Electron Diffraction and Imaging
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Lecture – 33
Revision 2

Welcome you all to this course on electron diffraction and imaging. In the last class, we tried to review some of the aspects on electron diffraction and imaging which we have covered. We will continue with that in today's class as well. Before we go further in today's class, what we will do is will just have a recap of what all aspects which we considered in the last class.

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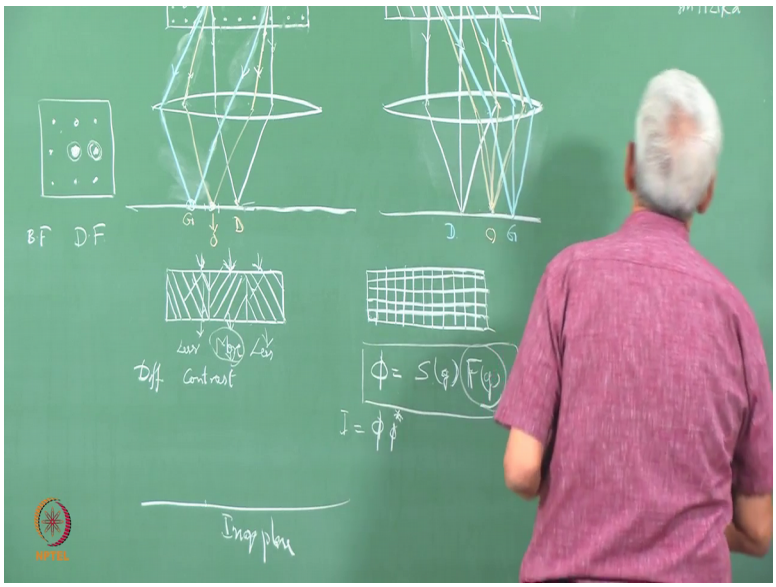

So, what we did essentially was that we looked at how for a lens. It gives rise to both diffraction as well as the image of that sample. This is a property of the lens. This is the aspect which we considered and this is the aspect which is used to get diffraction as well as image from the same region of the sample.

What we will do today is look at the various aspects of the microscope and see how we can get the maximum information about that sample in the microscope; what I have done here is that I have considered that sampled as individual atoms which are there because the reality of the sample. If you look at it is that atoms are at regular particular positions. They are sitting in the sample. So, with a particular periodicity, when the electron beam

enters into that sample or we can consider this as a electron wave which we enters into you know plane when you plane wave which enters into the sample it is scattered from each of the atom in different directions.

What we do in the way diffraction is try to find out; what is going to be the intensity of the beam at a point which is very far away from the sample in a specific direction. The beam which has been scattered from all the; in a specific direction from all the atoms at the amplitude of the waves and see what is going to be the resultant amplitude when all the bus add together then we say that the constructive interference has taken place and it gives rise to the diffraction spot here; what I have done. It is that I had considered a case where a wave is scattered from one atom here and the another atom here 2 examples and the un-diffracted beam which comes which is travelling in this direction they are all focus to a point and this is call the direct beam.

At the one which is shown with this blue line these waves all of them when they meet at a particular point the amplitude of the waves all add together because the path difference between the different waves is multiples of a lambda. So, when they add together we get a constructive interference and this is what a diffractions part which is denoted by g then, but we know that from every point the incident wave is scattered in various directions. So, if you look at these particular direction in these direction the wave which is coming at this particular point when we find out the amplitude of the wave net amplitude of the wave then what it is going to happen is that all of them have different signs. So, the net amplitude turns out to be 0.

That means that only at some specific scattering angles the amplitude add together giving rise to a constructive interference other cases the amplitudes can be less than this and in some cases the amplitude can become 0 finally, this results the form of appearance of a diffraction pattern on the screen with a central beam and then there will be some spots where we get this sort of reflections are present this same case can be considered in an another way where what we do is instead of considering the individual atoms, we can consider the sample of consign of some planes when the beam is entering in a specific direction. This is the transmitted beam. These all join together to give rise to the direct part and the wave. The blue ones are the ones which the first difference between each of these wave scattered in this direction is lambda.

