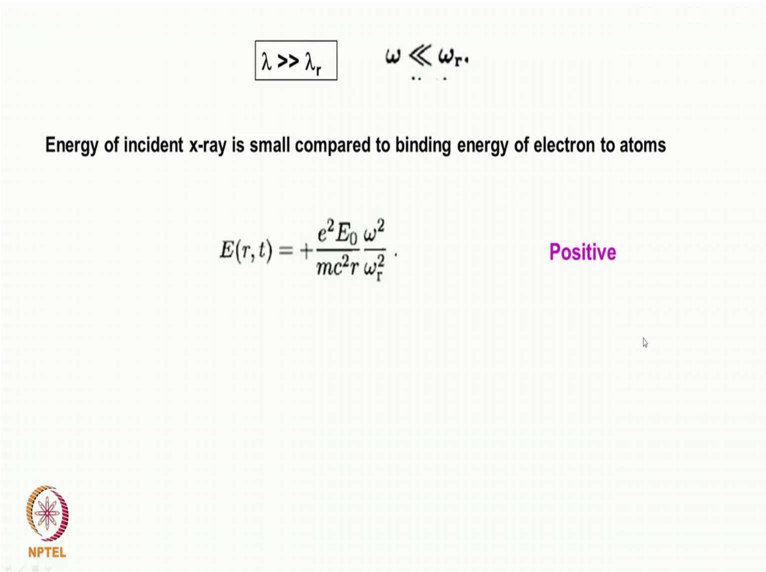

Now, but what is essentially is going to happen is that when it is going to be high this is a case which we can take it is that suppose I use copper k alpha and I am trying to look at a germanium; germanium as I said which is larger then what is going to happen is that with respect to k level if I consider it k level has got a higher energy. So, it cannot frequency is high whereas, for all other levels l l level and energy is going to be very small l alpha. So, in that case if we look at it with respect to others it is l levels and all electrons which are going to be there the energy of the incident radiation is high the other one the incident energy is small compared to that in that case if we look at the amplitude of the scattered wave it is going to be positive this is something which one should remember and its going to change with respect to the essentially.

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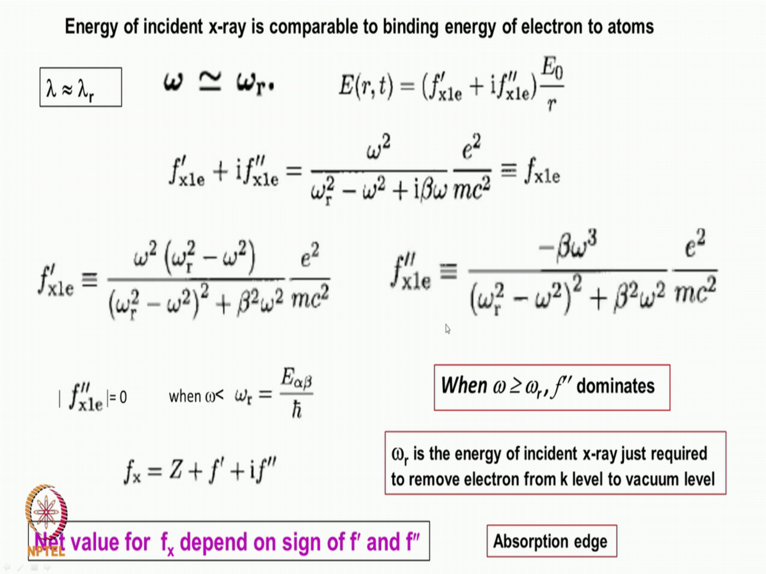

The ratio of these 2 which decides interesting part is when it is going to very nearly the same since this equation itself has got a complex function we can write it into 2 terms this essentially a simple mathematics. So, it will turn out to be f x l dash and another is the i the complex the imaginary part f x l E this is 2 terms are going to be there essentially what is going to happen is that this factors are now going to change.

Let us assume the case with respect to copper k alpha itself suppose I take the case of cobalt.

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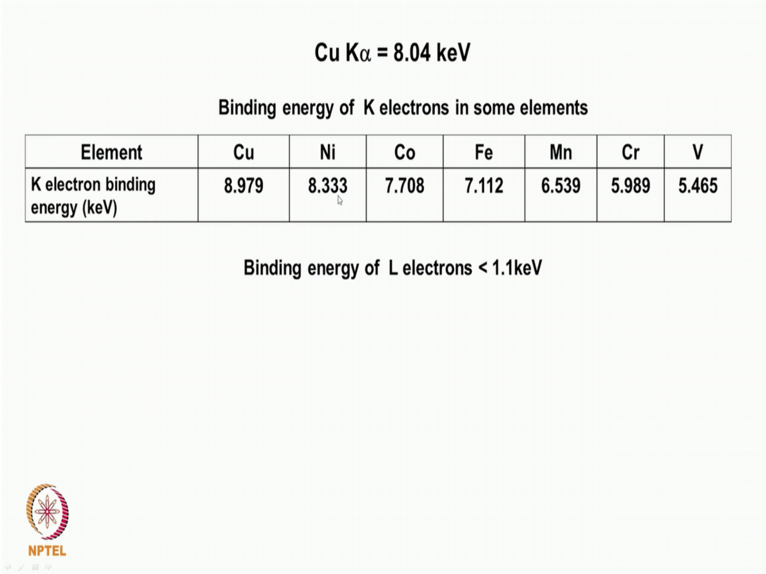

An example which I consider it because then one will be able to understand it much better k alpha energy is 8.04 keV whereas, for k electron binding energy in copper is eight point nine if a sample is containing nickel 8.33. So, it is higher cobalt if it is contains one point we know that if the incident beam has got a X-ray has got an energy which is close to that of the binding energy of the electron to that level it will be observed and re emitted with this energy. So, this we call it as fluorescence which it will be taking place.

