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Lecture - 26 Phase Contrast Microscopy - 02

Welcome you all to this course on Electron Diffraction and Imaging. In last class we discussed about the simple basic principles Phase Contrast Microscopy, but in today's class we will talk about when the lenses have aberrations how to go about and get information about phase contrast microscopy. So, what essentially did in the last class is we assumed a plane wave which is entering into that sample, ok.

(Refer Slide Time: 00:48)



And when the material has got a periodicity associated with it since it is crystalline, it gets part of the beam passes through without any interaction the other beam which gets diffracted they would gives these primary beam, and the diffracted beam we allow them to join them together.

When they join them they give rise to an interference pattern and that interference pattern if you look at the spacing of that pattern is essentially depended upon the g vector of the diffracted beam. So, essentially the intensity fluctuates with the periodicity d the which is that d spacing, and this is equal to 1 by modulus of g. This is the expression which we have derived for this interference of these two beams this gives rise to intense.

So, intensity is essentially fluctuating that is what we can make out; and when we consider only pattern beam ok.

(Refer Slide Time: 01:52)



The intensity fluctuation is essentially the having that iso intensity lines, they are perpendicular to the g vector. So, we get essentially a fringe of one type.

(Refer Slide Time: 02:12)



When this is a typical example which we considered to show that how a lattice fringe we get it. From this we can get information about the periodicity in that particular direction.

(Refer Slide Time: 02:24)



When we use many beams multiple beams ok to interfere then each beam will give rise to a fringe corresponding to each one of this diffracted vectors and this gives rise to crossing of fringes due to different gs and this gives rise to an intensity fluctuation which look similar to this gives rise to a dotty contrast, and this we can call it as atomic resolution, but one should remember that here though we get some information this is essentially about the fringe spacing which we get it, in the last class I mentioned that what all the pitfalls of this sort of an analysis.



(Refer Slide Time: 03:16)

Now, in today's class what we will do is that we will look at high resolution in a different way. The way we consider essentially is that we have a beam and it is a plane wave, the plane wave is a propagated. How the propagated as that wave enters into the sample, the sample gives rise to scattering; what we assume in this case is that the sample what essentially is does that it changes the phase of the wave which comes out at the back of that sample that is how we look at that sample. And this wave which comes out of that sample essentially what is being done is that a diffraction pattern is at the form at the back focal plane, and image is formed at the image plane.

So, what does that lens do as it enters into it in earlier class on lens aberrations I mentioned that the lens itself can be considered as a phase shifters. So, it introduces it brings about a shift in phase of the intern ray, not only that as because of that aberrations we find that as we go away from the center of that lens, the aberration which introduces also increases gives these spots when we try to interfere we will be getting that image or in the back focal plane the diffraction pattern which we get it is nothing, but the reciprocal of the real spacing information, when we try to joining all these spots we are doing again an another Fourier transform of it, and that should give rise to the real space again which is what called as the image plane.

(Refer Slide Time: 05:00)

Incident spherical wave
$$\Psi_{in}(r) = \Psi_{in}^{0} \frac{e^{ikr}}{r}$$

Wave propagator $p(R) \equiv \frac{-i}{R\lambda} e^{ikR}$
Lens distortions $q'_{lens}(x, y) = e^{-ik(x^2 + y^2)/f} * F\left[e^{-iW(\Delta k)}\right]$
Specimen $q_i(x, y) = e^{-i\sigma \phi_i(x, y) - \mu(x, y)}$

So, let us look at sequentially start with an incident wave. The incident wave though it is a plane wave from every point, how does that wave is being propagated. It is essentially spherical wavelets which are emanating from each of these points.

(Refer Slide Time: 05:27)



And this spherical wavelets they do constructive or destructive interference, this gives rise to essentially a wave front which is moving. So, here psi in 0 is what that intensity which at any particular point at the spherical wave. As it propagates at a distance r this will be e to the power of I k r by r, this you know how this is coming.