So, they add together giving rise to a diffractions part and in between regions the waves are interfere destructively. So, there is no reflection is same. So, we can consider it; either as a lave individual scatters or we can consider it as planes, but both of them give rise to the same sort of a diffraction pattern, then when we have to get; we are bright field or a dark field picture; what we do if we put an aperture around either this reflection or around this reflection; then what we are essentially trying to do is that if you put an aperture around this reflection then what we are trying to do is that we can consider in with these example; here what we are doing it is a sample which is there in which the diffraction planes are inclined like this here the diffraction planes are inclined like this.

In these 2 cases, where the diffraction planes are inclined like this they satisfy the Bragg condition for the beam which is entering into the sample, if we make that assumption then the lot of the beam will be scattered away. So, in the direct beam the intensity is going to be less in this particular case what is going to happen is that the direct beam since this is not satisfying the Bragg condition diffraction; the beam is not diffracted away are scattered from the direct beam is the scattering of the direct beam is less because of which the amplitude of the wave which teaching here is more are the intensity of the transmitted signal is more in this region intensity of the transmitted signal is less. So, from region to region there is a variation in the transmitted intensity this gives rise to a contrast and this contrast we call it as a diffraction contrast.

So, if you put on aperture around air diffractor in spots then and then what is going to happen if the beam which has been scattered from this in a specific region are the beam which is scattered from this in this region we consider it and this will also give rise to a contrast which we complimentary that we call it as a dark field imaging, but what we should understand is that when the rays are scattered in all the directions all these rays will join together in the image plane. So, when all these things join together in that image plane that is where we get a sharp image of that sample; that means, that the rays which are scattered if I consider any point here all the rays which are scattered from a corresponding point on that sample scattered in different directions they are all brought back to this point.

So, it is essentially equivalent to the image corresponding to all the diffraction parts to superimpose one on top of the other such a condition normally what happens is that the sharpness of the image is not good, but this is the condition under which the maximum

information about the sample we get it, but when we put aperture around either a central beam or a diffracted beam; what we are essentially trying to do is that nothing, but essentially magnifying this diffractions part putting an aperture like this and cutting of all the others parts we are essentially trying to magnify the intensity variation in the diffractions part and that is what we are giving it. Later I will show you some pictures to tell that what sort of information which we get it; how much the information we get it; if we use a bright field or a dark field or if we use all the different diffractions parts to get the image.

In fact, if you use bright field or the dark field the maximum information is not passed on that is the true representation of the sample we do not get it because in reality the sample is individual atom positions the true representation is that we should be able to see that all the atom positions, but in bright field or dark field images we do not get such images its essentially some variation in contrast, but that variation in contrast we use it to and analyze it to find out what all types of defects which are present in the sample then when we wanted to quantify it we should know what is going to be the intensity of each of this reflections that intensity. Essentially if we try to find out that phi that depends upon 2 terms 1 is S g the sheath factor or this is the amplitude and another is f g the structure factor to determine the intensity what we do is essentially we can consider the sample as unit cells which are stacked one on top of the other.

Suppose it is a primitive unit cell. So, primitive unit cell contains only 1 atom per unit cell then what we are essentially trying to find out is that from each of that atom what is going to be the contribution to the intensity and that we add together suppose the atom contains more than that suppose the sample contains more than one atom per unit cell. So, it is a non primitive unit cell in that case each of the unit cell itself will contribute to some intensity that is what is given by the structure factor consideration and then the number of unit cells which are there which are eliminated by the beam we and the intensity is from each of them together that is what is given by the sheath factor.

So, this gives the total amplitude and this structure factor formula depending upon the position of the atom which is going to be there in that sample that gives rise to depending upon the type of crystal structures there are some systematic absence of reflections will occur on that basis we can identify, but when we have to find out the intensity; intensity will be nothing, but phi phi star because this is a complex quantity this yes itself if you

try to look at what is going to be the yes this is given by this formula . So, as you can make out the number of atoms in this direction the other number of unit cells which are in this direction is about the phi bar six the number of unit cells in this direction is going to be more depending upon the number of unit cells in the particular direction.