So, the incident electron which is available for now scattering to take place their intensities getting reduced considerably correctly. So, if for all these elements if we consider it l l electrons are 1.1 keV only or less than that; that means, that compared to this k alpha energy is very high. So, only copper k alpha energy is very high. So, for the incident beam what matters is with respect to cobalt suppose an alloy is nickel cobalt or nickel ion or nickel chromium then what is going to happen is that the atomic scattering factor is going to be different though if its high energy what the value is now its going to be 2 different values and this is what is written here as a f x equals is that plus another factor f dash plus i and we know that depending upon if lambda omega is slightly greater than lambda r omega is the that is lambda is if it is slightly less than lambda r the resonance frequency then this term is going to negative.

So, now if you look at the atomic scattering factor it is not going to be that same otherwise it is only the disadvantage we consider when its high energy its varying with respect to atomic number no more that happens this is what we can see in.

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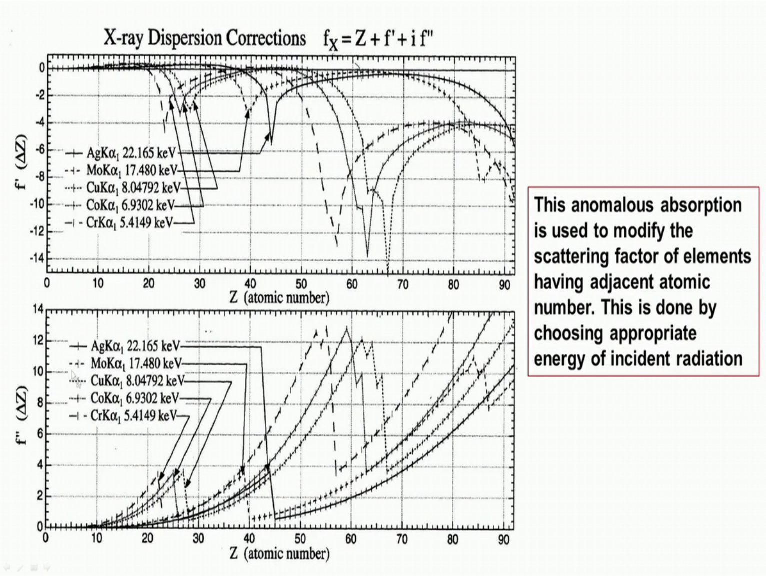

This case that f dash there is a sudden dip quiet it is become negative and if we look at that f 2 dash this also has been calculated you can see that for the same copper if you use it copper k alpha for nickel one it is reducing and another which is increasing. So, the net atomic scattering factor changes this is what is called as anomalous scattering this anomalous scattering could be used to find out ordering in materials that is if the elements have got the atomic number which are closed by if we are not able to differentiate between them suppose an ordering has taken place by using an X-ray which has an energy such that it is above k alpha for 1 and less than k alpha for another then artificially we can change the atomic scattering factor and; that means, that the super lattice reflection intensity when we look at it we write it as f a difference f b and if a and b these values are closed by then it almost turns out to be 0 like that of a disordered material we could not see that order is there by artificially changing these values we can still find out information about ordering this clear.

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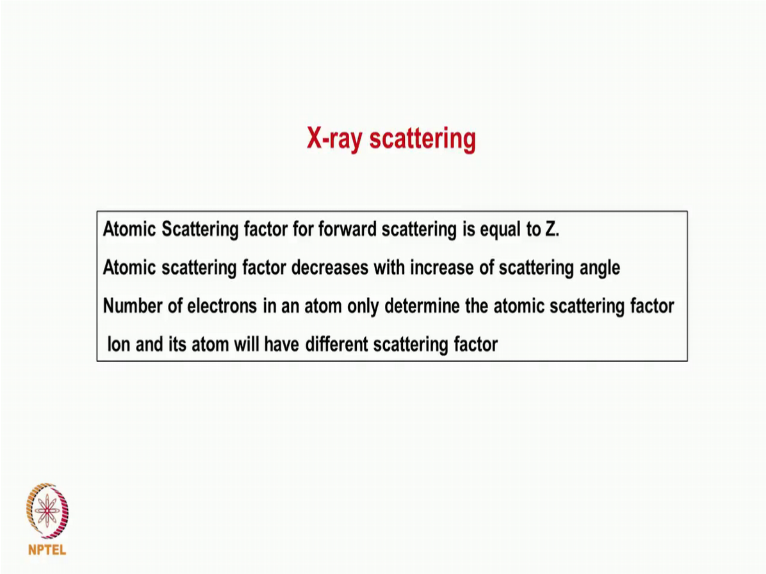

So, in short if we look at an X-ray scattering atomic scattering factor the forward direction if we consider its proportional to this or equal to z, but for all other angles we have to use the table to find out what the value is and that has to be used essentially it decreases with increasing the angle of scattering then number of electrons in any atom only determine the atomic scattering factor then nucleus has no effect what is the information which we get from each of this experiment that is suppose we use X-ray as the probe the information.