And since this wave is being propagated a propagation vector also has to be taken into account, then only we can completely describe what is going to be the amplitude of the wave at a particular point, anywhere on this wave front that is what essentially is being given by a wave propagator you just take these were the term which is being used. Then this is that wave which is entering into the sample, what does the lens do? Lens essentially as I mentioned it introduces phase shift and it magnifies that image also in addition to it the lens distortions which are there that is going to introduce another phase shift. So, that phase shift is again all the phase shifts we multiply we can introduce a factor e to the power of i into the some phase factor, ok.

In all these processes what we are essentially doing is one is the incident wave which is entering, and that is modified by the lens distortion. So, this is what we called as a convolution of the wave or essentially an envelope of this two waves together this what we take it. Then the specimen if you look at it how do we describe this specimen is itself described at because the sample itself is a very thin simple if we take it. Any point on that sample can be described with coordinates x y and z, z if we take it together propagation direction this is the direction of the beam. So, we can make out that one particular plane if we concerned x and y is changing ok.

What it does is essentially a phase shift which is being introduced, e to the power of i these interface which we are introducing it. That is as the wave passes through the sample its phase has been shifted, and this phase shift depends upon what is the inner potential of that sample this we will come to it how it happens. And then there is an another time e to the power of minus mu x y this term is a real term, this real terms whenever we introduce it that essentially shows that there is a absorption which is taking place, that is when that electron beam enters into the sample suppose that is some inelastic scattering is taking place. So, part of the electron is lost that absorption term is given this particular factor.

(Refer Slide Time: 08:42)



Now, let us look at how we have to consider that specimen. Earlier we consider the specimen for most of the diffraction as well as for the last class or phase contrast microscopy, there where atoms are arranged in a periodic way and then that gives rise to a diffraction that is how we considered. Now how we will consider here is that as the beam passes through the sample when we enters, then atoms are arranged at specific

positions these are positive ions and which are distributed periodically in a c of negative c of electrons ok.

Since, there is a coulomb potential which is acting between them. So, there is a periodic potential which is there that sample which is varying in a regular interval. Then what it will happen when it enters into a periodic potential? The effect of it will be that the wavelength of the radiation will change. So, if the wavelength of the radiation when it comes with a wavelength lambda if it enters if it becomes lambda dash, with respect to the wave which has not undergone any interaction which comes out, this introduces a phase shift that is what essentially we are looking at it.

And using de Broglie formula, we can find out wavelength lambda equals h by root of two m e electron charge into e the applied voltage, this is essentially is non relativistic correction which has been taken. And in the case when it enters into the sample this the voltage increases by this potential which is essentially a positive potential these two when it adds together, we get that lambda dash which we calculate and what is the phase difference between these two. So, this is what 2 pi d z by lambda pi.

So, this when we try to do it finally, what happens is that this turns out to be a formula of the type, the phase difference which is being introduced pi by lambda into E into V x y z is nothing, but the potential at every point and if we assume that sample is extremely thin and this is going to be a constant at particular point, then we can write it as sigma into this factor. Now we integrate this over the full thickness then we get the phase difference which is there that is the if this is the thickness of the sample then that integration will give you what is going to be the total phase change which is occurring at the back of the sample.

So, that will turn out to be nothing, but sigma into this integral is written as phi x y. This sigma is nothing, but pi by lambda e. The details you can see in the standard text books and get it. So, f x y essentially becomes exponential since it is a phase which is introduced I into this minus I into this is the factor and then this term is essentially as I mentioned is the absorption which is what is responsible for it. Now, the specimen is represented as a phase object. A phase object approximation this is what it is called this is how the specimen itself is represented and what we consider this phi is nothing, but a

projected potential which is being taken and what is the effect of this projected potential as the beam passes through on the phase shift which is introducing.