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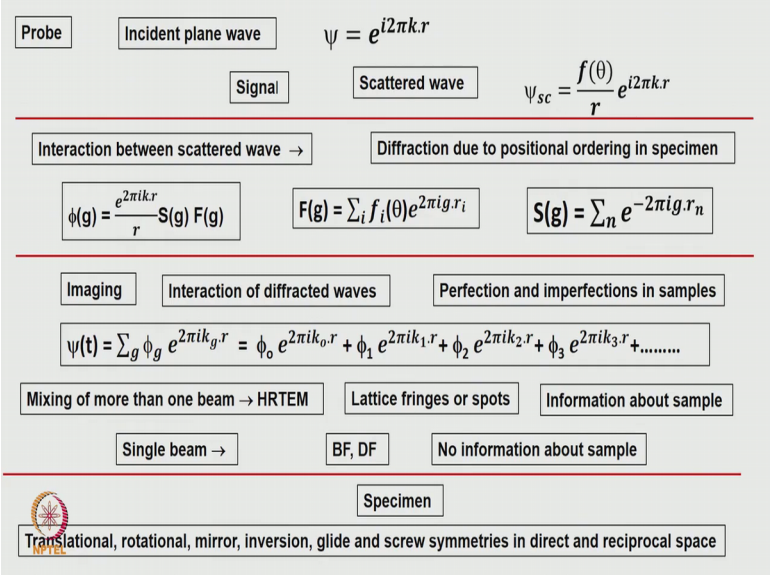

The sharpness of the diffractions part in those directions will change. So, that is why this factory is called as the shape factor looking at the shape of the diffraction part; we have seen that we can find out what is going to be there shape or the morphology of the sample as I mentioned here the bright field or the dark field images which we get it is nothing, but magnification of this magnified view of these different diffractions parts so; that means, that as a function of x and y because this intensity itself you can conciliated x y along different you said each correspond to some particular value of x 1 y 1. This may correspond to x 2 y 2 at these regions depending upon the suppose some defects are present in the sample then what can happen is that the effect of the defect maybe that the atoms in this region maybe a tilt are rotated that will be essentially equivalent to tilting of this unit cell.

So, this will have an effect on the intensity in this particular column. So, essentially using this methodology we can find out the intensity for different x and y values intensity along different points that is what is going to be the intensity at the back of that sample if you try to find out there will be some variations will come if it is a perfect crystal and

just a single crystal then the intensity whatever is going to be there is uniform or the amplitude of the wave which is going to come at the back of it is going to be the same everywhere where as when some defect is being present and it is rotating the unit cell then there will be some variation in the amplitude will be there and that will be reflected as a variation in intensity ok.

This how it can be here when we try to find out the intensity the way in which we can do it is that in these terms or in these terms we take it as a summation we know that from mathematics the summation can be taken as an integration also.

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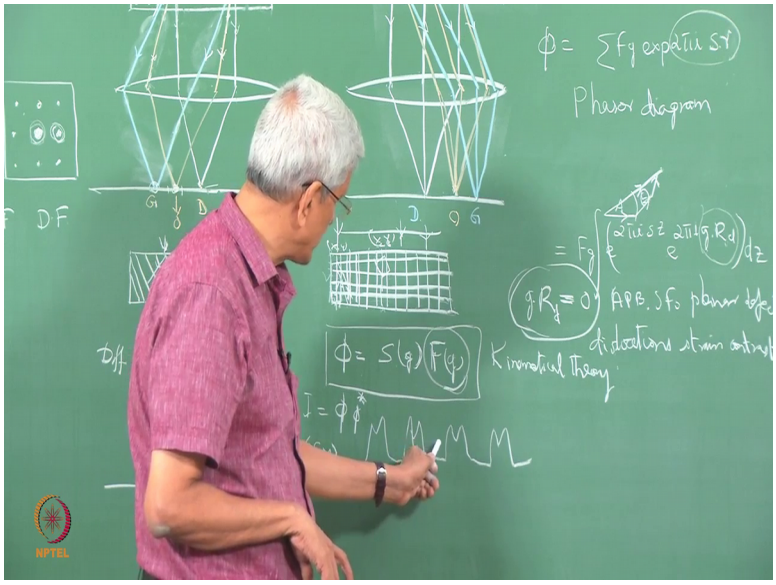

