Electron Diffraction and Imaging

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Lecture – 19
Kinematical and Dynamical Theory of Diffraction and Imaging

Welcome you all to this course on diffraction and imaging. In the last few classes I had covered the different modes of diffraction like, parallel beam diffraction, convergent beam diffraction, and divergent beam diffraction and some of the applications. In a microscope apart from getting diffraction from different regions of the sample we can get information about the, how the image itself looks like right in addition to diffraction. So, how the contrast arises in the microscope? That is what we will discuss about it. Earlier itself I mentioned that in crystalline material the contrast comes from or we call it as a diffraction contrast; that means, that the whatever the diffraction phenomenon which is occurring is responsible for the main contrast mechanism ok.

So, essentially we have to use the formulas which we have derived for finding out contrast from different regions of the sample, that what has to be done. And this is one with respect to a perfect sample and mainly the contrast arises in a perfect sample if it is a polycrystalline material, from one region to another region orientations could be different. The extent of scattering could be different that will give rise to a contrast. And if it is within a grain various types of defects which are present. They would also bring about displacement of atoms from their normal position which will give rise to contrast.

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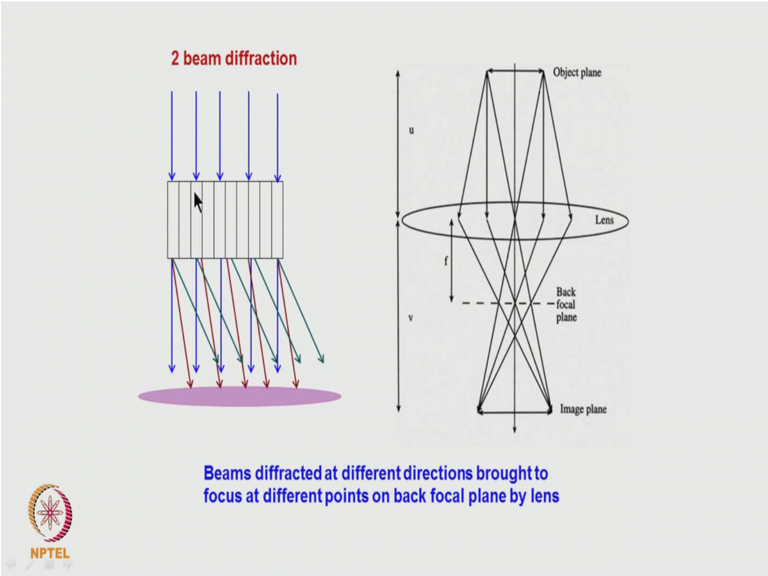

So, these are all the various types of defects this which I had mentioned long time back. So, I am not going into it. So, essentially when we have a sample like this and all the planes are arranged like this. If you consider a beam which is entering like this and when it comes out as the beam passes through the sample, this may be consisting of many unit cells arranged one on top of the other.

So, if there is variate so, even if it is a perfect crystal, if there is a some scattering which is going to take place from every depth into the diffracted direction, the amplitude of the wave which comes out is going to be different right. So, depending upon the composition suppose this region contains ordered alloy another region contains a disordered alloy. So, they extent of contribution to the scattered wave will be different in these region and may be from this region. So, there will be a variation in the intensity of the transmitted beam itself. So, if we look at the back of the sample in a what essentially we get it is a variation in amplitude of the transmitted beam. Beam which is transmitted in this particular direction the same as the direction in which the beam has entered.

Similar to this, in the scattered direction also there will be variation is going to be there. So, this variation if we see it in the transmitted beam alone and try to magnify it by using lenses then we are able to get some variation in contrast that is what we call as that image right, that is what we normally do.

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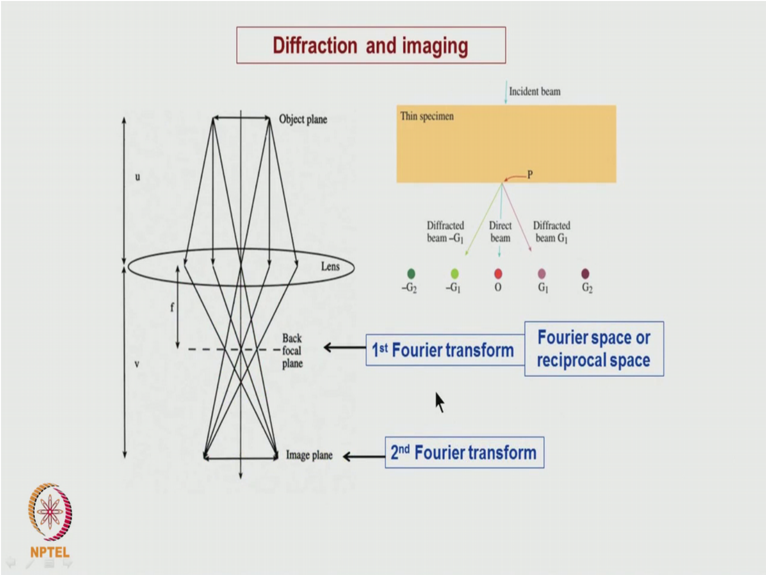

So, this we can understand it in a way that when the beam an incident beam enters this is the direct beam and there is a waves which are scattered in different direction. And the we have derived earlier expressions for finding out the intensity of each of that amplitude of each of the diffracted beam and also it is intensity right, that is under a kinematical condition ok.

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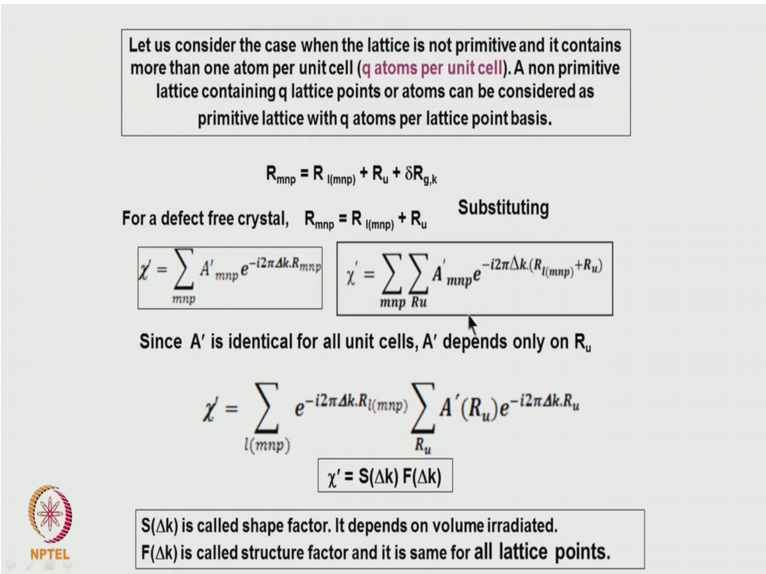

What we will do it is now we will go back and we extent it further. So, the total amplitude in a particular scattered direction essentially depends upon the intensity which is scattered in that particular direction from the full volume in which, full volume of the sample which is illuminated by the electron beam. Correct? That is if an electron beam is falling onto the sample like this ok.

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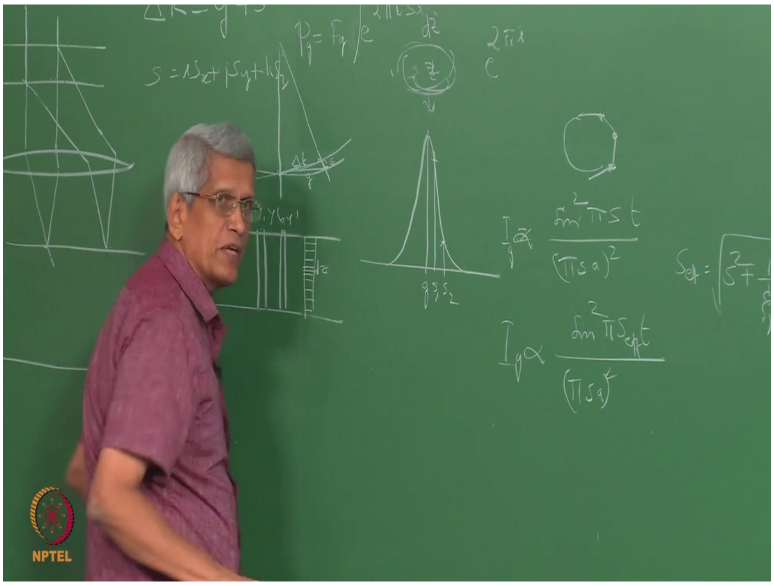

This is essentially the transmitted beam and you see that from this region diffracted beam is going to be there. If we put a lens what the lens does it is at the back focal plane, all these rays are focused together ok.

So, we get the diffraction spots, but since the diffraction spot is a concentrated one. We are not able to see the variation in intensity there right, but if that same area which is there is magnified and we see it in the image plane. So, the image plane we are able to see the contrast which arises, but essentially what we see it is nothing but the variation which has taken place because of the diffraction which is occurring in a specific direction. So, many directions it will be taking place, normally when we do microscopy we use a technique which is called as a 2 beam condition. That is a transmitted beam and a diffracted beam; that means, that the sample is tilted in such a way that only one space particular planes are stronger, oriented for strong diffraction ok.

So, if we consider that, then we know that that every atom position which is there that volume can be taken as one corresponding to a unit. primitive unit cell plus the one which corresponds to primitive or a non primitive unit cell, that is as one cell plus one which corresponds to that atoms positions in the unit cell plus this corresponds to a position which is the if a defects is there in the defect there is a slight displacement of the atoms from that position, this is what it tells about the atom positions in the. And this finally, the expression which we have derived earlier, is one which it corresponds to within the unit cell which we call it as a structure factor. And the whole volume which we consider is essentially the shape factor. This together gives the amplitude of the each of the scattered diffraction spot which will be coming, correct? Ok.

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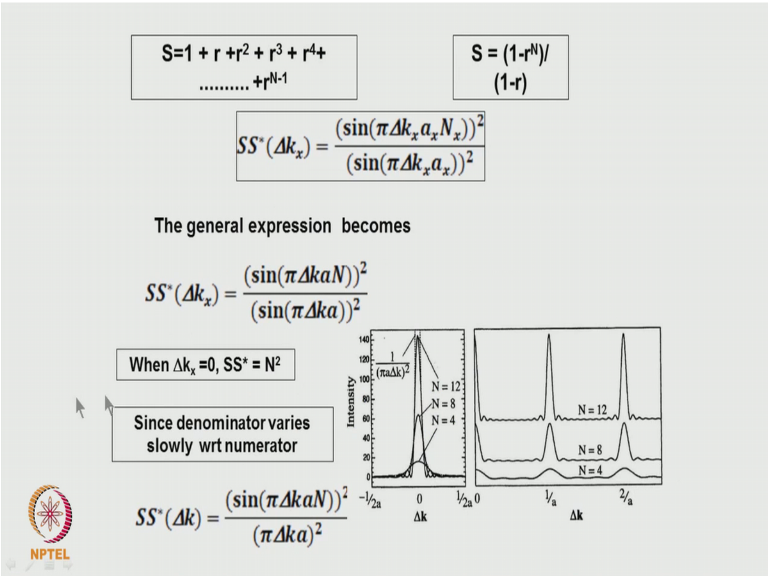

Then we have derived this expression that is the structure factor we know that for every unit cell it is going to be the same, but the shape factor turns out to be this sort of a value will come sin pi. And if you look at it how this shape looks like, this is how the shape is and here we can make out that away from the exact brag condition also there is some intensity which we can see it. So, that condition we normally write it as delta k equals is that as g plus S the right essentially this is equivalent to suppose diffraction spots are here like this if the ewalds sphere passes through 2 spots together then we say that the there no deviation exact Bragg condition is satisfied. If the ewalds sphere is slightly tilted, then we can do it is from here to here this is g, this is the delta k from here to here this will be g plus s. And that sin depends upon how we have fix the coordinate ok.