(Refer Slide Time: 12:40)



So, this has already been explained and in a general formula if we write it at every point a x y, and what is essentially important is that when the beam passes suppose this is one point this is one point when the electron beam enters come or here or here or here we know that depending upon where exactly it is entering, the potential is going to change.

So, depending upon that there is going to be a phase shift, when the comes out of it at different point this is what it has the exit wave function at various points if we try to calculate, the this function f of x y is going to change depending upon the what the projected potential in that direction is.



Then this called as a weak phase approximation that is the sample is approximated as one which is introducing just a phase change, and how this phase change is being considered? Essentially looking at we are not looking at the details of that interaction, but we finally, look at what the change which it introduces into a phase of the incident wave ok.

Then suppose the thickness of the sample is very small if we make that assumption, then what is going to happen is that this potential pi could turn out to be very small similarly this absorption is also assumed to be small. So, if these two are small then the exponential this one can be a expanded into a series expansion, and then if you omit the higher order term this is how it will turn out to be finally, this turns out to be one minus I sigma into phi of x y minus mu into. So, this is the phase term and this is the absorption term ok.

But generally when we deal with lenses and the lens aberrations and when we look at the back focal plane, we always look into Fourier phase similarly for many calculations doing it in a Fourier space is very ad advantages. So, what is essentially is being done is that the Fourier transform of the weak phase object, is this is what essentially it is given this is f of nothing, but the Fourier transform of this factor that finally, gives rise to one function a delta function, this is an another function which depends upon the absorption and this is the third function which depends upon the phase which it has introduced ok.

It has been noticed that this sort of approximation works very well in many cases, but realistically if you look at it in many cases you find that for uranium atom. Essentially the size of the atom is such that the thickness of the sample for this approximation to be valid turns out to be smaller than the atomic radial. So, there are some limitations are there, but what has been noticed is that this has been working very well in the case of most of the material, and this is what it has been used in many of the computers programs which are used to simulate the images as well.

So, essentially what we have considered is an object which represented as a phase which brings about a phase change, and then we do what is called as a weak phase approximation. So, that it can be the higher order terms in the exponential can be removed, and then it turns out to be in this particular form. So, this is as far as this is how an object will be behaving.

(Refer Slide Time: 16:31)



And now, let us look at what does that lens do. We know that in a ideal case the for a point object for an objective lens, we should produce a point image. But normally all the lenses have got spherical aberration associated with it what is the effect of the spherical aberration? For a point object we do not get point image in the Gaussian plane, but what we do get essentially is this is the particular plane in which an image which spread out its a Gaussian distribution and then another is a disc of least confusion where that all rays

converge that is the minimum size of the in the image which we can obtain for a point on the object.

The same sort of distortion takes place for chromatic aberration as well as the spherical aberration. We know the lens aberrations which are there spherical aberrations coma astigmatism curvature of that field, distortion these are all the lens aberrations, but if the astigmatism can be corrected and eliminated the other aberrations are also can be corrected corrected, but what is essentially going to happen the spherical aberration is inherently is going to be there.

So, this aberration by designing and making the lenses properly we can minimize it, but we cannot eliminate it and this is the one which is responsible with a Rayleigh criterion, to give an optimum point to point resolution which for a wavelength of 0.025 nanometer, the point to point resolution turns out to be 100 times poorer around point two nanometer correct ok.

(Refer Slide Time: 18:28)



As I mentioned all the aberrations this is spherical aberration can be corrected for a lens. Let us look a little bit in detail how this spherical aberration gives rise to phase shift that is what it is considered in this diagram here.



If we look at it this is an point on an object for which the ray which is travelling very close to optic axis is focused at this point at the back focal plane at the image, and the ray which is travelling to further away that is assuming to be the one which is coming to a end of that lens, this ray satisfying the Snell's law the ray diagram if we try to calculate it will be focused to a particular point here ok.