So, if we consider that way, the amplitude can be written as sigma of F g exponential 2 pi a D into I z or S into this will be R and we know that when the beam enters into the sample what we can consider it is that at different points of R, they are getting scattered depending upon this. This factor S dot R will be changing then when the S dot R from different points. It is going to change we have to add together and finally, we will get what is going to be the intensity at this particular point.

For that this can be we can use the phasor diagram here what we do is essentially we can amplitude and the phase this represents nothing, but an angle theta using this we can represent it as that with an amplitude and then the next how it is a different point. So, the net amplitude we can find out and the net angle which it can make out that is what essentially the sum of this formula also this formula itself can be written in the form of

an integral as well where if F g is a constant we can take it out e to the power of 2 pi a S in to z whenever defect is present due to the defect also there will be an another term will come should be 2 pi a g dot R d.

This into d z; this is the sort of formula which we have derived when the for the particular what is g? G is the reflection which we are using it for imaging it and R is the defect vector if this g dot R turns out to be 0 then only this particular term will be coming then the intensity of that image look like that of a perfect crystal this is the one which is used to this condition g dot R g dot R d equal to 0. This condition can be used to find out the defect vector are the for all various types of defects like and if it is boundaries stacking faults these are all the inner defects.

Similarly, for defects like dislocations which gives rise to strain contrast in this particular case planer boundaries there is only going to be a relative shift of the planes and in the case of dislocations essentially displacement of atoms is going to take place around the line direction. So, we can find out the burgers vector of the dislocation the line direction all this information could be obtained using this sort of a analysis in the derivation of this expression we have assumed that only once scattering even takes place for the beam which is entering. So, that is why this is called as a kinematical theory, but in fact, when electron beam enters into the sample multiple scattering takes place for which the dynamical theory has to be evoked what is being done in a dynamical theory is that.

Here we assumed that point scattering centers; the scatter and for the scattering; we give some atomic scattering factor as a term which decides how much of the amplitude is going to be scattered in different directions how the amplitude is going to change in the dynamical theory. What is being done is that the sample itself is considered as a wave which is entering into that is in the dynamical theory as the electron beam enters into the sample. We considered that electron beam as a plane wave, then there is a coulomb potential which is going to be there and that potential can have different shape with some particular periodicity we see this. This is not a simple sine wave, but we can see that there is periodicity which is associated with this sort of a function what we can do is it is using Fourier analysis. We can find this out we can express this in terms of a different sine for or cos for a sin and cos functions with some fundamental frequency which corresponds to the separation between the atom positions, then double the separation first that is first harmonic second harmonic and all these

This wave; we can represent them when we do that then similarly, what we try to do? It is see that what is going to be the effect of each of this harmonic onto the scattering function or that is what we assume that depending upon the first harmonic or the second harmonic each one of them is the one which corresponds to scattering of the beam in some specific directions. All these aspects have been covered in detail what we have to consider here is that as I mentioned earlier when the beam is the scattered from a particular point.

What we have to look at it is there when the scattering is taking place from this particular region; the electron beam is scattered in various directions the way the raise which are scattered in all the directions they are joined together to give this image. So, if you look at that image at each point whatever is the amplitude of the wave which is going to reach here corresponds to the amplitude the wave which is scattered in this direction then depends upon the amplitude of the wave in this direction depends upon the amplitude of the wave in this direction, but essentially what is it which is which we are seeing in is when the waves are scattered in the various directions. This will have some amplitudes which using this formula we can find out in addition to it that is the amplitude with the wave coming this wave what is going to be the component of this wave in this specific direction because as particular parts when we consider in this particular direction that is at this particular point what is going to be the; it is the back of the sample.