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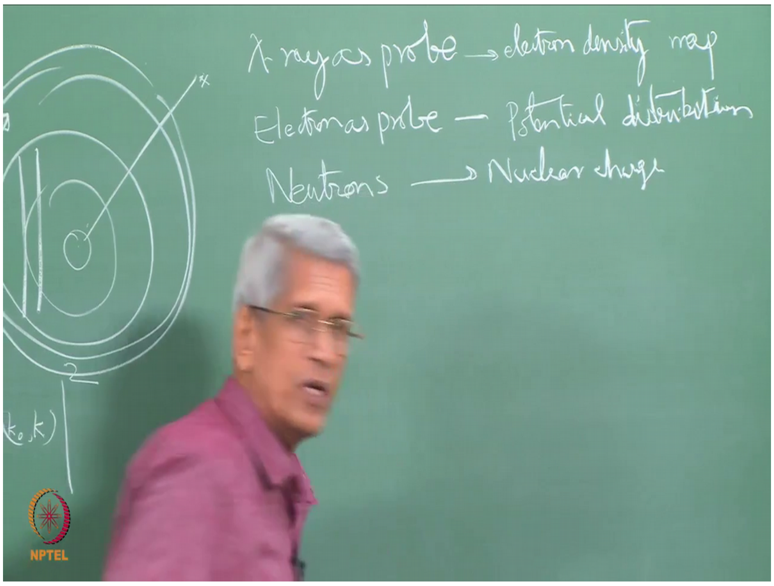

Which we get it is essentially electron density distribution or electron density map on the sample which we can get it if we use electron as a probe the information which we get is essentially potential distribution in the sample because it is essentially the columbic potential with which the electron is interacting. So, how that varies in that sample that mapping what is being done whereas, if we look with neutrons it talks about the nuclear charge. So, how it is getting distributed suppose there are 2 different isotopes are there for the same element each isotope can have a different type of ATO scattering factor and one it could be positive only neutron you find that another could be negative.

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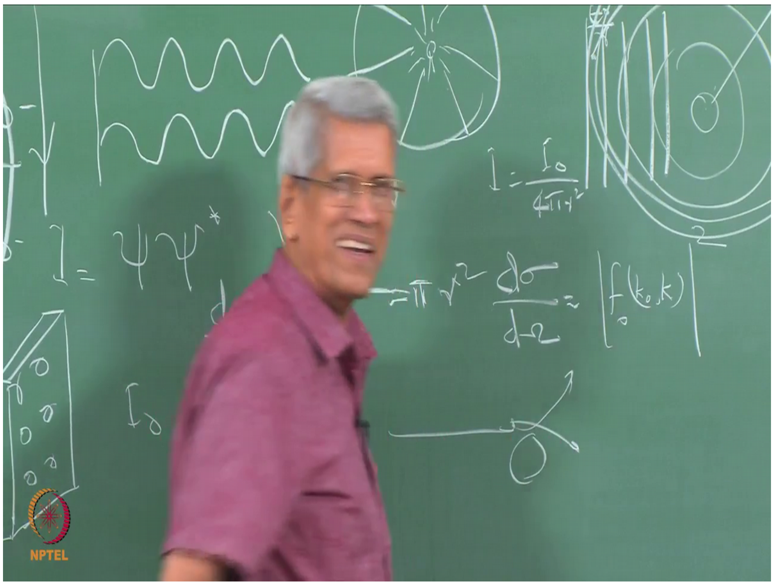

So; that means, that essentially if an it is comes like this in one case its scattered another it may be scattered in this direction. So, this sort of things also have positive and negative atomic scattering factor is possible with neuron. So, isotopes if they are present we can find out how they are distributed in that sample that information neutron can give no other technique can give.

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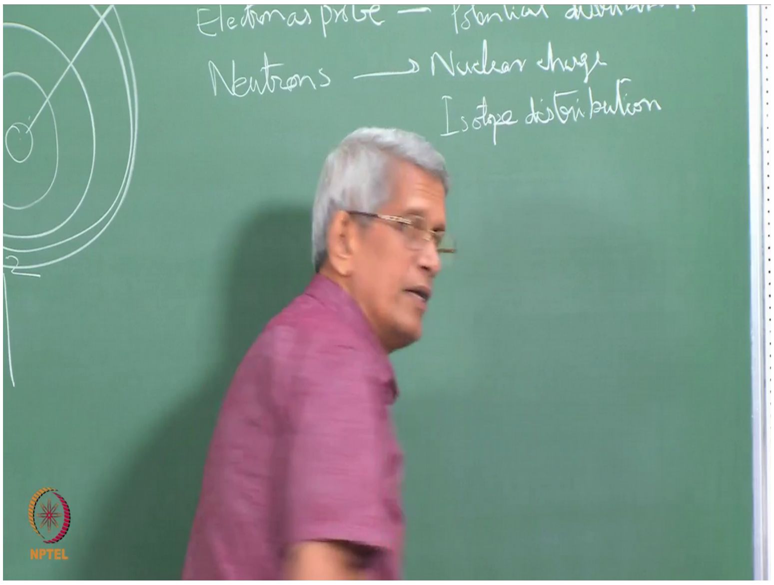