So, because of that for a point object now we have essentially a spread which is going to be there this spread is what we call it as delta r so that means, that if the lenses has no aberration associated with this the ray which is reaching this point should also have been brought this is focus. So, what it has done it is as bend the ray a quiet a bit. So, what is the angle which it has changed that epsilon as that is what is as given in terms of C s the spherical aberration, the radius of the lens and the focal length this is given by this formula this is from a geometry, it is very easy to derive it that one can calculate.



Now, let us what is essentially important is that we have looked at spherical aberration. In a lens what happens is that if we defocus the lens. So, what essentially is being done is that look at it. So, this is that object when it is in perfect focus it crosses over the along the optic axis at this particular point, where that image should have formed. Now if the lens is defocused a little bit so that this is the particular point in front of it is being; that means, that essentially if we take it this is though this point it comes this is equivalent to some spread which is going to be there. So, when it is being focused here for this ray.

If we look at it this is the way it bends and it is essentially coming to a focus at this particular point; that means, that now compared to that we had seen in the case of spherical aberration, the beam is deviated in the opposite direction. So, this also we can relate it to this deviation in the angle bend which its bringing out to be delta f into R divided by f square or in terms of this angle theta if we try to into interpret this, will be [mi/minus] minus delta f by f into theta this also one can derive very easily.



Now, let us compare these two ray diagrams. This is what its very interesting that is the spherical aberration what it does is essentially makes a ray bend closer towards the optic axis, the rays which are travelling far away from the optic axis whereas, the defocus what it does is makes the ray deviate away from the optic axis. So, it acts in an opposite direction.

So, for a particular angle of theta or the particular distance from the lens where the ray is getting scattered, if we try to find out what is going to be the net angle of bent which it is going to take place that will be a sum of these two.

(Refer Slide Time: 22:34)



So, it will be one is this and another is. So, the net effect will be some value that spread delta r that is going to be rather small that is what essentially it is being given epsilon s equals this is the term corresponding to spherical aberration, this is the term which is corresponding to the defocus ok.

This bent essentially what it is doing it is if we look at it here is that, introduces a path difference in the ray which is coming because of this bent. So, this bent angle itself what we try to do is convert this into a phase difference, path difference is given by epsilon into d R and what is the phase difference corresponding to it. So, this is exactly the value which it, but this phase difference will be continuously changing as we go as the value of R changes. So, essentially what is the maximum which it can introduce phase difference which it can introduce is by integrating this function we can get out, and this is what when we substitute this value of epsilon into this equation we get a term like this ok.

This term can be written in forms of theta also, but what is essentially important or assuming theta equals delta k by k, this we can easily derive it we can write in terms of delta k which is nothing, but the wave vector or the diffraction vector. Essentially what this delta k means that if we have a lens.

(Refer Slide Time: 24:17)



The rays which are coming parallel to optic axis all of them are entering into here and focused at this point on the optic axis, the ray which are far away from the optic axis there will be all coming like this ok.

So, they are all focused to a particular point this is equivalent to with respect to lens if you try to see it here the distance this delta k equals g. So, essentially delta k equals 0 means this is the transmitted beam for different g values, that the diffracted spots this will have different values of delta k this is equivalent to beam entering the lens at different distances from the optic axis. That is what essentially which is being taken care of. So, this is being explained position of g vector from optic axis in reciprocal units from optic axis in the lens in reciprocal unit ok.

Now, what we can see that the defocus and spherical aberration can compensate for each other c, but normally depending upon the value that we can calculate also for this epsilon equals 0, what should be the specific value of theta for which they will be compensating. So, they compensate only for one particular value they do compensate, but for different g vectors g occur at different positions away from the optic axis in the lens. So, there will be a different value of W which is going to be there.