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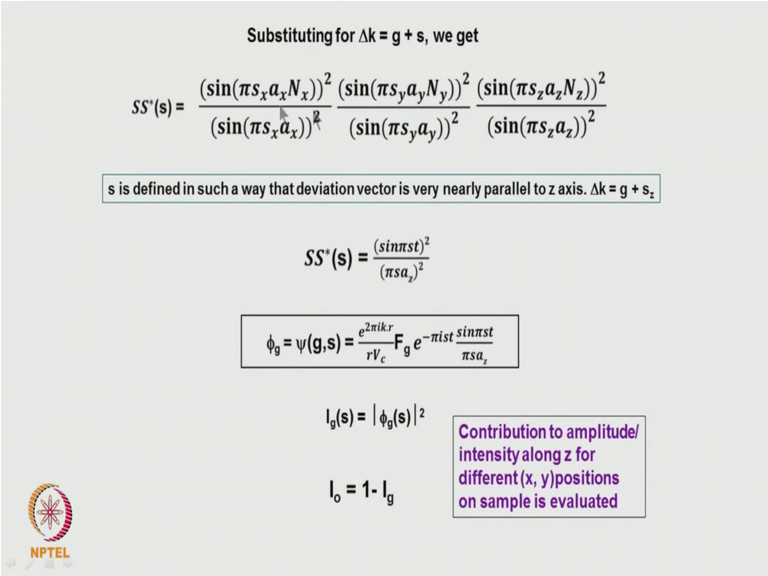

So, instead of this delta k if we substitute this is an expression which is a general one, but x y z is a direction this will have components. So, this is what the expression for the shape factor turns out to be. The total intensity if we look at it this multiplied by the structure factor will give the structure factor square will give the total intensity. And the when we put g plus S, then what is going to happen is that g dot a because a is a lattice translation vector a x. So, if g x plus this one if you take it that is a integer. So, because of that what is going to happen is that all these terms that only the S will come into the picture, the factors will not be there. Here what we have considered as S equal to the vector is written as i into S x plus j into S y plus k into S z. But normally in microscopy one assumption which is being made. The assumption is that the deviation in the Bragg condition is only is only in the exact direction, other directions the directions the deviations are 0 ok.

If we make that assumption then when S y and S z becomes 0 then what this term will turn out to be? Will turn to be that N y square and N z square, right? Because from the, the hospital rule this will. So, only this term which is going to be there, correct? So, this will be the amplitude which will give, this term which is because when a scattering takes place from a particular point and the intensity we are measuring it to the point which is far away are then this will give e to the power of 2 pi k dot r by r will come. And this is the divided by the volume of the area if you take it per unit volume we will be getting this amplitude. So, amplitudes square give the intensity correct, and intensity of the if it is a 2 beam condition, intensity of the transmitted beam will be i minus i g. This is all along a particular value of is a that is for a specific value on x and y that is we are doing it. Right because this intensity if you look at it, this a z into n will turn out to be t. So, this is the expression which we will get it ok.

This is along the sample along a particular column which we are doing this calculation. So, with respect to a coordinate system which we are chosen. This may have some value of x and y and z. So, like that we can say another x and y value we can have. And along this column is that we can find out what the intensity Is, this is how an intensity has to be calculated to find out how the contrast is going to come. Is it not? If we do that essentially we get a mapping of that intensity at the back of the sample, with respect to a transmitted beam we can find out. Similarly with respect to that diffracted beam also. Is that clear? So, that way we can find out the intensity distribution.

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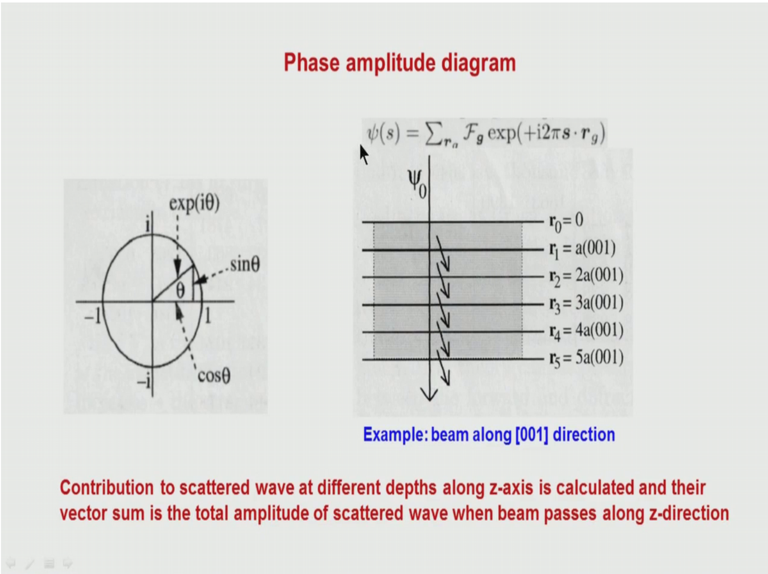

There is an another way which it can be done, that is because when we look at the scattered intensity with respect this is sigma into r g over the various unit cells which are there F g into exponential 2 pi S dot r g it will comes. R is that position of that x y and they said position. Essentially in we are adding the various waves, Right? This is mathematical way in which we can do it. There is a graphical way in which we can also do it. In a graphical representation what we do it is since it is a complex one, the real part and you know, in a complex plane this can be represented as an amplitude and an angle theta we can represent it. Correct? That way also we can represent if we represent it that way, then from here when it comes something has been scattered, amplitude. Then if you see from here the position of r is changing right, as we go along this column; that means, that here r 0 x y it is a x y z 0 it is consider origin, e z equals 0. Then the e z value is going on changing it; that means, that this phase time is continuously changing this phase time changes in the change in phase time is equivalent to change of this angle theta, e to the power of i theta. So, now, we can plot this as an amplitude phase or phasor diagram right.

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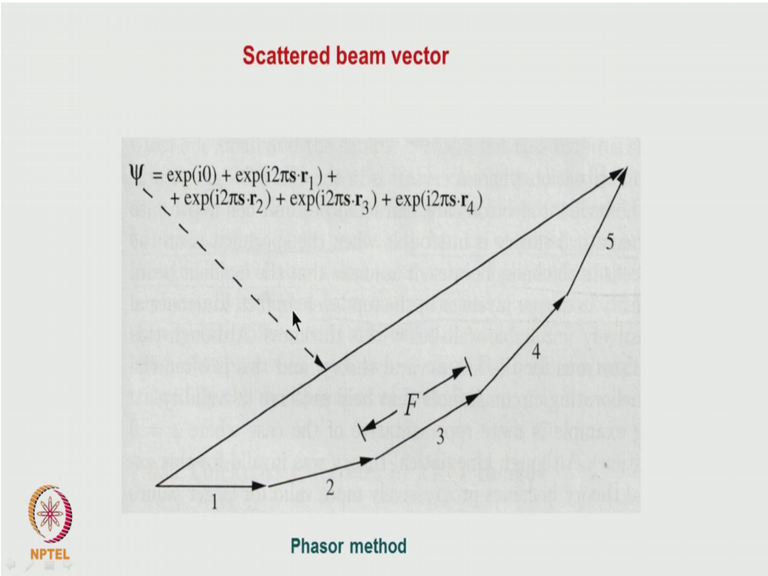

That means that this is a first wave at the top the next one. So, like that it comes and now if you see the resultant amplitude, this gives the amplitude of the wave, right? This is one this is an another way in which we can look at it. Is this clear? Because one we have calculated using the mathematical expression which is there directly found out that intensity.

Another is along that column using this ah, phasor diagram also we can find what is going to be the amplitude, and what is going to be the angle theta which we can find out. And then this is suppose we assume that this is the net amplitude of the scattered wave ok.

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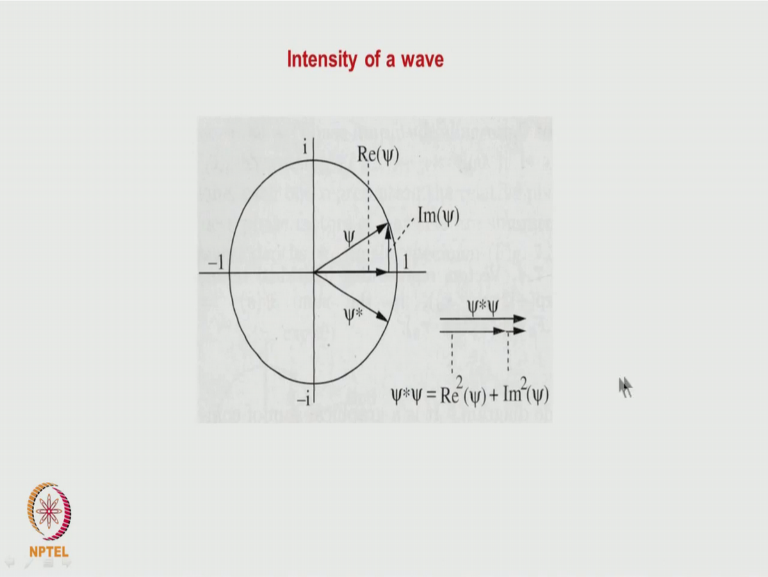

Then if we have to find out the intensity the psi psi star has to be taken. That will always be, if you take it is going to be the intensity is going to be in the real always. That is it is going to be in the plane which is going to be in the real plane or the x axis plane, right? The y axis plane is the imaginary plane when we consider it. So, this is what it gives that intensity. So, irrespective of what the orientation of the amplitude orientation of the wave in the complex plane, if you look at what the intensity is going to be, that does not depend on that, correct?

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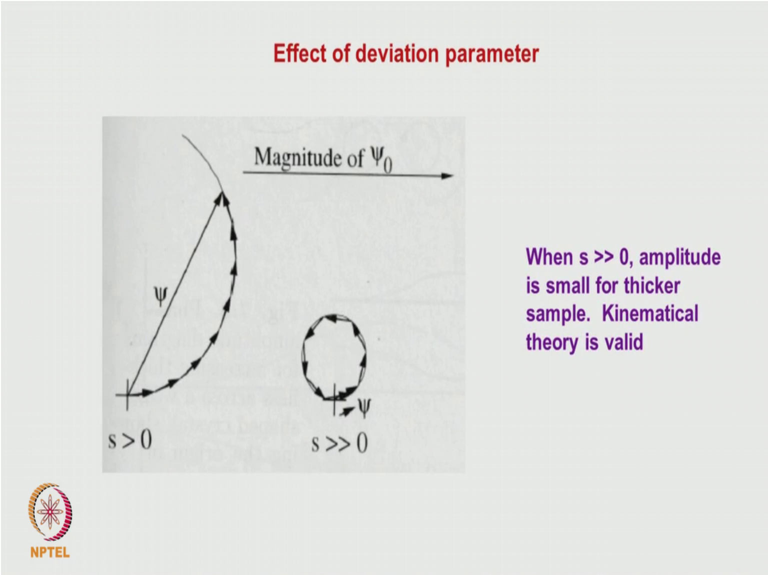

This has some consequence. The consequence essentially is that that expression which we have derived, ok?