Similarly that is isotope distribution that we can get similarly what we can happen is that when the magnetic since it as a magnetic spin associated with it how the magnetic moments are aligned that distribution also we can get it using neutrons where as in this case its only the electron density this. So, depending this is what is the sort of an interaction which is taking place that interaction is with respect to the in the case of X-ray which is only with respect to a electron. So, how electron density varies that distribution comes in the case of that is in the case of X-ray in the case of electron what is essentially is going to happen is that it is interacting the coulomb interaction with the positive charge or the negative charge or the screen potential

What it is going to be there depending upon that it will get give information about how the potential distribution is going to take place neutron has got many more information all that, but it does not talk about any of this things about potential distribution it talks about with respect to a nucleus isotopic distribution then magnetic movement how it is getting this distributed this sort of information we can get it. So, essentially from X-ray diffraction the information which we get it is it just tells about how the electron density distribution is varying in the sample and generally it peaks around the atomic nucleus that is the way that is information we are actually getting it from an X-ray diffraction work.

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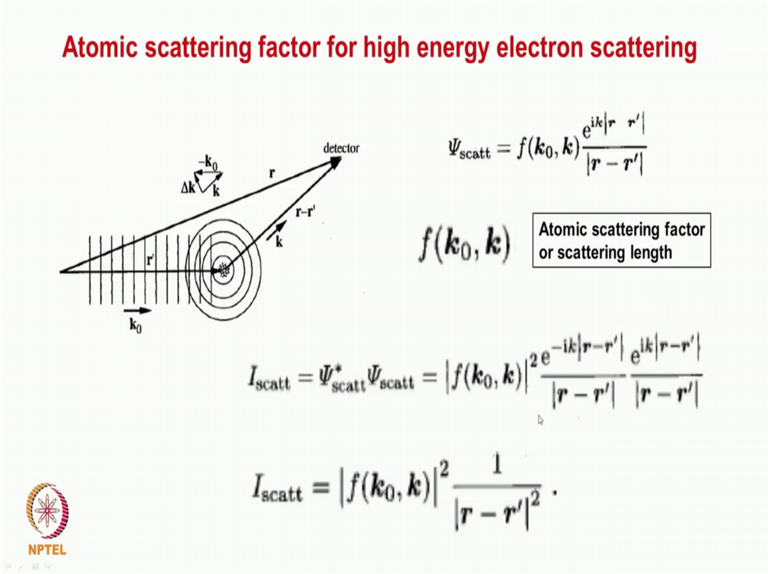

Now, let us take the case of an electron in the case of an electron what is the sort of interaction which is going to take place we could understand what is going to happen in the case of an X-ray in the case of an electron its essentially a interaction between the 2 charges electron the charge of the electron charge of the nucleus and the charge of the electrons which are there surrounding the nucleus in the atom this is essentially a columbic interaction which has to be considered. So, the structure factor when we cont if we look at the scattered intensity we can write it its proportional to sum term for each electron and that depends upon the distance where it is going to be E to the power I k r by r minus r dash because this is essentially from here the primary beam when it is coming electron it is a plane wave when we can just coming and hitting it here spherical wave is being emanated. So, what is going to be the scattered intensity at this particular point this is r minus r dash this is essentially what it has been given this has to be summed over all the this one for each electron and together then we get it with respect to nucleus also has to be taken into consideration.

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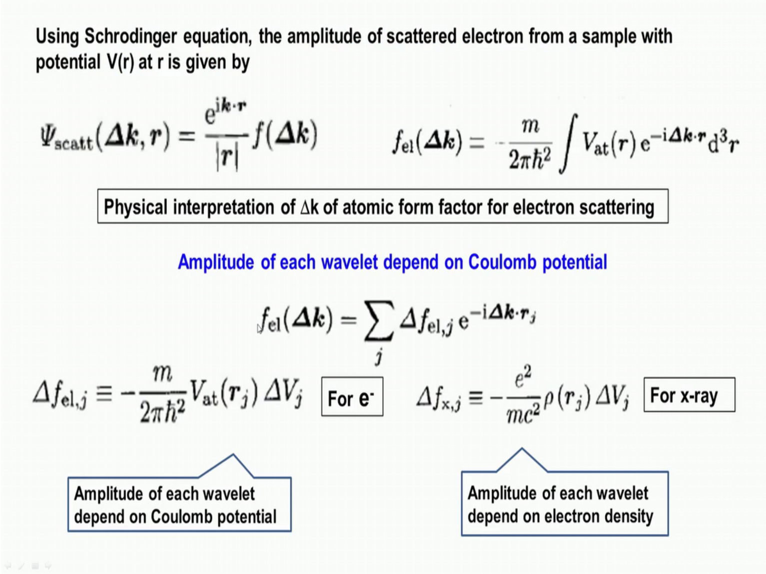

The way in which it can be done is that rigorously if you try to if you want to find out it is a essentially the Schrödinger equation we have to use it, it is an potential field that is a nucleus is there it has some coulomb potential that a high energy electron is coming how it is going to interact that we have to write and the solution will turn out to be is this sort of a form.