(Refer Slide Time: 26:08)

Lens aberration on lattice fringe imaging
$$\begin{split} & \stackrel{k}{}_{k} \\ Q_{\text{PTF}}(\Delta k) = e^{-iW(\Delta k)} & \text{Phase transfer function} \\ & \psi_{\text{tot}} = \phi_0 \left(e^{ik_0 \cdot r} e^{iW(0)} + i\frac{\Delta z}{\xi_g} e^{i(k_0 + g) \cdot r} e^{iW(g)} \right) \\ & \text{Corresponding phase shift added for each beam} \\ & I_{\text{tot}} = |\phi_0|^2 \left(1 - \frac{2\Delta z}{\xi_g} \sin(g \cdot r + W(g)) \right) \\ & I_{\text{tot}} = |\phi_0|^2 - |\phi_0|^2 \frac{2\Delta z}{\xi_g} \left(\sin(g \cdot r) \cos(W(g)) + \cos(g \cdot r) \sin(W(g)) \right) \end{split}$$

What we will try to do now, with these is that take this particular value for a specific g vector. So, this W is nothing, but it is the phase which is being introduced, this phase will introduce a phase shift into the in that sample ok.

(Refer Slide Time: 26:18)

$$\begin{split} \mathcal{E} &= \mathcal{E}_{\mathrm{S}} + \mathcal{E}_{\mathrm{A}} , \qquad \mathcal{E} = C_{\mathrm{S}} \frac{\mathcal{R}^{3}}{f^{4}} - \Delta f \frac{\mathcal{R}}{f^{2}} \\ W(\mathcal{R}) &= \frac{2\pi}{\lambda} \left(\frac{1}{4} C_{\mathrm{S}} \frac{\mathcal{R}^{4}}{f^{4}} - \frac{1}{2} \Delta f \frac{\mathcal{R}^{2}}{f^{2}} \right) \quad \text{W(R) phase shift to wave introduced} \\ & \text{by spherical aberration and defocus} \\ W(\theta) &= \frac{\pi}{2\lambda} \left(C_{\mathrm{S}} \theta^{4} - 2 \Delta f \theta^{2} \right) \qquad \theta = (\Delta \mathbf{k}/\mathbf{k}) \\ & W(\mathcal{A}_{\mathbf{k}}) &= \frac{k}{4} \left(C_{\mathrm{s}} \left(\frac{\Delta k}{k} \right)^{4} - 2\Delta f \left(\frac{\Delta k}{k} \right)^{2} \right) \\ & \Delta \mathbf{k} = \mathbf{g} - \text{Position of g vector from optic axis in reciprocal units} \\ \\ \text{Defocus and spherical aberration can compensate each other for a specific } \theta \\ & \text{value only since the dependence of each aberration on } \theta \text{ is different} \end{split}$$

That phase shift can be written as e to the power of i W into delta k, depending upon which g vector will use it this value will be changing

So, suppose we consider a one transmitted beam and a diffracted spot. So, that transmitted beam is represented e to the power of i k 0 dot r, and e to the power of i W 0

becomes the phase shift is introduced by the lens for the transmitted spot which will turn out to be 0, and the scattered reflection as we have derived earlier this will be i into delta i z by psi g because i is because scattering (Refer Time: 27:13) in a 90 degree phase shift e to the power of k 0 this is the direction in which the diffraction beam is coming, and into it multiplied by an another e to the power of i W g this is the phase shift which is introduced by the lens.

So, what will be the total intensity? I is equal to psi t psi t star. So, if you do it finally, we get a term like in this term if we look at it this is the transmitted beam, the total intensity at any point is this the intensity can transmitted beam minus this term it is a sin g r into cos W g, and then an another term which comes is that that is when the spot is very close the cos term turns out to be that is when the this particular term the sin term will turn out to be 0, but that essentially means that when the sin term turns out to be 0, the spot is very close to it we may not be seeing much of a fluctuations ok.