It contains e to the power of 2 pi i S into S z or S into t for a thickness of the sample into F g the pi g will be equal to, into S into over a (Refer Time: 16:49) that full region if you see it will be an integral which will come into z d z it will come. Otherwise it can be written as over the full column we have added that also that term, correct? Both the ways we can represent it. The other expression which we have to, I think I will come back to that later.

Suppose the value of S is very large or the value deviation is very small. What will be it is effect on the phase? The phase factor if you consider if S is for a S into r, if you it r S into z is a if we take it if S is small, this term is going to be a small value, right? So, the angle theta is going to be rather small, correct? So, if we take that way, that is what we are trying to do is that, the beam is falling on that sample, but it is not at exact orientation, but there is a small deviation S is there. But it is very close to the Bragg orientation. In such a case what is going to happen is that, if you look at the net amplitude which is going to be there, is going to be rather very large, correct? And there is a problem which comes in that. Because kinematical theory is based on the assumption that only a very small intensities getting scattered amplitude turns out to be large then, when we try to calculate intensities they can be 0 the lot of problems are going to be it does not explain the results also correctly. Instead suppose the value of S turns out to be very large, ok.

Then what is essentially it is going to happen is that, that is if it is g that is we let us consider 2 values of S, S 1 and S 2. S 1 is close to So, the intensity of the or the amplitude of the scattered wave it is going to be very large here. Whereas, here compared to the intensity which you should have at exact Bragg orientation, the intensity is going to be very small for this value; that means, that this corresponds to a condition where the amplitude of the scattered wave is much smaller, much small compared to that of the ah, incident wave, right? So, the kinematical theory is valid in this case. Here how it happens is that, when that is very large since the angle theta what will be the effect of this large S? Because for the same is that S into z is going to turn to be the phase angle is going to be large. So, when the phase angle is large, even for the same it will be one will be coming like this, another will be coming like this, for a few vectors this can go like this can move around in a circle, but overall the amplitude is straining out to be very small compared to the original amplitude of the incident wave.

So, in this condition we will have the kinematical theory is valid. What will be the consequence of it? Which we can we will see it in 2 cases ok.

In this expression also what we are writing is 2 pi i because that intensity when we write it is sin square pi S into t intensity of a transmission is proportional to here, correct? This is a sort of an expression which we have. For a particular value of S you can have a value of t so that this term turns out to be an in small integer, correct? Then what will happen is that the intensity will become 0, depending upon that value the intensity can fluctuate, correct? So, it is for the same value that for a particular value of S we have multiple values of t for which the intensity can go to maximum and come down to minimum, ok.

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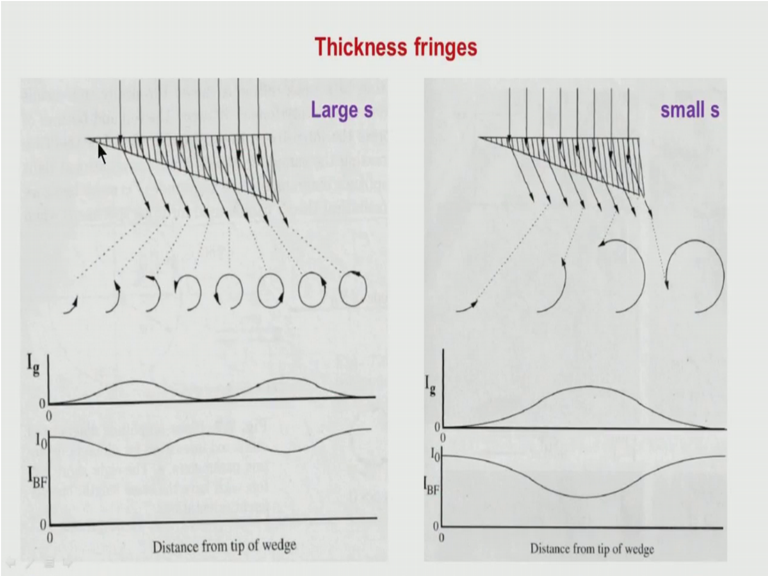

That is what essentially is being shown here. Suppose we have wedge shaped sample. The same parallel beam is falling onto it. Intensity of the diffracted beam if we try to look at it, for this particular thickness, this is using the phasor diagram it has been shown, but essentially what is what we will see it as we go such that either intensity becomes 0. It reaches a maximum value, then it becomes 0, it fluctuates like this. Opposite effect we will be seeing it in the case of a intensity of the diffracted beam or in the bright field or in the dark field, we will getting complimentary contrast, correct? And as per this if S becomes small, what it will happen? The thickness has to be at a larger value the separation at which this from bright to dark and bright dark this fringe contrast will change. So that means, that this is how it will go. Suppose S becomes 0 what happens? There should be uniform intensity that is what a kinematical theory says. What is it seen in practice? That is not the case, there is a variation.

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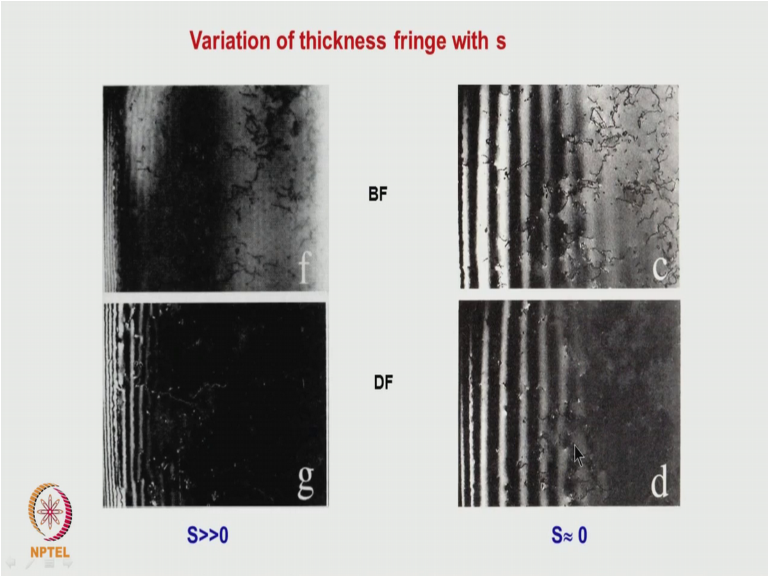

Here this is with the large S been we see that, it is a bright field micrograph closer to the end of it you can see some fringes. And this is in the dark field you can see complimentary fringes could be seen it is taken from the literature. The same sample when it has been taken to S equals 0, you see that the fringes have still seen if the large width bright field bright phenomenon. They are much better contrast. This is what the observation is; that means, that though the kinematical theory is able to explain some of the features under some conditions it is not able to explain completely all the features which we observe in the microscope, especially when a strong diffraction is occurring. Because when, we say that S equals 0 means that it is satisfying the strong diffraction condition ok.

Student: sir why you are saying positive .

No not positive that I am telling yes when it becomes 0. This x this is the expression which is derived know when S becomes 0, what it says that? That is it has to be only uniform intensity, but that is not what is being seen so; that means, that there is something is wrong with the theory which has been developed. This is valid only for when we have a, this theory can be applied only because when S is small or the or the S is large, the deviation from the Bragg condition is large the intensity of the diffracted ray is much smaller compared to that of the transmit. When the intensity of the transmitter and the diffracted beam become very close to each other that takes place under the condition when S becomes equal to 0, under that condition this theory is not able to explain the observed contrast.

So, we have to develop a theory which, that theory is called as the dynamical theory of contrast.

Student: sir this theory does explain the.

At when S is large it is able to explain us, but when S is equal to 0 it is not able to explain; that means, that under all conditions it is not to explain the contrast so.

Student: S 0 we are getting the a large contrast.

The S equals 0 is what we are getting it, by theory there should not be any fringe contrast, but now we have a fringe contrast.

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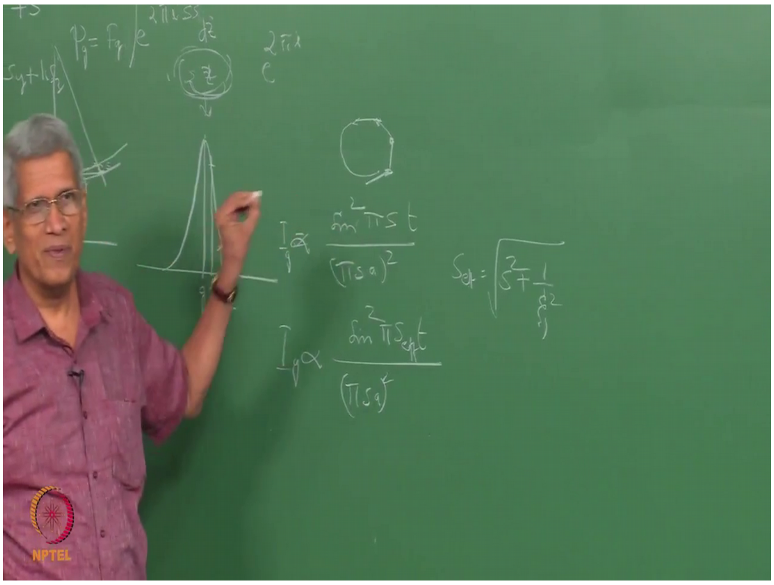

Essentially what happens is that the dynamical theory also gives an expression which is equal to sin square pi it will be written as S effective into t divided by pi S into a the whole square this all will be turning out to be the same. Only thing is that the S now which written as S effective equals root of, this S square the deviation from Bragg condition by 1 by 1 by psi g square it will turn out to be. This we will come to it, how this expression is being derived. I will not go into a full detail of it because it requires great hill of understanding of condensed matter physics we have to go through it which will not do it, but what happens is in this when S becomes 0 still, the S effective is going to be one by psi g, correct? So, this term nowhere becomes 0, you understand that that is why it is able to explain, is it clear?

So, far what we have considered all the amplitude derivation which we have looked into, we are not taken the absorption of the beam as it passes through. That is as if that only the phase is changing there is no other change. But if there is an absorption is, what do you mean by absorption? It is essentially is that if any inelastic scattering is occurring, the primary beam is lost. So, all these things contribute to the reduction in intense reduction in amplitude of the wave, ok.

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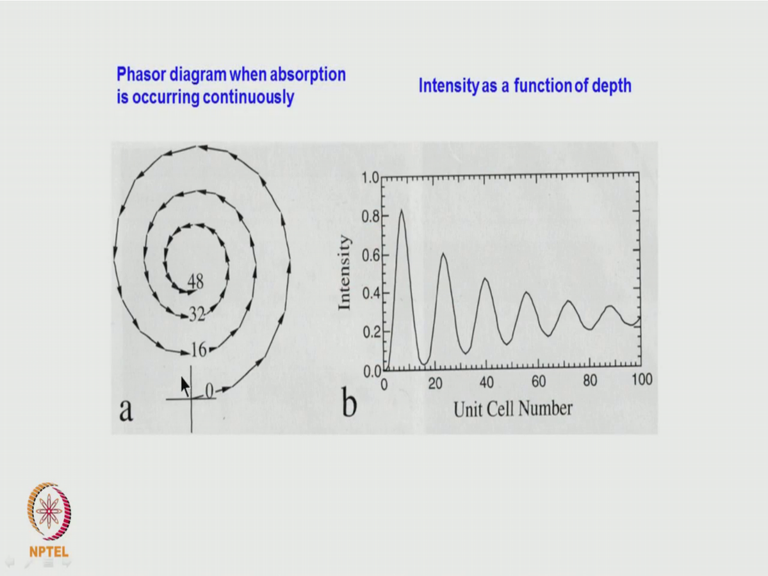

that we call it as an absorption. If that happens then in the same phasor diagram, every time an as the beam enters into the sample, gradually the absorption is also going to increase as it passes through the sample that as it is that increases. That affect will be that amplitude will be reducing, but the phase remains that same the deviation.