What is the contribution of this which is going to be there then we have to take a phase factor into consideration that is this phase factor will be e to the power of 2 pi I; if this direction is k 1; k 1 dot R, if this direction is k 2 e to the power of 2 pi k 2 dot r, all these ones that in the direction this is the direction r if you consider it R. This corresponds to a with respect to a beam. It is a wave vector k 0 then this k 1 dot R k 2 dot R; this nothing, but the projection of the amplitude; what is going to be in this specific direction. The net sum of all this amplitude is what is going to be the wave which is going to be there at the back of the sample.

This wave is called as the exit wave. This depending upon the scattering which is going to be take place at different points; it will be varying from region to region the image of this exit wave is what we are seeing it as image in the high resolution microscope.

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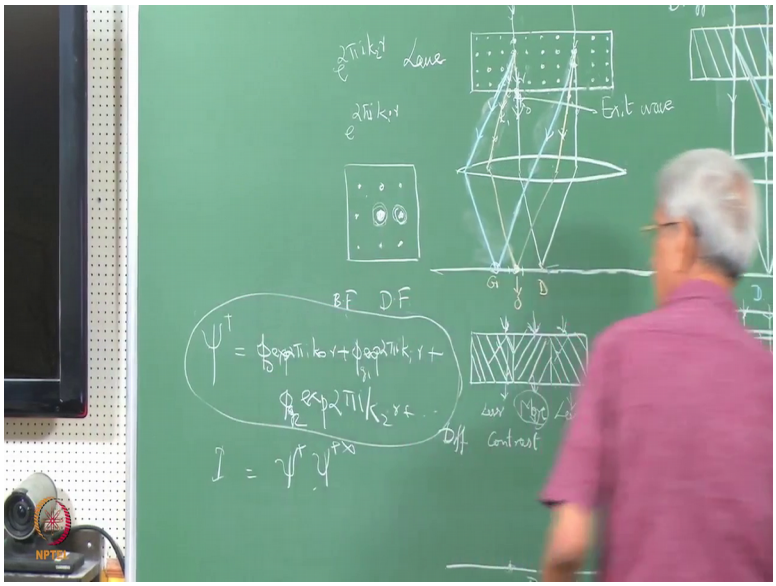

So, essentially what is going to happen is that then at every point on that image; the amplitude when we try to find out that is going to be 1 corresponding to phi 0 into exponential 2 pi I k 0 dot R plus phi g 1 into exponential 2 pi I k 1 dot R plus phi g 2 into exponential 2 pi I k 2 dot R. Like this all this ones when we summit up that gives the net amplitude which is going to be there with the net phase factor and this psi; psi star psi t star. This is going to be what it will be giving at the intensity at every point on the sample.

Suppose we assume that the lenses what does the lens do lens only magnify the information which is available on the back and gives it as a magnified image. So, that it can be resolved very clearly with our eye; that is how we can see it on the screen this high resolution images this expression which has been derived is derived under basis that the lens aberrations are 0 for are point object a point image can be obtained.

But we know that all the lenses have got some aberrations associated with them these aberrations are one spherical aberration, then coma astigmatism, then pine cushendun pincushion distortion, then chromatic aberration out of which the spherical aberration is inherently a property of the lens this aberration can be minimized, but cannot be totally eliminated in a conventional transmission electron microscope, but what are being seen is that the defocus produces some phase error that compensates further spherical aberration for some particular angles.