What is this? This is in the integration there is a v atomic potential which comes as a function of r and E to the power i delta l k dot r the nucleus itself when these electrons are going to screen it. So, the nucleus charge which the electron depending upon where it comes is going to be different all this factors are coming into the picture suppose we take as like a density this potential also is going to vary we can write this as potential at different points into this factor which we can write it some and essentially that some if you integrate it this sort of an expression will come into the picture the same way we can write it for X-ray also X-ray then that density at each of the point from the nucleus how it is going to be that is what we have to take it. So, essentially amplitude each wave let we take it and that depends upon the coulomb potential.

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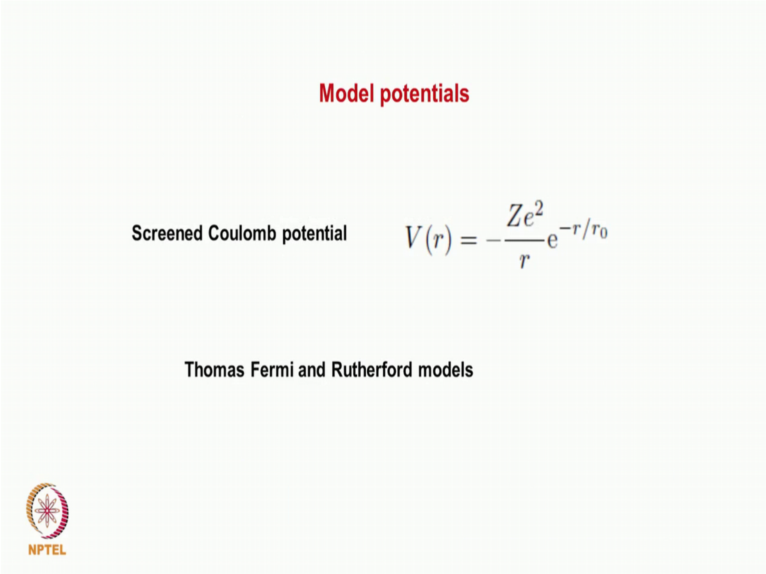

There are many model potentials which we can use it one is a screened coulomb potential we use which depends upon minus z E square by r into E to the power of minus then there are Fermi Thomas Fermi Rutherford models, there are many types of potentials are there their rigorous calculations which are being done as far as the structure factor consideration is concerned there is a different way in which it has been calculated that is what I will talk about it.

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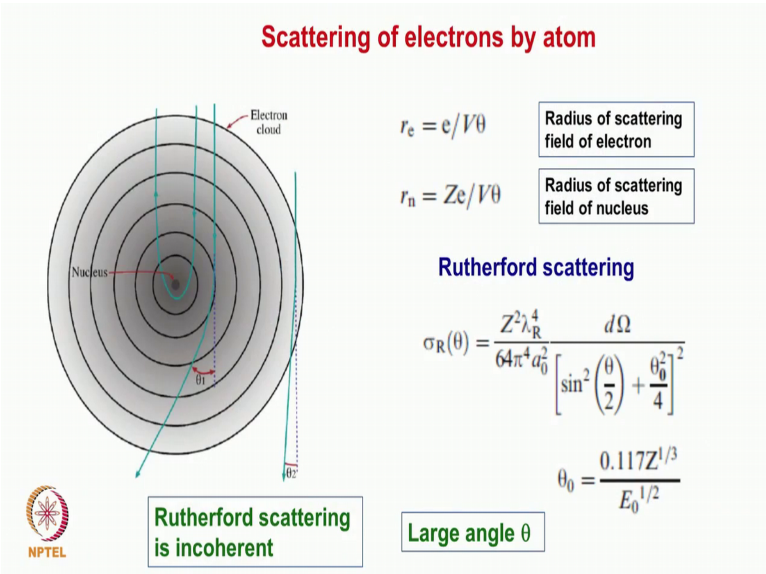

But if you look at the scattering of an electron by an atom if the primary electron is entering which is far away from the atomic core then what it will happen it will be a repulsive interaction between an electron; electron when it is comes close by its going to be a attractive interaction as it is close to the nucleus if it enters it will be deviated at large if it is very close because its moving. So, what it will happen is that it is this itself will be it can come back also as a back scattered electron all this pro type of processes which could occur.