So, now if we look at the phasor diagram it will not back not a circle. It will be a helix it will be just going on spiraling inward, but still the same thing could be used to explain how the variation in contrast, this is what it is being done, with the number of unit cells the intensity how it is going to change. But now if we look at it when the thickness is small whatever is the variation in intensity which we see as the sample becomes thick the, intensity variation is going get smeared out gradually, is this clear?

Now So, far we have considered the case, which is for a perfect crystal. Because we assumed that there is no defect which is present. When a defect is present in the sample then in this term delta k dot r m n p that g plus S will come into r l corresponding to the lattice ok.

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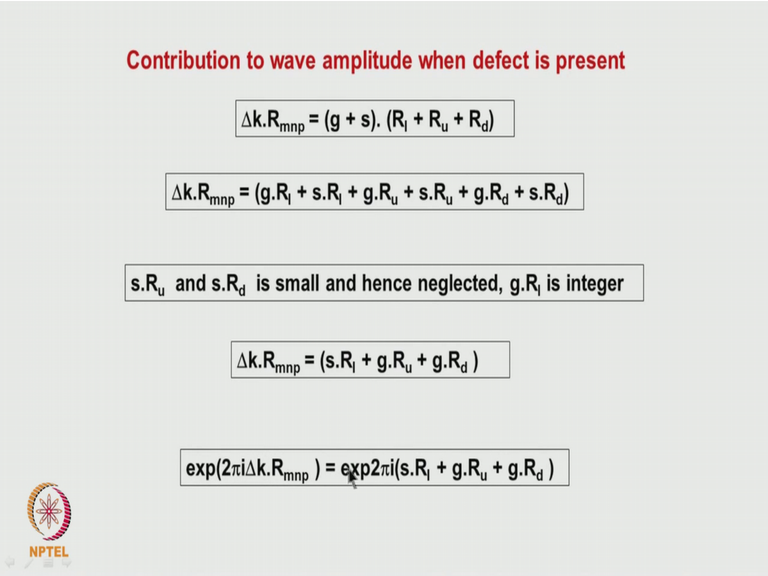

Then r u corresponding to the each of the unit cell, plus r d which is corresponding to that defect which is present at some location. Now if we just expand this expression, g dot R l is the term which is essentially going to be a integer, correct? G is the perfect translation vector, R l is corresponding to a latti different lattice points which represent each different point which represents each unit cell. S is a deviation from the Bragg condition. Because of it what we can see that this dot R u, R u with respect to unit cell, unit cell is a specific cell which we are considering it. There the r u vector is cannot exceed the lattice parameter of the unit cell. So, this if it is small this S dot R u can turn out to be small. Similarly R d is the deviation from the correct position of the atom closer to the defect. So, that deviation is also very small. So, S dot R d will also be small then. So, this can be neglected, because the effect of this close this becoming equal to 0. G dot

R l is going to be an integer. So, now, we will be left with only 3 terms which are going to be there. S dot r l plus g dot R u plus g dot, so.

Student: what is r a r u ideally.

Ah.

Student: sir what is r a r u.

R l.

Student:. So, r l.

R l corresponds to the each unit cell is represented by a form in a lattice point.

Student: r u is.

R u is that with respect to each unit cell, the positions of atoms in the unit cell. R d is corresponding to the defect. That defect which is present at that point the it is deviated from it is not r u that is a small deviation is going to be there.

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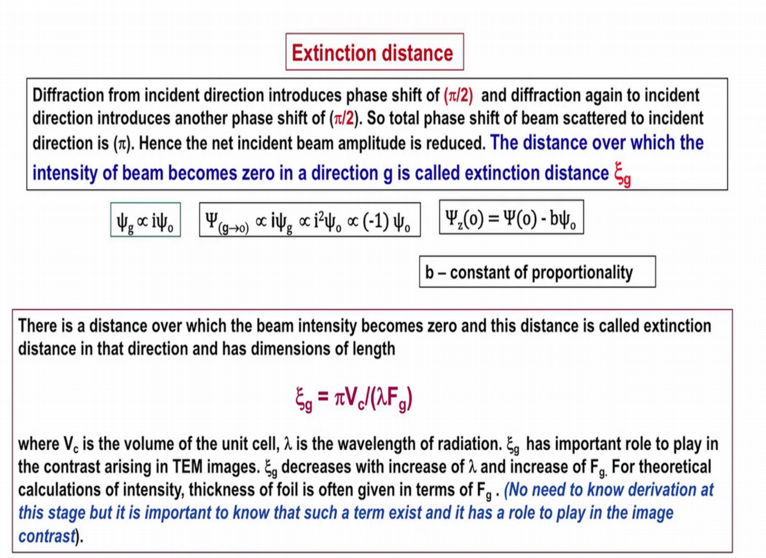

Now, that intensity for, this we have to write it in a expression exponential. This if you try to write it you can see that 2 pi i these 2 terms come together. This term is with respect to a unit cell. If you take summation over R u what does this term turn out to be? Structure factor structure factor and this is summation over the different full volume, but the way this summation we can do it is 2 different ways we can do it. One is the summation over the volume is you take any x y point on that sample and take along insert, like that you go on intra do that summation ok.

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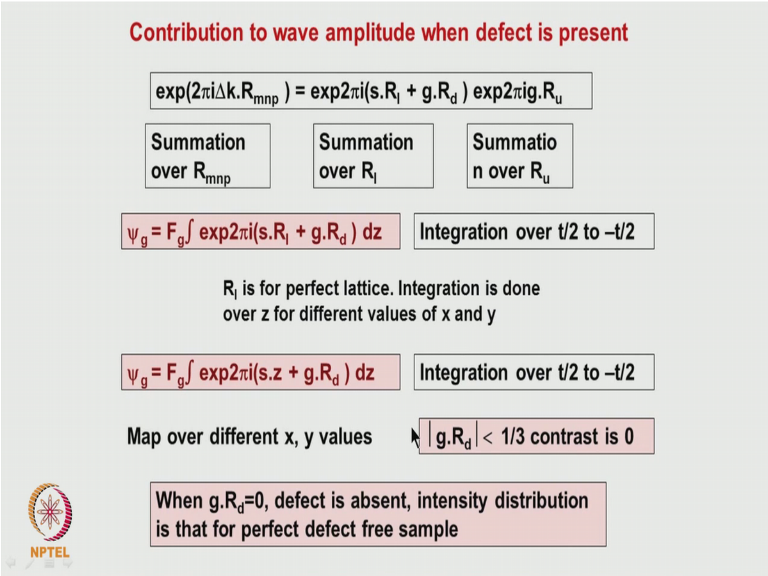

And this summation we can write it as also can be written on integral form. Because since we are taking it with respect to different depths like this in that sample as that is that varies d z. The different unit cell if they are there. We are essentially it is a summation we are taking that can be written as the integral over the full thickness of that sample. If we write it this will become F g into integral 2 pi i, these are all the terms which are going to be there. This term if you look at it, what it corresponds to? With respect to a perfect lattice.

But there is a deviation from the Bragg condition, is it not? What has this term corresponds to is g is the with respect to a reciprocal lattice vector. R d is the deviation from the defect vector, is it not? At some particular position, suppose in this sample we assumed that at this particular region we have the defect is there, so that the lattice parameters there is a expansion or contraction or that could be a rotation. There are different ways in which the replacement can manifest itself. If that is what it happens, and this some integration as some mathematical convenience it is being taken from middle of the sample to minus t 2 by 2. Do not bother about all those. Finally, when we get the integration over z for various values of x and y, we can find out at the back of the sample, how the intensity is going to vary from region to region. So, where the perfect crystal is going to be there in those region intensity will going to be uniform. Where the defect is going to be there will be a variation in intensity or the variation in amplitude will come.

this is that suppose, for some particular value of g because the g is the reciprocal lattice vector. We are using one particular g reciprocal lattice vector for which the displacement vector r d is such that the g dot R becomes 0. Then what will happen? The defect will not be visible, correct? So, as if then the intensity variation is going to be only with respect to whatever is the deviation from the Bragg condition. That, that is what essentially this terms tells is that exact Bragg condition you get some intensity. If the beam is tilted slightly away from the Bragg condition also you get the intensity due to the defect, but the intensity contrast varies. That is what this expression allows you to calculate, but you should remember that all these expression which we are talking is all for kinematical condition, correct? The expression which we are using is a kinematical condition, but if this g dot R d becomes much less than one third, effectively the contrast is going to be very small for all practical purposes we cannot see it. So, this is what it happens. So, with this sort of expression we can do a calculation and that is being done also. I will come to some defects I will take it later and show you how the defect ah, that I will not do it in this class in an another class we will do that ok.

Now So, far we have considered for a perfect crystal when S varies how the intensity is varying, how to calculate the ah, intensity at different points on the sample surface. Then when a defect is present, how the intensity will be changing? That formula we have looked at it using this we can calculate the defect, but specific cases we will consider, but we have seen also that this has the problem. The problem essentially is that all the experimental observations of the contrast this theory is not able to explain completely. Qualitatively it explains quantitatively there is a serious issue, for which we have to develop the dynamical theory ok.

What is dynamical theory? Let us try to have some basic understanding of it, is that if since the electron interacts strongly with matter as the electron beam enters into the material, if it is satisfies the Bragg condition as we were discussing before the class started, what are the Bragg condition? Electron will be strongly scattered ok.

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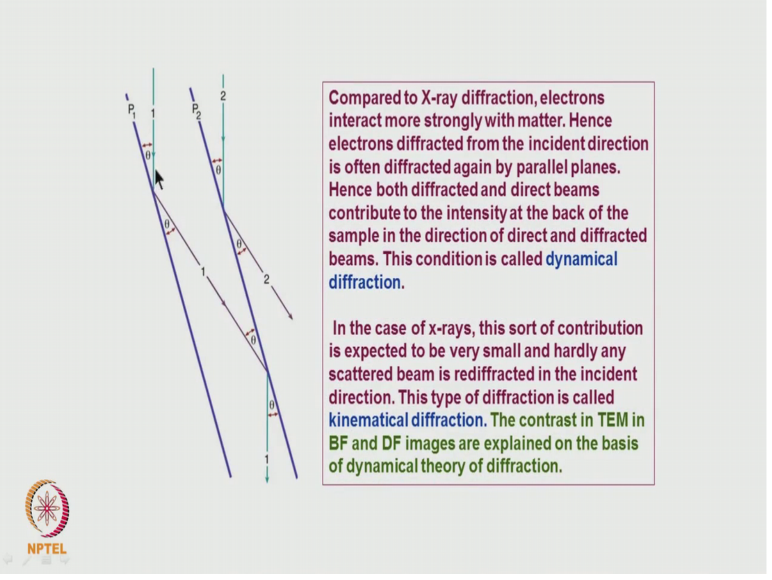

When it is satisfies Bragg condition, and from this plane it will again be scattered back into the transmitted beam. Similarly this beam when it is from the next plane when it scattered will be scattered into. So, like that back and forth there will be a scattering of the intensity is going, but what we should remember that when the wave is getting scattered from one to the other always, there is a factor i comes into the amplitude, correct? That is if we take any beam, a plane wave which is entering the scattered wave if we look at it that intensity will be some proportional to i into psi it will be.