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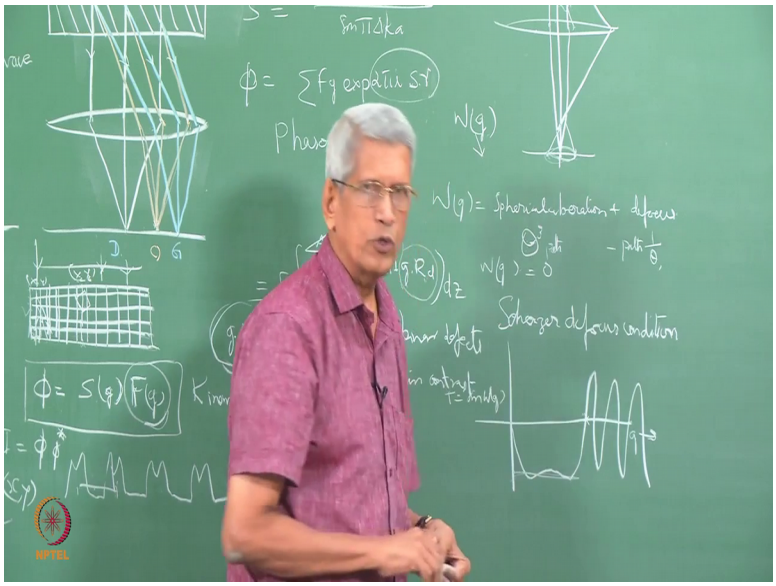

Since we consider the electron beam as a wave which is passing through that sample what does that lens 2 as we have studied earlier there is which are traveling close to the optic axis they are focused at some particular point and the raise which are travelling far away from the optic axis they are focused. So, essentially this should also I have been brought this points that is not happening because some path difference are the phase has been introduced to the beam which are scattered in different directions by the lens itself. So, some additional factor this factor is essentially phase factor, if we normally we denote it by a term w g. This factor will be added to all the terms and this factor is going to be not that same depending upon the angle at which the angle which the scattered beam makes with respect to the optic axis or what is the distance from which it reaches the lens depending upon that this value will change.

So, that will correspond to in these cases that is another factor phi g 1 plus here and another factor g 2. This will be added to the various terms what is going to be the net effect of this sort of an error is that for a point object; we do not get a point image in the Gaussian plane, we get a spread in the intensity. So, this makes first the resolution very poor though the information is coming from one particular point, but be a that information is spread over a particular area in the image and another important aspect of it which we have to consider it is that in this expression this is the one which corresponds to contribution transmitted beam this is from the various diffracted beams if all of them add together with a particular phase the net amplitude this psi is going to be.

If each one of them contributed in different way. So, that the amplitude becomes 0 are randomly give to various values then what is going to happen is that whatever is the intensity which we get it that is going to be different and its going to be difficult interpret. So, only when all of them have got a particular phase relationship which you maintain with respect to them they will add together. So, that the contrast which arises from point to point. This variation in contrast is what we are trying to interpret it in high resolution. So, to get a good contrast what is essentially important is that these terms, the w g 1, this phase error which are being introduced by the lens all of them should be of some sin. So, that the amplitudes add together.

What is the terms up to which they add together that is what it says how many of the diffractions parts which should be chosen. So, that we get better contrast and the information which we get is interpretable. So, this is exactly what is being done in a high resolution microscope is that is choosing specific values for the defocus because that w if we consider this w g. This consists the effect comes from spherical aberration plus defocus spherical aberration gives ways to some path difference and this is opposite of that the path difference it adds to it, but only difference is that that why this depends upon the angle to theta to the power of three with respect to the angle which them beam which makes this angle beta theta.

Whereas this is one by theta because of which for all angles they will not be certain a matching exactly that is what I mean is that for some specific value of that angle theta is w g can be made to 0, but what we see is that since we are using. So, many diffractions parts each will have a different value if we can optimize the condition such that for most of this reflections this value turns out to be having some specific value and close to each other. So, that the all of them each of difference parts they add to the contrast add to the amplitude that condition is called as the Scherzer defocus condition Scherzer defocus condition.

For this particular condition, the value of this phase error turns out to be almost that same and this is what we are trying to part it what; the term exactly will turn out to be this will be some factor of sin omega is psi g will come and this what is the this is with respect to g; what is the distance up to which this value turns out to be of uniform factor; that is called as the Scherzer resolution also. So, these are all the factors which are very important in high resolution imaging. So, essentially what is being done in a high

resolution imaging is that we use an aperture to take maximum information put an aperture in such a way that all the diffraction spots contribute to the image are essentially, what we are doing it is all the words in Layman's language if you take say all the words which are scattered in different directions from each point their allowed to join together at the back. So, then we get the full information.