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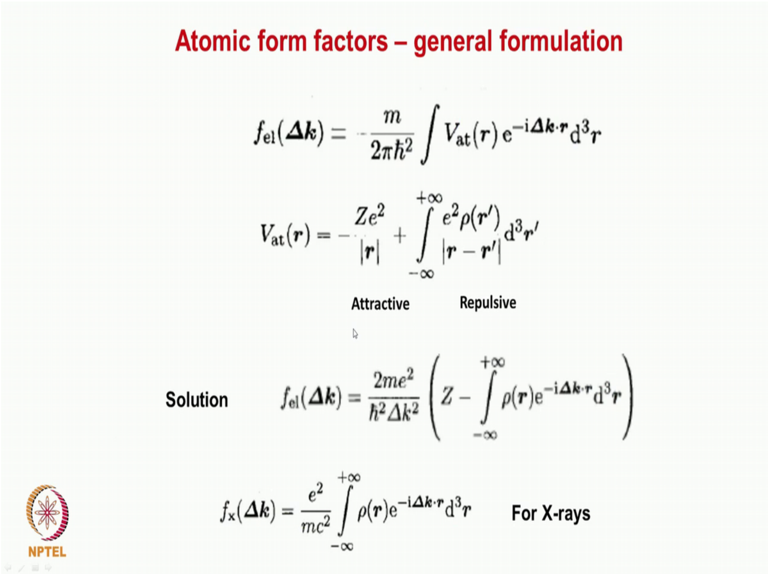

So, then essentially what is important is that depending upon that potential which the electron as it enters whether it enters here or here or here the potential we are is going to change that is what we have to look at it. So, how we can write this; this potential can be written as one there is an attractive potential which depends upon r that is what it is plus there is a repulsive potential away from it this way we can write the potential and if you try to substitute and solve it the details mathematics one can find it turns out to be 2 terms one is depend upon z one term and another is a factor which is depends upon the density of the electrons which are repulsive interaction which is going to be there.

We know that for X-ray the same thing the atomic scatterings are factor if you look at it only this 3 terms E square by m c square otherwise this is the same. So, this term can be substituted with respect f delta k divided by the pre term which is going to be the; that if you substitute then we will be able get an expression like this.

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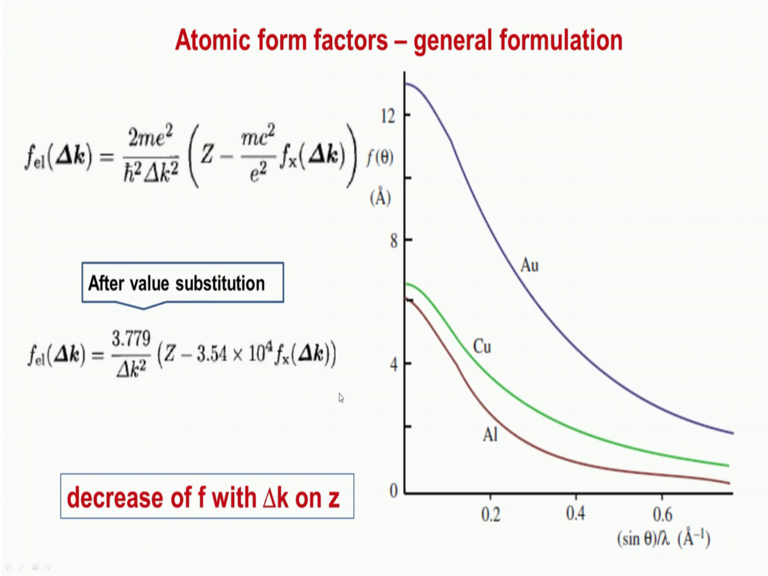

And so, both the nuclear as well as the attractive as a repulsive force both are going to act we can substitute all this values then this is the sort of the expression which we get it now we know z is a charge this has been calculated and this is for f of theta how it is going to be vary as function of sin theta by lambda it is plotted here again we can see that as we go away there is a reduction in the atomic scattering factor maximum is in the forward direction, but now if you should remember that these values no more correspond to the atomic number, but it is as a maximum value for example, if you take copper and then as the angle of scattering increases the contribution is going to decrease.

So, depending upon the type of reflection which we are using it we have to use these values in the case of electron and essentially decrease f decreases with the increase of delta k we can see it is that if it is for aluminum the way it is changing for gold if you see it, it is not that same the drop is going to be different these are all the things which we can qualitatively make out looking at this plot.

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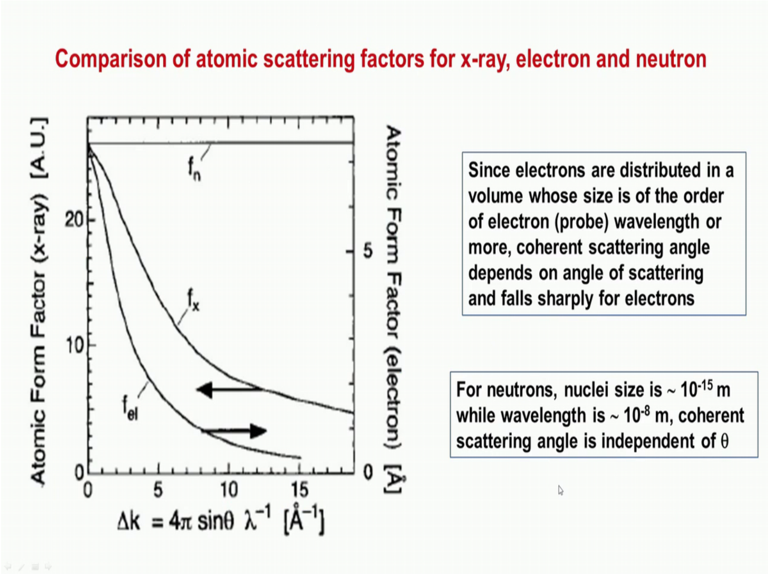

Since the same type of behavior we see both in the case of X-ray for the for the incident cases where the incident beam is an X-ray as well as an electron it is better to have look at a comparison between these 2. So, in the case of an X-ray if you look at it f x if you see the way it drops is rather not that sharp because this is a normalized plot whereas, in the case of an electron it drops very drastically why it happens because for X-ray the wave length is almost the same as that of the intra atomic spacing right whereas, in the case of electron diffraction the energy of the electron is very high.