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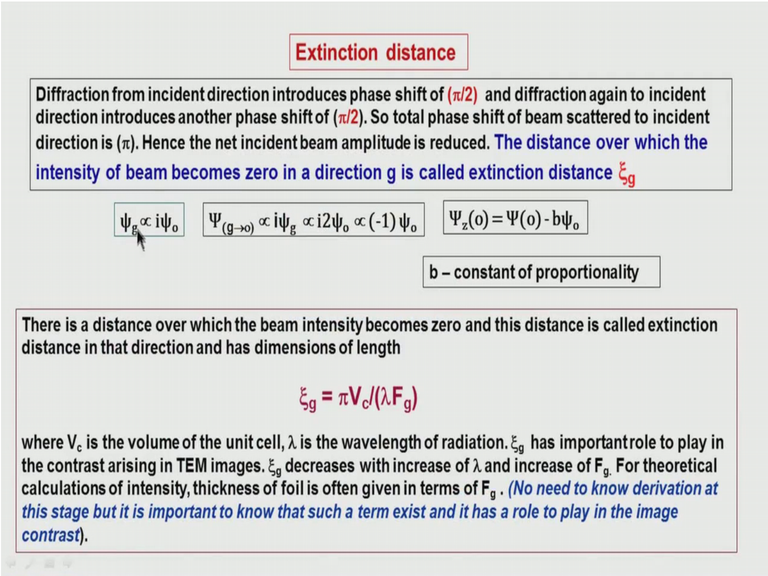

So; that means, 90 degree phase degree always it introduces. So, because of that in the scattered direction g the Bragg diffraction first diffraction which has taken place, this i into psi 0. Then from this g when it scatters back into the original direction, then again i into psi g will come. So, these id you multiply this turns out to be minus into psi zero; that means, that the beam which has been doubly scattered it is out phase with respect to amplitude. So, because of that the amplitude in the scattered direction.

If we try to look at it or amplitude in the transmitted beam if we look at it, it gets reduced faster. The same thing So, there is a particular distance at which the amplitude of the transmitted beam becomes 0. That distance we call it as the extinction distance. That distance depends upon the periodicity in that particular direction. And what all factors this and this called psi g, what all factors it depends on? One it depends upon the volume of the unit cell, that is if the volume of the unit cell is large the scattering is going to be small. So, this psi g becomes large because number of atoms are going to be less. And what is F g? That there is F g is the structure factor, structure fact means that structure factor for a particular scattering. If the structure factor is going to be strong or the structure factor is high, then over a short distance the intensity of the transmitted beam will get reduced; that means, the psi g becomes smaller. So, psi g and structure factor are inversely related.

Similarly, you take the case of the wavelength. If we go on increasing the energy of the electron beam, what will be it is effect on the material? It penetrates, but what happens? It is in a it is the scattering power gets reduced know, as it enters through it is effects will be that psi g will be. So, this will be also in inverse relationship. So, essentially this psi can be written in this sort of a form with pi, but all this things could be derived, this is a qualitative way in which we are looking at it, but this expression is an exact expression, which is derived from the dynamical theory ok.

Now, we will go into a dynamical theory just get some brief idea about it. Because this requires an understanding of quantum mechanics ok.

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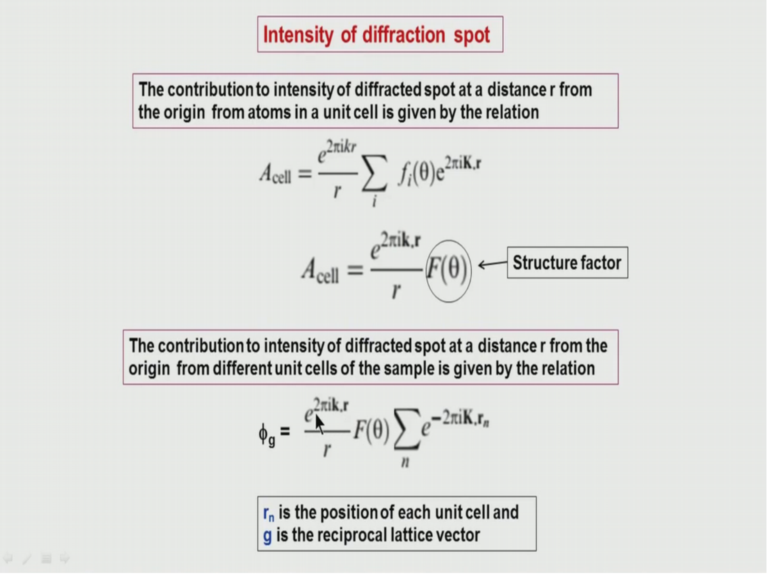

Before going to it what I will try to me tell you is that, that psi of the scattered wave depends upon this term f of theta is the structure factor, correct? And the sigma n this is over the full unit cell which we have to consider. This how phi g for each wave is going to be right.

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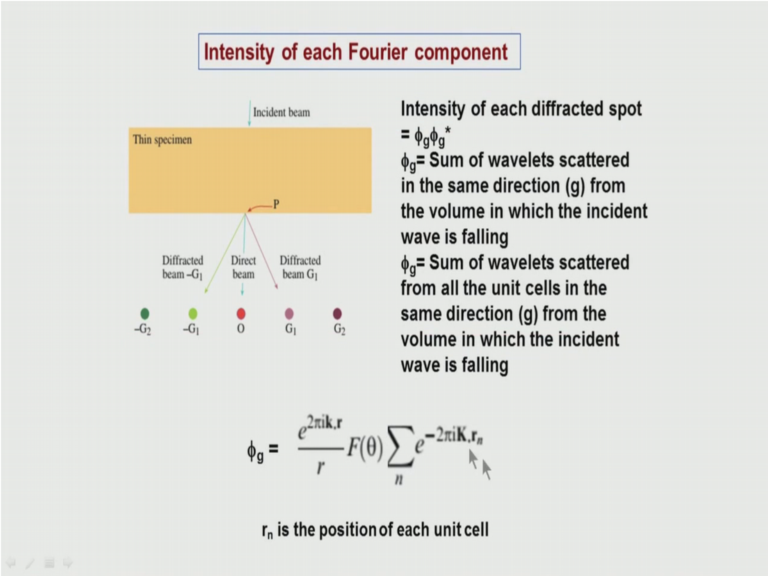

And when an image when we look at it, at every point on the image plane the intensity at the point depends upon how has been scattered in each of the direction, correct? So that means, that the total intensity of the scattered beam, if we look at it.

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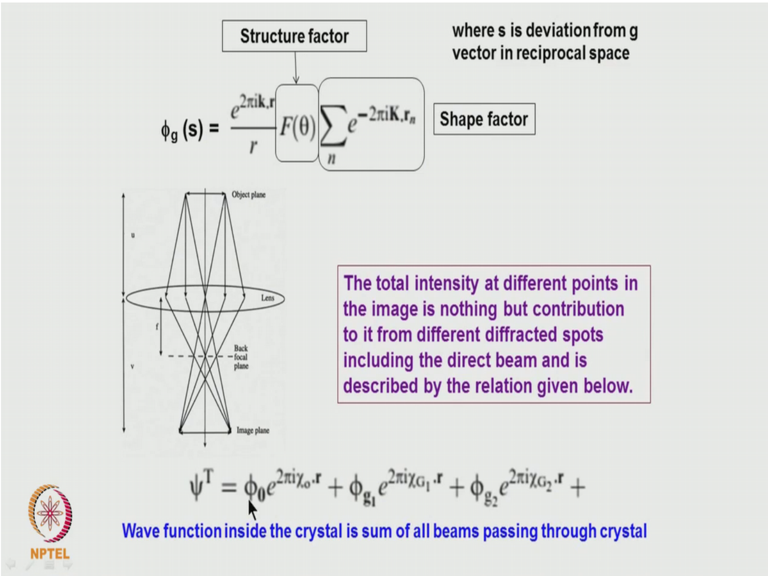

Depends upon the transmitted beam with some phase and then, psi g is with respect to amplitude of the diffracted beam and the direction in which it is coming. Then with respect various beams all of them together determine the total wave amplitude at every point in the image ok.

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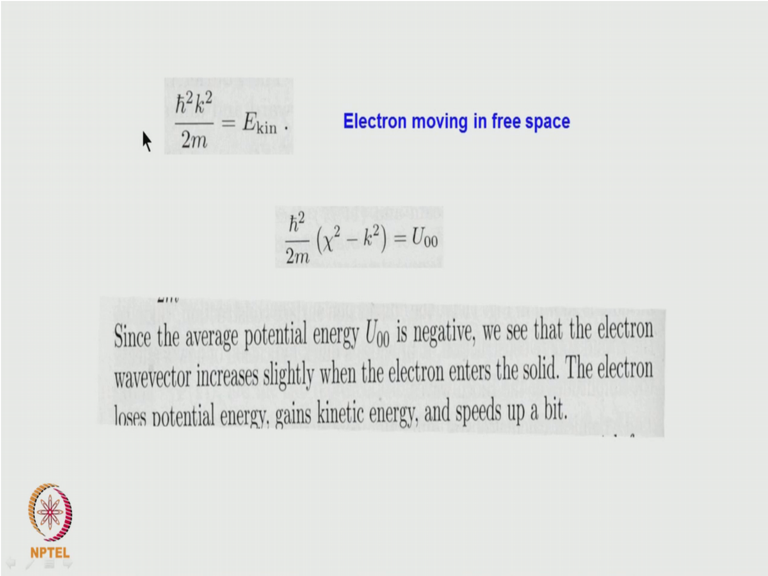

Now, let us come back to the sample again. In a dynamical theory what we assume is that, essentially it is solving schrodinger equation. Electron beam with a high energy and with a value of kinetic energy equal to particular value, which is beyond the accelerating voltage it is entering into the sample. So, for that when it is in vacuum h bar square k square by 2 m will be kinetic. From which we can find out what the value of k is going to be. When the beam enters into the sample ok.