In the case of a bright field are the dark field, only some specific direction which we are looking at it; that means, that the wave which is scattered only in this direction gives some contrast in the image, but that does not contain complete information about that sample only a some small part of that information which is coming. So, in the high resolution image if you look at it that complete information is coming because we use as many reflections as possible, but since their phase error is introduced by the lens that puts a limitation on up to what a g vectors can be used for getting an interpreter build image R up to what g vectors the amplitudes will add together.

Afterwards what is going to happen is that there is some fluctuation. So, there will be some variation in amplitude will be taking place that is essentially because of the phase error which is responsible for it in such a case the interpretation of the results become very difficult even then what is essentially important is that to interpret the high resolution images we have to simulate the images using the conditions which is used in the microscope then assuming some model for the sample generally what is being done is that how what do we assume about that sample we assume that when the electron beam enters into the sample in the case of diffraction we consider is the point objects or in this particular case we consider as a Bragg condition that is the planes which are responsible for diffraction.

Here it is each atom is considered as a point scattering centre for getting interpreting the high resolution image what we essentially do is that assume that as that electron beam enters into the sample its essentially it is a coulomb interaction with the periodic potential of that sample takes place takes place and as the beam passes through the sample we assume that the potential what it does is essentially at surface to the wave and no other change which is taking place. So, the wave which comes out at the back of it will have its phase which is altered that is how we write this as F of x y a sample is a of x by some amplitude exponential I into phi of x y is it.

This we assume that this can be taken as that phi itself can be taken as some integral of the potential x, y, z. This is integrated over D z. This is a sort of an assumption which is being made this is called as the phase the sample is now called as a phase object this is the way the sample has been assumed to be and these how theoretically we try to interpret the image contrast which we in the high resolution images.

In addition to it since we use some apertures then a chromatic aberration of the sample is going to be there. Here we assume that the beam is parallel to get a perfect parallel beam maybe difficult the beam can have a some till in such conditions are the there is a drift of that sample itself is going to be there all of them will give rise to modification of the contrast which is going to see all these effects have to be taken into account to get correct interpretation of the images.

So, when we have to interpret that image; you can an electron mayor especially the high resolution images the simulation of the image is very much essential in all this talk what I mentioned essentially is that we use for a bright field or a dark field image when you wanted to obtain from that sample we use either a transmitted part or a diffracted part I told that the information which is being passed on to the sample is very small we get some variation in contrast, but that just does not tell any information about how the atoms are distributed in the sample.

If we take king more diffractions parts and the image due to all of them allowed to join and correct all the lens aberrations and if the resolution of the microscope is such that it can resolved the separation between the atoms then we should be able to see this high resolution image then what we are essentially getting on that image is nothing, but a dotty contrast this dotty contrast has got some relationship 2 distribution of atoms along the columns not the distribution; it has something to do with the columns through which the atoms are present the sample this.

These I will illustrate it; this will be illustrated with a example which is taken from the literature.

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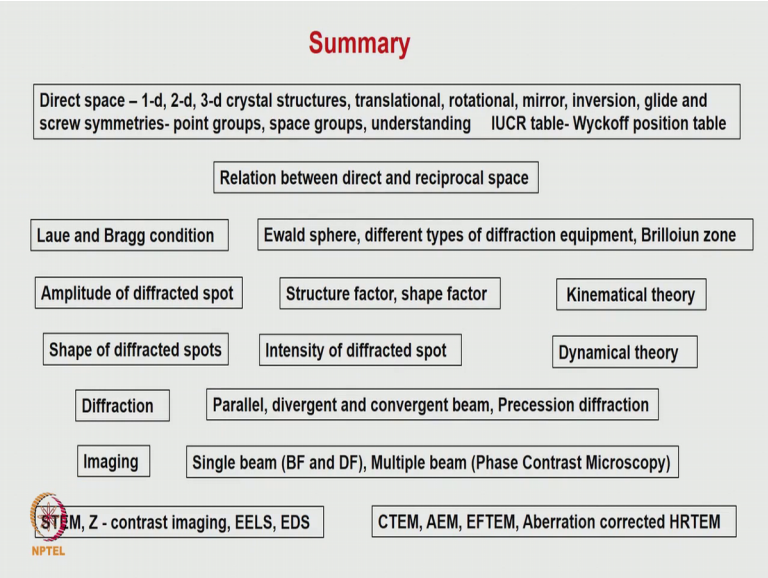