(Refer Slide Time: 28:46)

$W(g) = -\pi i$	2, when diffraction vector is far from optic axis. This condition gives best
contrast for minges. This is for a specific fattice minge.	
More g ve dot appea one g. co	ectors have to be used to get intersecting fringes giving black or white arance in image. But spherical aberration is compensated best for only s W and sin W now affect fringe intensity and appearance of image.
lt is not c can chan	lear whether columns of atoms should appear as white or black. This ge with defocus and thickness of sample

But when the W turns out to be pi by 2, then what is essentially going to happen is that the cos term will become 0 and this is the term which is going to determine how the intensity is going to vary. This is what the various conditions which are being chosen that is W g equals 0 means that diffraction vector is very close to a optic axis fringe spacing depends only on the second term. When W equals minus pi by 2 it is far from the optic

axis this condition actually in fact, this condition gives the best contrast this is for a specific lattice fringe.

But normally what happens is that not one diffraction spot we use it more than one spot is used to get high resolution. Then e g will have a different value of W g corresponding to it then this methodology of trying to find out the how the intensity varies, the variation will be different for different ones, this method has got some limitations in which is associated with it. So, though this in principle conveys how the lens aberrations modifies the diffraction contrast ok.

(Refer Slide Time: 29:54)



What we normally do it is the weak phase approximation which has been derived for that object that is the one which is being used. So, here we represent the ray in reciprocal space, the object can be represented reciprocal space in this way, and the then the lens introduces another distortion this distortion we can add to it.

So, now with this if I total will be that this and a W star of it the star of this one. So, this turns out to be this is the delta function, and there is an another term two f this is function and this is the third function which represents on sin W delta x because delta k x delta k y is nothing, but from the center of the lens where in reciprocal space the diffraction spot is entering. And if we assume that absorption of the sample is going to be 0 this corresponds to a intensity corresponding to a direct beam, this corresponds to absorption.

If the absorption is assumed to be 0, this term is going to be for a thin sample this negligible then essentially these two terms decide.

So, the how much is the contrast which is being transferred intensity variation between the direct minus this term is going to decide and intensity at every point. So, that is what is going to decide how the contrast is going to come is decided by these functions sin W.

(Refer Slide Time: 31:39)



So, this correspond to a direct beam, this is what is written this term corresponds to amplitude contrast and the third term is essentially are all absorption this is the phase contrast which comes. And when W equals minus pi by two sin W equals minus 1 and that value of mu is considered to be very small, then as I had mentioned earlier only these two terms are important. So, finally, this is how the intensity turns out to be when sin W equals minus 1 ok



This depends upon what the value of W is, what is this W let us look at this that sin W as we have derived earlier this depends upon this particular term which is corresponding to a spherical aberration, this terms which corresponds to a defocused term.

Here this is term is varying delta k to a power of 4, here the defocused term is turning out to be delta k to the power of to the power of 2 and finally, this is what it decides the net what is going to be the phase change which is being introduced. Here what is being plotted is this phase error is being plotted as a function of C s and for various values of delta k for a 300 k v microscope, where the wavelength is 0.196 nanometer and a C s of the lens equals 2.3 and this is being plotted from the when the defocus becomes 0 this term becomes 0 since the variation is essentially delta k to the power of. So, essentially this will be varying like this.

And then when the value of defocused increases initially what is going to happen is that this term dominates and the value of W becomes negative, then afterwards as a value of this delta k terms becomes large that effect of delta k terms increases, and then we find that as you shell it increases and the effect of this term gets reduced. So, it is a very complex term, but what is essentially important is that this phase error as we can calculate it, for some particular value we can see that minus pi by 2 that is for specific value if we consider it, here as we mentioned it when that W equals minus pi by 2 the maximum contrast comes and that corresponds to in this specific case some particular value that is what essentially it is being given here depending upon the delta f the range of value of, but if you look at these terms as it turns out to be from here to here, there is a value which is going to be there between minus pi by 2 and some other value which is very close to it so, that the effect of this phase error on sin W, if we calculate it that value turns out to be approximately nearly the same value which we get it.