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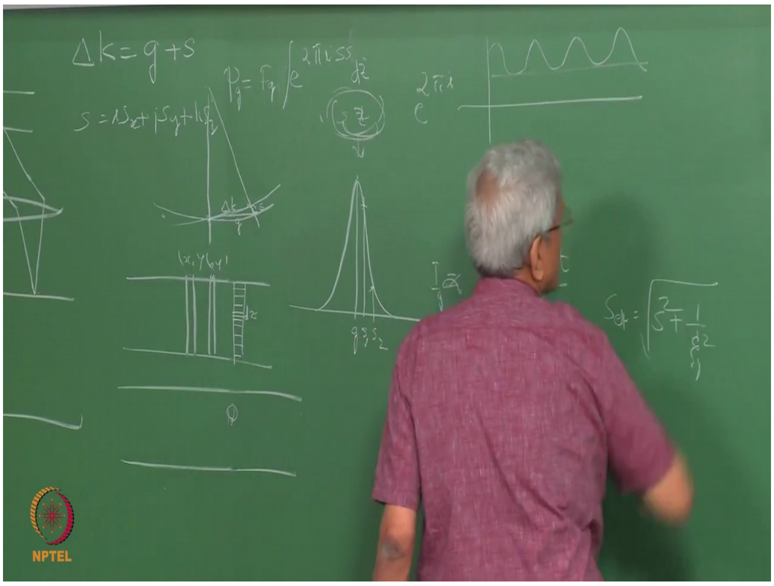

The sample consists of ions which are arranged in a specific position, this gives raise to the periodicity of the potential, right. This periodicity has got 2 aspects which we have to consider it, that is potential may be like is if you assume it is varying; that means, there is an average potential is there over which this fluctuation is going to take place. This average potential, what is going to do? This is a positive phenomenon when the electron enters into it is attracted towards it. So, the energy of the electron as if it is increases a little bit. So, when the electrons enters into the sample, it is k vector is going to different inside the sample compared to when it is outside the sample ok.

Then there is an interaction which is going to take place with respect to the potential. And generally the potential of the material if you look at it most of them are may be 20 to 25. From may be few electron volts to 25 to 30 electron volts whereas, the kinetic energy of the electron which is coming. If you look at the voltage which we are given is 100 or 200 keV. So, it is orders of magnitude difference is going to be there. Still what is essentially it is going to happen is that, there is going to be a variation.

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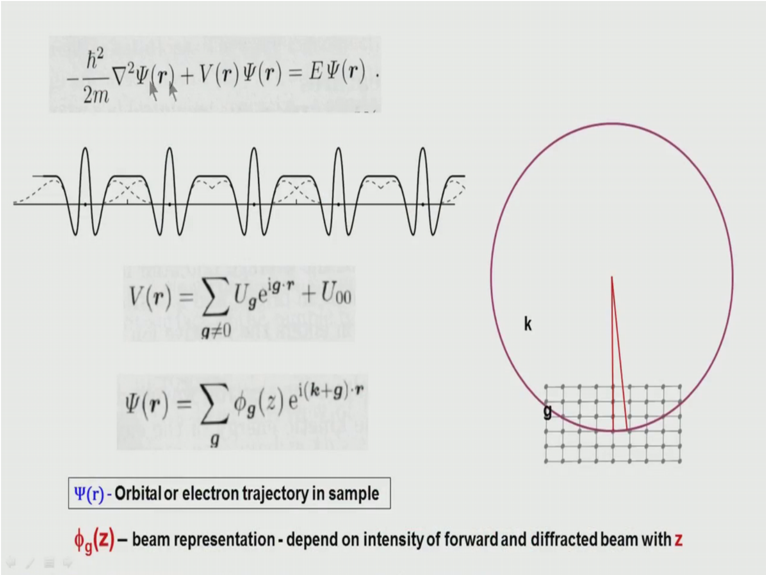

So, in this expression this is the, I had just taken a potential like this. This potential how we can because if we look at it, this is periodically varying potential correct, but it is not sin function right. So, this can be written as, this periodic potential can be written as sigma. We can separate into a Fourier series we can do it. With some period corresponding to g, that is it will this distance if we know that one by inverse of it will be. So, with respect to that 2 g, 3 g like that we can find out then we can write that sigma of this one that sigma of this one, this u g and all for each of that wave which we consider with a particular g frequency.

What is going to be there coefficient corresponding to that Fourier coefficient corresponding to that. This is the way the potential could be represented is it not in the sample, is it clear? Because since atoms are arranged in a periodic fashion, as the electron beam enters into it depending upon where it enters it going to see a different type of a potential. It is kinetic energy is going to change this potential is going to be different. That psi r is that amplitude at every point is also a function of it is written as phi g, which is essentially nothing but the amplitude of the scattered beam it primary beam or the different scattered beam, into e to the power of I k h psi. This is the direction k in which the beam is entered ok.

If this is the next position which corresponds to a reciprocal lattice position, or the atom position is corner there is reciprocal lattice also will be with a inverse in this direction. You assume that this is a reciprocal lattice, then from here to here what it represents? G. So, this vector will represent the beam which the direction in which the diffracted beam is coming. This will represent the diffracted beam coming in a another direction, this will represent the diffracted beam in. So, this terms are going to be essentially that is what in k plus g over all g values. So, in each of the direction you have a wave function which we can write it for that, it is all that is each corresponds to that phase factor plus this is the one which gives which is related to the amplitude of each of the scattered wave. That is how the total intensity, if we substitute in this and try to solve it this is d square psi by d x square. One of the things which we have to keep in mind is that this g can have k can have component k x, k y, k z.

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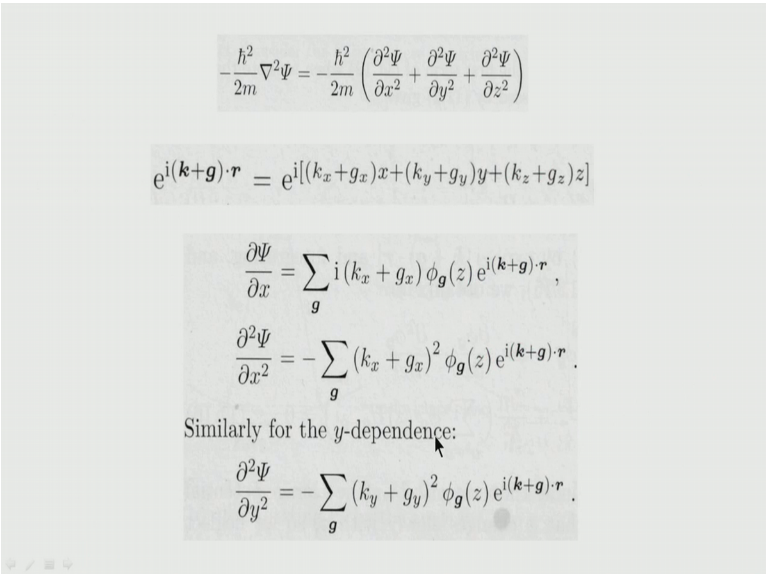

Similarly, g can also have component g x, g y, g z correct? But what normally happens is that, since the energy of the electron beam is very high and compare to the separation between the atoms is going to be small, and we are assuming that the beam is falling in the z direction then the g is almost perpendicular to r right. So, because of that what is going to happen? The g z will turn out to be a 0 term. Only g x and g, then if we just this is just an mathematical you just substitute, The this one simplify it algebra.

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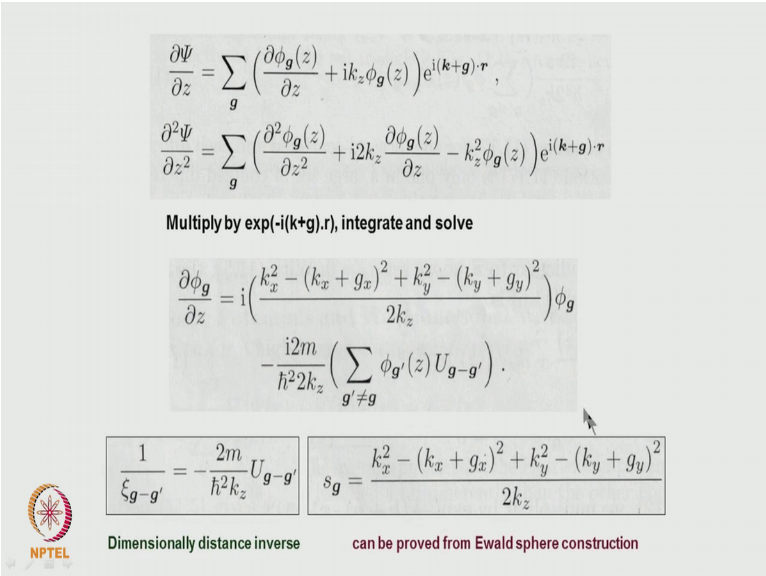

That is essentially what is being done. When it is being done we get some expression like that d phi g by d z into i into some terms will come. This is k x, k g x, k y g y, k z ok

This phi g is another there is this is the amplitude of the scattered wave plus one more term which comes, i 2 m by h bar square 2 k z. This by I am not going into it you can do all these algebra, then this will turn out to be this phi dash, phi g dash into this u g comes; that means, that in this term it is for different values of g which we are considering it. It is between the Fourier coefficients of the amplitude of the wave at every point is coupling with is multiplied by the Fourier coefficient of the potential corresponding to each of this, correct? This is this Fourier coefficient of potential because how we have written this expression V r, U g right ok.

This comes from some orthogonality relationship, but you can because this like dummy suffix because, when g dash equal to not equal to g only summation is taken when g dash is equals g this becomes 0. There are some conditions are there, that is why I am just not going into any of the mathematics. But what is essentially important is that, this term is going to be there know each one of this is equals one by psi g. So, what it essentially means that that extinction distance depends upon in a particular direction g that is g to g dash means that from one particular value of g vector to another value of g. That tells the periodicity in that direction. For that periodicity what is going to be the Fourier component of the potential which is going to be there. That is going to decide the extinction distance, you understand that. So, extinction distance directly depend upon the potential within the sample. The potential is very weak, then what is essentially is going to happen is that the psi g is going to be large. And when the potential is very small that psi g is equal that is going to be small. This is what it happens in the case of suppose you take aluminum along 1, 1, 1 direction if you take psi g. You will get a value which will be very high. We take for the same 1, 1, 1, or you normalize it by the lattice parameter because otherwise lattice parameter.

Take the case of a tungsten, tungsten the value of psi g is going to be extremely small because that the potential is going to be high, you understand that. So, it is a related to potential, but the potential itself is not a simple sin wave or a cos wave, it is a complex wave. When it is a complex wave that potential can be represented in terms of a Fourier series with respect to the Fourier series, but the Fourier coefficients are there, and what is the frequency which we consider? It is with respect to the reciprocal lattice vector g 2, g 3, g like that it will go. Various gs which we have to take it.

Student: one diffraction.

This is with respect to this g dash can have any value. This is with respect each diffraction vector this values will change. Suppose instead of, suppose instead of 1, 1, 1 direction suppose I take 2, 0, 0 direction. So, the value of psi g will be different, because the potential Fourier coefficient is going to be different, you understand that? And then this term is essentially is nothing but S g, S g is the deviation from the Bragg condition. This comes only from the quantum mechanical expression when you write it and try to solve it, you understand that?