So, the k is very small correct wave length and that is why we can make out that these and what happens in the case of a neutrons neutron is interacting with the nucleus the wavelength of the neutron also could be which we use this is same as that of the intra atomic spacing, but what happens with respect to the size of the nucleus each nucleon it has to interact with it, but the nucleus size is. So, small compared to the wavelength that from a region like this if we consider it if the wavelength is very large. So, the phase difference delta k dot r f, we try to find out this is going to be extremely small if that value turns out to be very small irrespective of that angle then what is essentially is going to happen is that this value of f n will remain a constant. So, that is what essentially what is going this is one of the advantage that in neutron diffraction the intensity over the angle of scattering which we consider it it remains almost the same is it clear.

So, essentially what we have to look at it is that now what we have to consider is that depending upon whether its electron or X-ray or neutron how as a function of scattering angle the atomic scattering factor changes is different the effect is maximum in the case of electron and nil in the case of neutrons suppose now we are coming back to the case of an the electron scattering.

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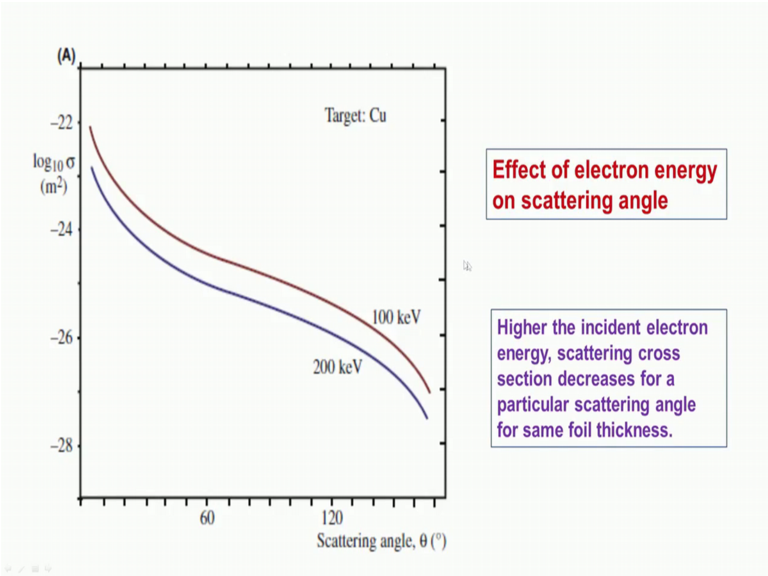

In this if we increase the energy from 100 to 200 keV then what is essentially is going to happen is that for a particular scattering angle we can immediately make out that as the energy is increased the scattering cross section is coming down what is going to be the effect of this; this we will look at it.

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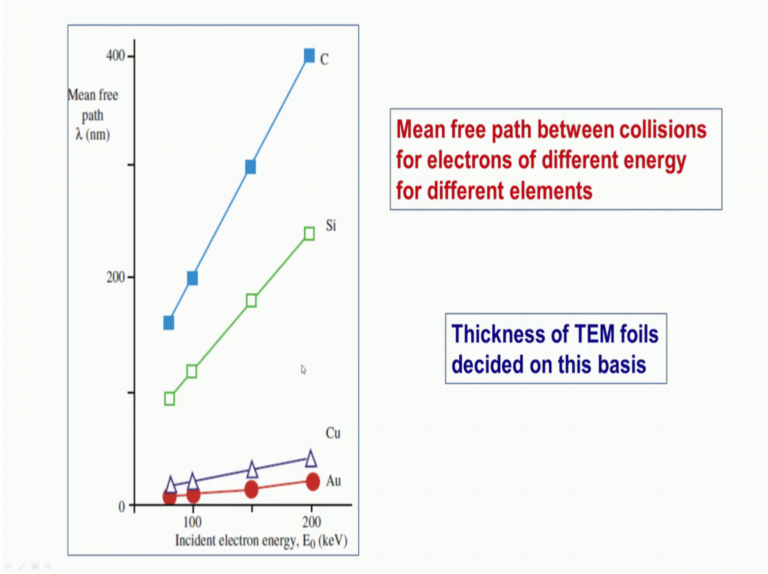

The scattering cross section is going to come down means that f is going to decrease that is one which is going to happen and the; if the interaction is going to be less the probability of elastic scattering taking place is high inelastic scattering is less. So, even a thicker sample could be used and that also comes out if you look at the mean free path also if we try to plot as a function of a incident electron energy we can see that depending upon the atomic number of the element or even for a specific particular copper if you see it that is gradually we see that even for 200 kV that is here we have to use a sample may be about ten nanometer thick this is the mean free path is the means that when the electron engaged to the sample between the first collision to the next collision what is the distance it will travel; that means, that that is where it is going to lose energy in-elastically. So, thicker samples could be used.