So, what one should understand is that the lens itself introduces depending upon the defocus, a phase error is being introduced and this phase error we can see that at a particular value we get an optimum value this called as the Scherzer defocus, that is where the range of values over which closer to it this phase error the effect of phase error on sin W if you look at it is very small. So, most the sin value turns out to be nearly the same for a range of delta k values range this we will come to it in a short while.

So, what is essentially important is that, from here to here when it is the negative value whatever be the value of this sin term; the sin term is going to be always giving rise to a sin some value because if we can take this intensity, intensity equals ok.

(Refer Slide Time: 36:14)



One delta function minus 2 sigma into phi into sin W. Suppose the value of W turns out to be a positive value then what it will happen is that for one value of g it gives a positive value and another value of g delta k value it gives a negative value, then what is going to happen is for a specific at a particular point when we consider the intensity contribution for all of them one adds to it another subtracts the net effects could be that the intensity of that spot could be as same as that adjacent regions, whereas for these values delta k the value is always negative; so they coherently and so the contrast essentially increases, ok.

(Refer Slide Time: 37:09)



So, this is what essentially is being done ok.

There is a specific value which is called as an optimum value of defocus for that optimum value of defocus if you try to plot it, we can see that from this particular value to this particular value T u is nothing, but twice sin in this particular diagram is essentially nothing, but equal to delta k, this is sin nu equals sin of W of delta k, this is what it is happening going to happen. So, here if you look at it though it is for small values of the delta k, that small values of delta k corresponds to spots which are very close to the primary beam, most of the diffraction spots depending upon the periodicity (Refer Time: 38:06) at some distance, most of the time for the planes which are like if it is a 111 is the close pack plane that is where the first diffraction spot. So, from which to some other spots where we can get it within that range of reflections we find that this value of that sin term turns out to be very close to a specific value.

So, this give rise to this means that, all the effect of all the spots to at a particular point at a intensity at a particular point is to coherently add to it. So, that the contrast the sharp contrast we get it and then where is that first term where it cross over? These are all the range of g values because this you can see that this is a nanometer inverse. So, it is an reciprocal space. So, these are all the g values if we use to form high resolution image used to interfere, then all these beams at every point they are going to coherently add and constructive or destructive interference will take place, this will give rise to a nice contrast and we will be able to see sharp.

But beyond this particular point we can see that there is a fluctuation it changes very rapidly for delta k value. So, the effect of this will be that this regions of k value if we choose it, they will be essentially one will be a enhancing the contrast another will be reducing the contrast, the net effect will be that in some places the contrast can become 0, in some places there is a variation in contrast, but in the reliability of interpretation becomes very poor in this case. So hence, we should use only this limit this range only we should use it. So, this particular value of u is the only one which gives useful information ok.

(Refer Slide Time: 40:23)



That is what we do when we have a lot of diffraction spots are there, we put an aperture and choose it, the size of the aperture should be decided by the we can write it in terms of the reciprocal distance, then that will turn out to be this particular distance.



So, here what is being done is that for different defocus how this value of sin is itself is being changed which is being shown. For example, when the defocus becomes 0 we can see that essentially this gives rise to a one where that value of sin wave becomes positive. And when the defocus gradually we increase the defocus value, we can see that the range of values over which that value of sin remains almost nearly the same that increases and for what we call it as a Scherzer defocus. This corresponds to a value of C s to the lambda to the power of it becomes half.

Then for this value of Scherzer defocus what is essentially is going to happen is that, for a long range high range of values of delta k the value of sin W becomes same, and coherently add to the contrast. This we can calculate it for the microscope which we are this is the range over which the delta k value changes and the Scherzer defocus this is 0.2327 nanometer this is another resolution.



How to find out this optimum value for the Scherzer defocus? For which what we can do it is that here what is written as (Refer Time: 42:21) which so far what we have done is essentially W of delta k ok.