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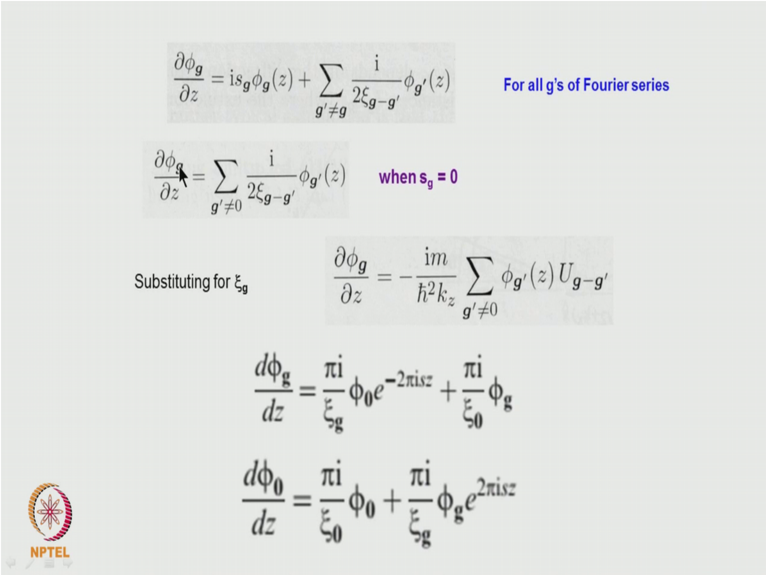

Now, what I will do it is that, this if we substitute this S g and this psi g which we put it and if we do some substitution, we will be getting explain, what is this term which it tells. What we have written is that the rate at which the amplitude of the diffracted beam varies in the z direction depends upon the intensity which is scattered in that direction. The amplitude of the wave scattered in the direction plus this corresponds to the defect means amplitude of the waves which are scattered in the other direction with psi they both have an effect, correct? That what we qualitatively talked about also earlier. Finally, under a 2 beam condition we will be getting an expression like this. That is the rate at which the amplitude of the wave that incident wave you look at it enters phi 0, as it passes through the sample rate at which it decreases is given by this expression. It can be derived from here. And the rate at which it amplitude of the scattered wave changes and here we have taken only one diffracted wave and the transmitted wave. This is what essentially this expression.

This expression We can substitute for phi g into this one, this we try to do it we will be able to write a differential equation like this. This I am not going to any of the derivation I, but want, but generally if this sort of an equation which is there what is the general solution? This all of you have studied in mathematics. No this will be into e to the power of 2 pi i some alpha into So, that sort of an expression you write it.

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$$\frac{d^2\phi_0}{dz^2} - 2\pi i s\frac{d\phi_0}{dz} + \frac{\pi^2}{\xi_g^2}\phi_0 = 0 \qquad \phi_0 = C_0 e^{2\pi i\gamma z} \qquad \phi_g = C_g e^{2\pi i\gamma z}$$

$$\gamma^2 - s\gamma - \frac{\xi_g^{-2}}{4} = 0 \qquad \gamma^{(1)} = \frac{\left(s - \sqrt{s^2 + \frac{1}{\xi_g^2}}\right)}{2} \qquad \gamma^{(2)} = \frac{\left(s + \sqrt{s^2 + \frac{1}{\xi_g^2}}\right)}{2}$$

$$\gamma^{(1)} + \gamma^{(2)} = s \qquad \gamma^{(1)} \times \gamma^{(2)} = -\frac{1}{4\xi_g^2} \qquad w = s\xi_g = \cot\beta$$

$$\frac{C_g^{(1)}}{C_0^{(1)}} = 2\xi_g\gamma^{(1)} = w - \sqrt{w^2+1} \qquad \frac{C_g^{(2)}}{C_0^{(2)}} = 2\xi_g\gamma^{(2)} = w + \sqrt{w^2+1}$$

Now, you substitute and try to solve it. This is all just the mathematical, I am just only showing some of the important results, when you do it this will turn out to be a term like this, with respect to gamma. The solution of this term because gamma is essentially contributing to a phase factor. It is something similar to S. This will have 2 solutions, gamma 1 and gamma 2. And if you take gamma 1 plus gamma 2 that turns out to be S the deviation. And if you take the product of gamma 1 and gamma 2 that turns out to be that 1 by psi g square just that is why this 2 terms are very important. These are all coming out of this mathematical operations when you do it. And then there are some expressions by which it can be written as or (Refer Time: 54:25) These are all mathematical manipulations and using which we can find out because in this what we require is gamma we know, but see what is the ratio of c 0 to this one that amplitudes also we should know, no. So, that everything is being derived in this way finally, what happens is that, when those sort of amplitudes are derived.

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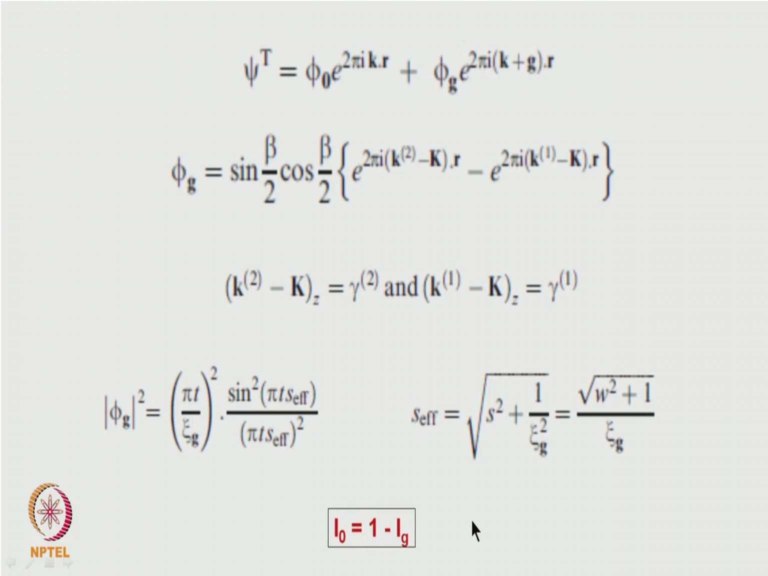

This is the term which we will have know we said that 2 beams only are there know; that means, that psi t will be equal phi 0 into e to the power of 2 pi i k dot r plus phi g into k plus g into dot r, correct? This how the expressions will be. This phi g when it is being derived this is sort of an expression which comes. You forget know finally, it turns out to be an expression that phi g squared will turn out to be pi t by psi g the whole squared sin squared pi t S effective by this factor.

This expression if you see it, is very similar to this expression, correct? For the kinematical theory, but the meaning of the terms are quiet different. This S effective turns out to be root of square plus, now all the derivations I had left out because it is a lot of mathematical which is there which is unnecessary, but what you should remember is that this is how the intensity of the diffracted wave is going to be. And when S becomes 0 also this will become one by psi g square, correct? So, you can substitute for S effective into it then you will find that there will be a fluctuation which will be taking place. Is this clear? And what will be the intensity of the intensity of the transmitted wave? This will be one minus i g ok.

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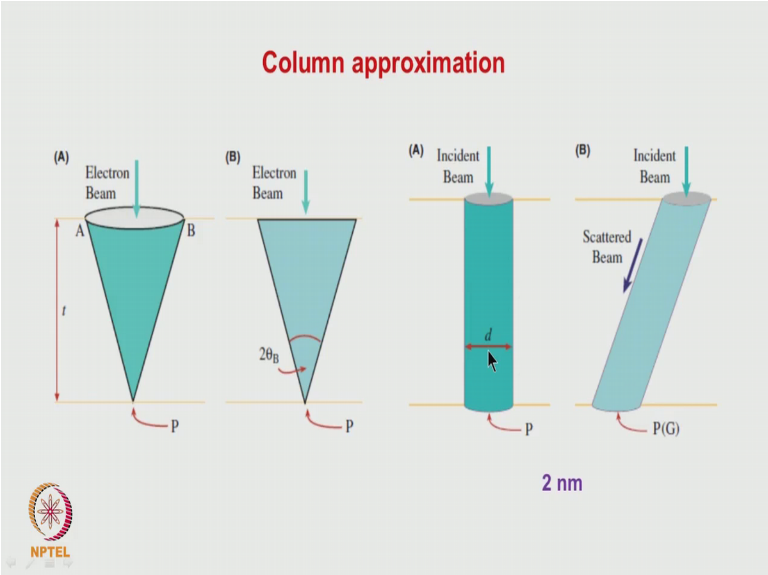

This is the way a calculation can be done. Then the whole issue comes is that practically when you have to do the calculation. What is the size which you take of that sample dimension? Ok.

Suppose I wanted to find out at the back of the sample at this particular point, what is going to be, what all, what is, what all beams which will contribute to the intensity here? Suppose a beam is entering here and the beam should come out through this. As the beam enters the beam gets scattered and it is getting diffracted back into this one. So, essentially the diffracted beam makes some angle theta, is it not? And with respect to the lattice parameter, that tells us that this angle is 2 theta b all the beams which are falling here in this direction, they will contribute to some intensity or other to it so; that means, that at this point intensity depends upon not from only just from this, because the theory we derived it on that basis, but practically it is going to be from this region as well. So, that has to taken into account ok.

Why I am telling is that these assumptions are already softwares are there where this calculations are being done, they take this into account. This is called as column approximation. Then what is normally done is that generally you assume that some thickness of the sample you take it. So, along this column within this, whatever is the beam which is going to entering that will contribute to intensity at a particular point. If we know this, if we know this what value of theta been normally in the case of a sample, in t e m sample, especially it is about less than half a degree. If it is half a degree if I assume that the sampled size is about hundred nanometer, this diameter will turn out to be about something like 2 nanometers.

So, in most of the sample the column size is taken to be 2 nanometers for the calculation. This is how the calculation is being done.

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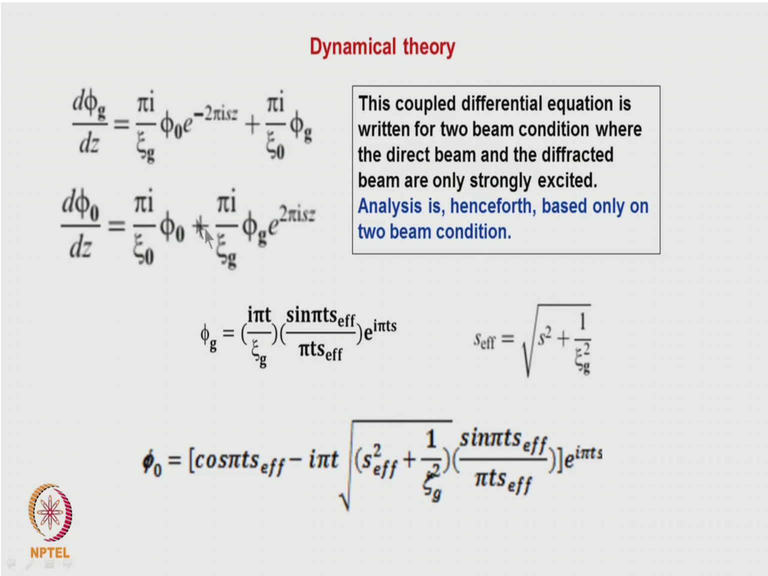

Now let us come back to it this derivation which we have done is that is, what we have started with is assume that, what is the potential of the sample we know? The wave function, what is the wave function when we write it as the expression? That tells us nothing, but what is the path which the electron is going to take as it moves within that sample. In the physics term we will call it as a wave function. Chemistry we will call it is an orbital function, right? What is the orbit which is going to take, correct? So, that is what we have done it. So, that depends upon, that wave function the sample depends upon what I psi g it is essentially with respect to the beam directions, right? With respect to a beam which is there in the transmitted direction, what is it going to be the amplitude? of the wave phi 0, phi g is the amplitude of the diffracted wave. So, the path of the electron within that sample is being controlled by amplitude of the transmitted beam as well as the diffracted beam. And that is related to the potential which is being, potential of the potential of the electron comes in terms of that i g, correct? And this the ex equation when we solved. We arrived at for phi g and expression like this and this is how we have got that final expression, ok.