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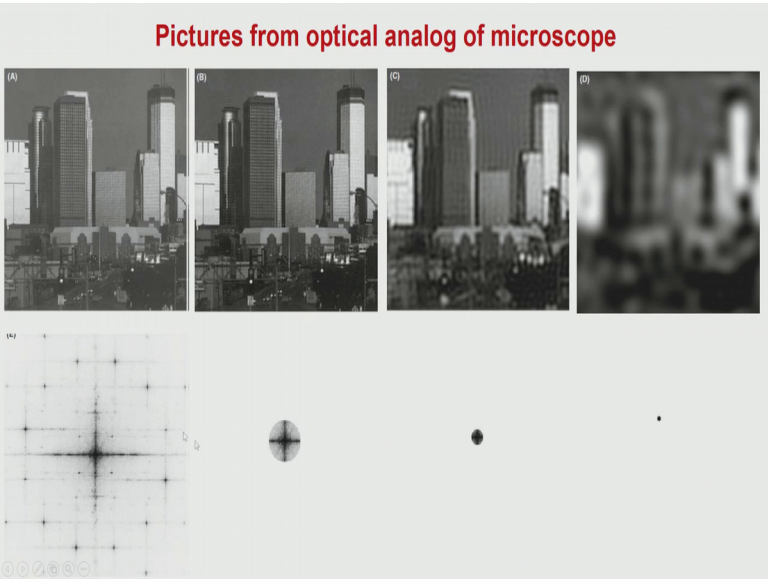

This is an optical analog picture which has been taken you see here we have the skyline of a photograph which is there; which is taken analog film in an optical analog; what is being done is that instead of an electron beam which we use it in a microscope what should be the characteristics of the beam you should be monochromatic and coherent the same type of beam in optical radiation we can achieve it using lasers.

Using a laser beam is passed through that sample exactly like this and then using lens we can get at the back focal plane the diffraction information could be obtained how does

this diffraction information looks like you see here this is the sort of a diffraction pattern which we get some spots some streaking which is going to be there some of which is an artifact and if I use all these information to join together put on aperture like this and I can collect it because this is what it can be done in an optical this one like here as I mention I can put on aperture. So, that cut off all these or I can put a choose an aperture such that all the beams are taken.

Here all the beams when they are taken the same sort of an image which is obtained the next is what is being done is that only this much region which is being chosen from this then you can see that some image blurriness, but still you can see an image of the same sample; it could be obtained. Now that aperture size is being made small. Now you can see that how the image is getting blurred now it can be its being made. The next picture is that it is only just the aperture is made such small that only the central beam which is used. Now you see how blurred that image there is the object which we have the true image of the object you get it when we choose as many diffraction spots as possible when we the less the number of spots which we choose it.

We can make out from this optical analog that the information which we are getting it is not the complete information about the object, but some variation in contrast is there in the case of a defect which is present in that sample this is a sort of image which we get in bright field and dark field and we are trying to interpret on the basis of interpretation of these sort of images we are trying to tell what all the types of defects which are present.

There are so many aspects which we are trying to analyze and interpret it, but we should be clear in our mind that whatever is the information which is being obtained in a bright field or a dark field does not give the complete information about that sample this is quite obvious from the set of pictures. So, what we will do is that I will stop here now essentially what I had covered is the various types of imaging briefly reviewed the various types of images imaging and what is the principle which is behind the various types of imaging we have considered in this particular lecture.

We will try to have a demonstration a lab demonstration of how images look like both in the diffraction plane are the back focal plane as well as that image plane this also we will try to demonstrate in the next class I will stop here now.

Thank you.