And the u is nothing, but equals delta k then you will understand that there is a these two expressions are that same. We differentiate it and try to find out that is the differentiation minimize it to 0 that gives value over which we can find out that where delta k value for which the value of sin x turns out to be almost a constant over a range of value differentiate it. And another imp parameter which we choose it is that we chose an two conditions one is sin 0 equals 1 and another is that this sin W can be command that twice sin W we take it this function t equals twice sin W so; that means, that when sin W equals half this value of T becomes 1.

(Refer Slide Time: 43:30)



If this value of T becomes 1 essentially what is going to happen is that this value becomes 1. So, essentially we get the maximum the contrast becomes the maximum contrast which we can obtain that is what essentially it is being taken here and solving these two equations together, we get a value of delta f which is called as the Scherzer defocus which is minus 4 by 3 C s lambda to the power of half. And another is this is gives rise to value of delta k which we can find out using this value of delta f and inverse of that will give rise to a distance.

And this distance also is similar to a point to point resolution which we have used earlier in the Rayleigh criterion this turns out to 0.9 lambda to the power of 3 by 4 C s to the power of 1 by 4, here this turns out to be slightly better. So, far a lattice resolution this is the term which decides what is going to be the resolution which can be achieved in a microscope ok.



But what we should understand is that, what all aberrations which we considered. We considered only this term which corresponds to the spherical aberration and its compensation by defocus to a certain extent, but in addition to it chromatic aberration can again corresponding to a distortion as we have seen, then spread of the angle if the beam is not parallel they can the specimen can drift the vibration of the specimen can take place.

There are so many factor each one of then add to some sort of a phase shift or a distortion and this will be added to the beam. What will be the effect of all these distortions is that when we calculate this value of T u which is essentially a product of all these terms, then it turns out that beyond the particular value this term becomes almost 0 what is the value of delta k corresponding to which we could observe this ok.

This is slightly better than this; this is called as the information limit of the microscope. So, this is the maximum resolution which we can get it, even if we try to get information which is beyond that in these slide what I have done is what will be the effect of the various effects like delta f becomes 0.

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And then when the convergence of the beam is being changed, all those effects are being considered, ok.

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And that is what essentially it is being finally, as I mentioned earlier its though this fluctuation takes place in an ideal case where only the spherical aberration is considered when we consider all other limitation the spread of electron beam, chromatic aberration all other contributions to the lens errors then what is going to happen is that we may not

be even able to go to this beyond before that itself it comes into a point. So, this is what it decides the information limit.

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What we are showing it here essentially is an image which is being an example which I am trying to show is that image which has been taken with 470 nanometer defocus. This is an optimum Scherzer defocus and this is where the defocus has been changed to a positive site. One can immediately make out that the clarity with which the dotty contrast is coming is much more better for the Scherzer defocus. Here we can see that there is a fussiness which is coming in both this regions, ok.

So, when we do a high resolution imaging what we should do it is always try to take the image a Scherzer defocus, but so far what we have done? We have done all these things a derivation to find out what the Scherzer defocus is depending upon the microscope conditions the sample thickness then at what voltage we operate it these conditions can change.

So, what is essentially is being done is that to get the best information normally closer to Scherzer defocus on either side take a series of images changing the defocus condition, and using this images and a computer simulation one can find out that image which corresponds to a Scherzer defocus, and how the contrast of that image itself is changing that can also be simulated that can be used to find out what is going to be the atomic structure of that sample which is giving rise to this sort of images. That is what is essentially important when we wanted to get or when we wanted to interpret the high resolution images ok.

How these sorts of simulations have to be done and that part we will discuss it in the next class. Similar to that in recent times microscopes have come out where the spherical aberration of the lens itself could be compensated and made 0 or negative, this also can drastically affect the contrast as well as the clarity of the image, and also it helps in interpretation of many of these images.

We will talk about these developments in that are both simulation as well as the aberration. These microscopes are called aberration corrupted high resolution microscope. These aspects we will discuss in the next class. We will stop here now.

Thank you.