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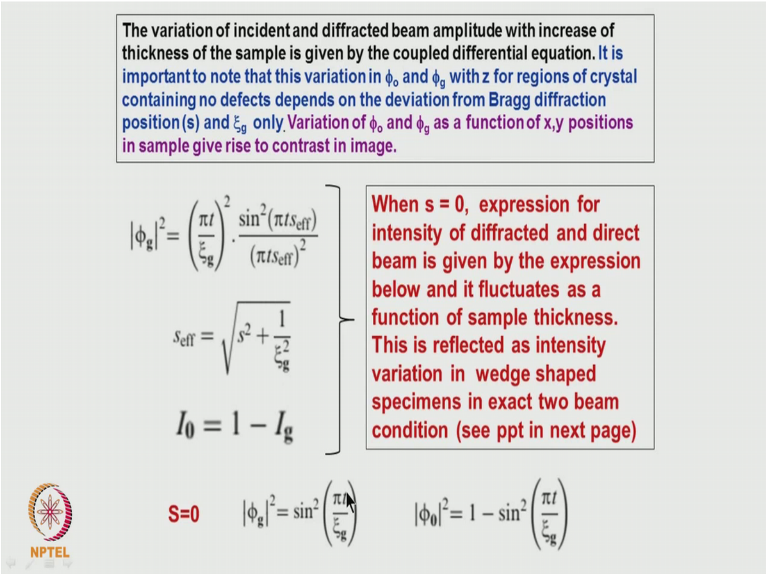

Now, when S becomes 0, what this will turn out to be? Phi this will become pi into t by psi g, correct? Then phi 0 square will be here now what is going to happen is that, as the thickness of the sample t by psi g becomes 1 half, 3 by 2, 2 like the intensity is going to fluctuate. It that is what is being seen when S equals 0.

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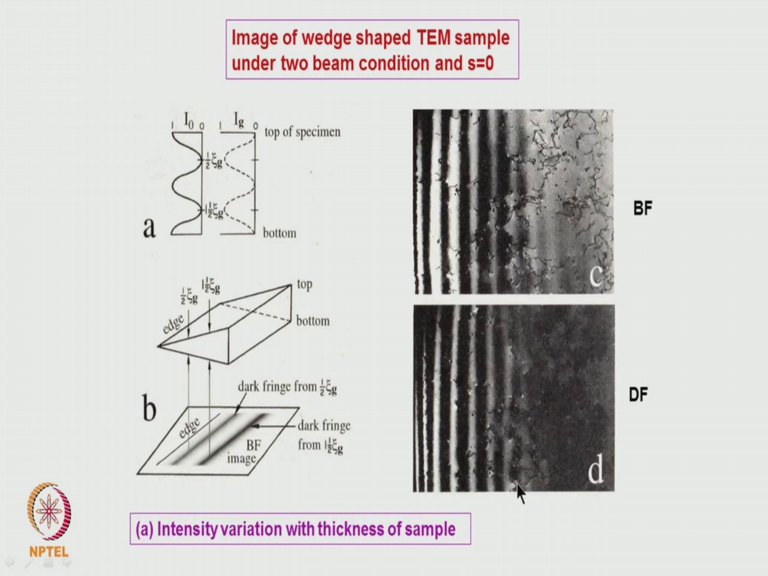

So, this expression the dynamical theory of expression is now able to explain all the experimental observation. Not only that, S effective is there then like the way we explained it for the kinematical theory S effective and t we can take it, is it not? The way explained in the kinematical theory, when the S is going to very large. Then what is going to be? This one by psi g is going to be the psi g will increase. That this term will become 0 S effective will become S then the kinematical theory is valid. So, this theory has it is a theory which explains under all conditions how the contrast will vary. Whereas, the kinematical theory can explain when the deviation from the Bragg angle is large, but not when under not under exact Bragg condition, is it clear? Ok.

(Refer Slide Time: 62:13)

Table 7.1. Extinction distances ξ_g [Å] for elements in a two-beam condition with $s = 0$ (100 keV electrons). [7.1]

Diffraction	Al	Cu	Ni	Ag	Pt	Au	Pb	Fe	Nb	Si	Ge
110								270	261		
111	556	242	236	224	147	159	240			602	430
200	673	281	275	255	166	179	266	395	367		
211								503	457		
220	1057	416	409	363	232	248	359	606	539	757	452
310								712	619		
311	1300	505	499	433	274	292	418			1349	757
222	1377	535	529	455	288	307	436	820	699		

So, this is where a table which I am showing it for different diffraction, this one for hundred k v electrons. What is going to be the psi g value which has been calculated for S equals 0? What is going to be the effect of this? The effect of this will be that suppose you have a multilayer sample, in which each layer has got at different element which is being present there. Or the composition from layer to layer changes, then the psi g will also change. The effect of the psi g that even under the condition when S equals 0 if the closer to the sam thin foil, closer to the hole of the sample, generally any of you are prepared samples for t e m, what is the shape it looks like?

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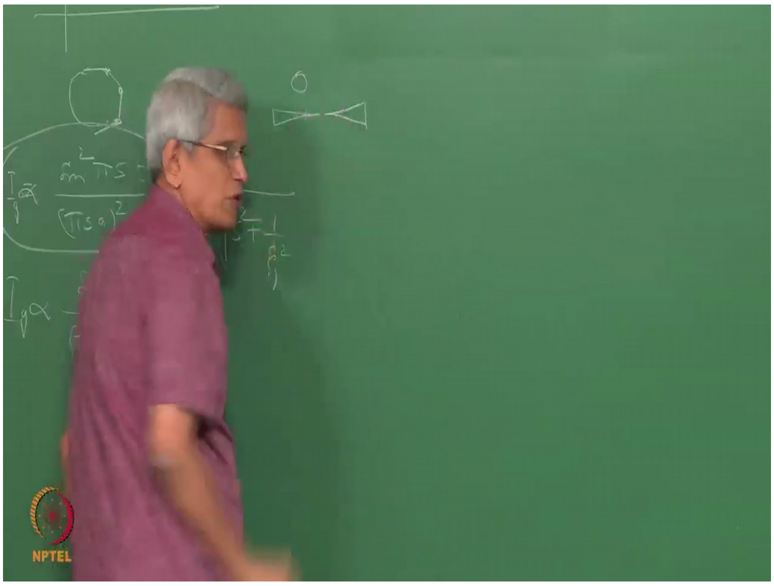

Student: circular

It is the whole. Sample looks like circular, but the thin foil thin region, it is the hole from here it go. So, essentially it will be something like this is how it is. It is essentially a wedge shaped which is going to be there, correct? Even under the Bragg condition. So, if the there is it is like multilayer it is going to be there psi will vary locally, that will have that effect on this periodicity of this bright and dark fringes.

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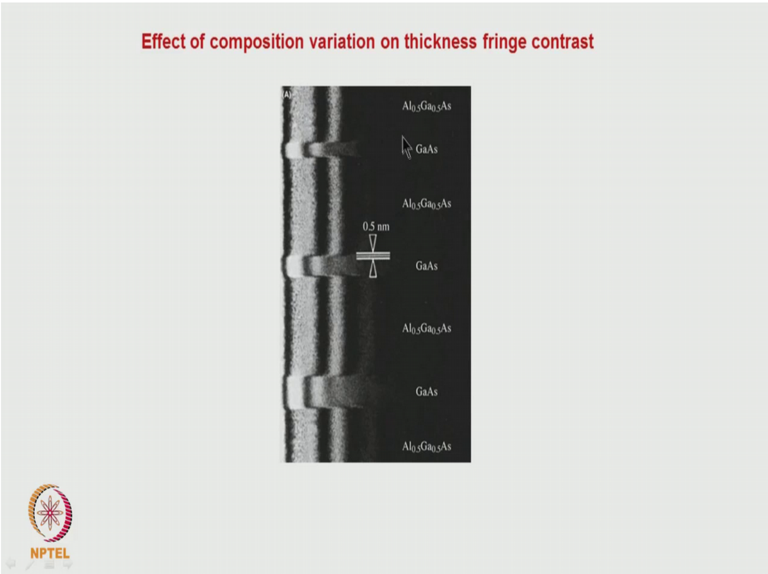

That is what you can see it here, you see this. This gallium arsenate, this is aluminum gallium arsenate. Now you can see that how the fringes are changing. So, gallium arsenate has got a higher this one so fringes spacing. So, here you see that when the aluminum is introduced the fringe spacing has changed, correct?

So, all the features which you observed could be, there are many situations where you will not be directly able to interpret it, the image can. Then under those conditions, that we will take it up in the next class, I will explain some case where we are done. Computer simulation of the image which you have done it to verify it ok.

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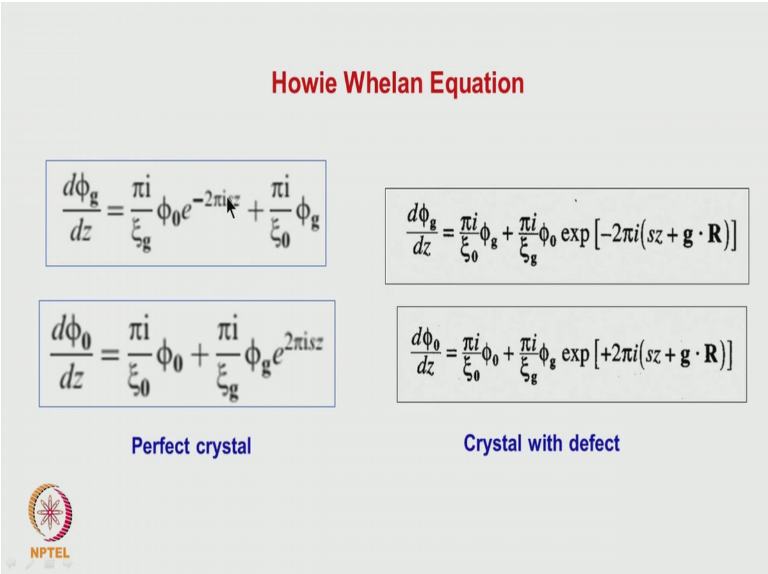

In such conditions you have to simulation to find for which you should understand all these theory. Software will be there, but you should know how to use it no, how to optimize it and use it for that unless you understand the theory it is going to be difficult. If somebody wants to do a serious microscopy anything which we do otherwise we are not sure what we interpret is correct or not. So, this equation which we have written it for the variation of incident, amplitude of the incident beam and diffracted beam this is called as the howie whelan equation, or howie whelan darwin equation ok.

This equation is for a perfect crystal. When it is going to be a crystal with the defect, like the way we have seen it wherever that S z is going to be there. There will be a term which will be attached h z plus g dot R where r is going to be the defect vector. Exactly this term will come like in that case if the g which we choose is such that, g dot R becomes 0 then it becomes the case of the perfect crystal. So In fact, that is used to find out the by just vector of the dislocations. And then about strain contrasted on precipitate all this things will be determined by this g dot R. Some examples, now I had just given the formalism, the mathematical derivation without going into it I said that what is the need for a dynamical theory, from the kinematical theory, how the dynamical theory differs? Just had the written the initial expression and in between this expression which comes, and what is the relationship of psi g with respect to the periodic potential all these things some expressions which comes out of it only just the expression which I had flashed. In the next class we will take it up because when we do the calculation all these things how do we put into a place and we have to do it. That is why I had introduced this. In the next class we will take some few examples of defects which both with kinematical and dynamical how we try to interpret it that part we will take it up we will stop here now.

Thank you.