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Atomic scattering factor for 200 keV electrons

s	0.0	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.5	0.6	0.7	0.8	0.9
Ti^{+4}	–	55.81	15.78	8.264	5.526	4.158	3.326	2.751	2.320	1.706	1.291	1.001	0.796	0.649
Ti	12.14	11.02	8.617	6.459	4.957	3.956	3.254	2.730	2.318	1.711	1.294	1.003	0.797	0.649
V^{+5}	–	68.76	18.75	9.421	6.075	4.451	3.499	2.867	2.407	1.771	1.347	1.050	0.837	0.681
V	11.50	10.53	8.404	6.423	4.993	4.014	3.319	2.797	2.385	1.776	1.352	1.052	0.838	0.682
Cr^{+4}	–	55.92	15.88	8.373	5.639	4.275	3.447	2.875	2.446	1.828	1.403	1.099	0.877	0.715
Cr	9.676	8.946	7.373	5.896	4.783	3.965	3.342	2.849	2.449	1.839	1.409	1.101	0.878	0.715
Mn^{+2}	–	30.55	10.41	6.471	4.891	3.986	3.358	2.875	2.485	1.887	1.458	1.146	0.917	0.748
Mn	10.40	9.649	7.950	6.270	4.986	4.069	3.401	2.893	2.490	1.885	1.457	1.145	0.917	0.748
Fe^{+2}	–	30.49	10.36	6.442	4.879	3.991	3.377	2.904	2.521	1.931	1.504	1.189	0.955	0.780
Fe	9.934	9.261	7.726	6.172	4.958	4.074	3.424	2.926	2.529	1.930	1.502	1.188	0.955	0.780
Co^{+2}	–	30.42	10.31	6.403	4.857	3.986	3.385	2.924	2.549	1.969	1.544	1.228	0.991	0.811
Co	9.503	8.899	7.505	6.064	4.916	4.067	3.436	2.949	2.559	1.969	1.543	1.227	0.991	0.811
Ni^{+2}	–	30.35	10.25	6.357	4.829	3.973	3.387	2.937	2.571	2.001	1.581	1.265	1.025	0.842
Ni	9.108	8.562	7.290	5.953	4.866	4.051	3.440	2.965	2.583	2.002	1.580	1.264	1.024	0.842

f – highly sensitive to chemical state of atom

Atomic form factors for other electron energies can be calculated by multiplying by the factor

F= ($\gamma = 1 + \frac{E}{m_e c^2} \simeq 1 + \frac{E[\text{keV}]}{511}$)/(1+(200/511)) ($\Delta k = 4\pi s$) (F in units of length)

Here again taken from the book i am just giving what is the for 2 hundred k v what is going to be the atomic scattering factor here what is essentially important is that if you see here titanium four plus ion or titanium for small angles if you try to see it that is the large variation in the atomic scattering factor the effect of this is going to be reflected in the intensity of the X-ray intensity of the diffraction peaks this could be used to tell also or to identify that whether which chemical state it is there if one tries to quantitatively determine the electron intensity we can do. In fact, the present day microscopes are fitted with detectors we can almost do every electron could be counted and the dynamic range is. So, large that X-ray diffraction pattern earlier the problem was getting information from electron diffraction counting all the electrons even the central beam is going to be difficult now detectors are available with which it could be done. So, that we can do one to one comparison and using the diffraction pattern itself we can find out in which sort of chemical state it is extinct that is also possible in principle.

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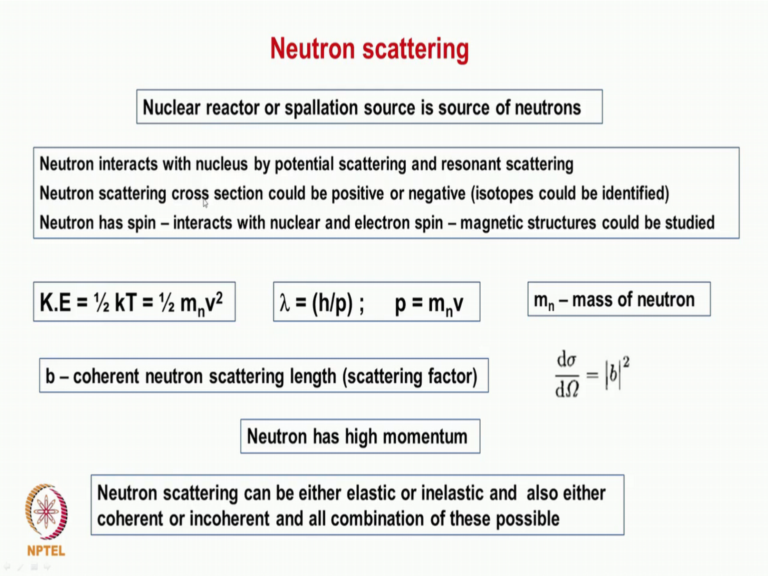

In the case of neutron scattering what happens essentially the mass of the neutron is high. So, the momentum is going to be k is going to be high correct momentum is that is what essentially we have to consider it, but the advantage is that since it has got a spin associated with it we will stop here now.