

Electron Diffraction and Imaging
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Lecture - 27
Phase Contrast Microscopy - 03

Welcome you all, to this course on Electron Diffraction and Imaging. In the last two classes we have discussed phase contrast microscopy are high resolution transmission electron microscopy or you can call it as atomic resolution microscopy.

Let us before we proceed further let us have a recap of what we have covered in the last two classes. In the first class what we considered was an ideal microscope, where all lens aberrations are assumed to be 0. And we assume that essentially coherent the elastic scattering of the incident plane wave which taking place within that sampled, and the wave length of the radiation is much smaller than that of the atomic spacing in the sampled.

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For ideal microscope when all lens aberrations are assumed to be zero and coherent elastic scattering of incident plane wave

$$\psi_T(x, y, t) = \phi_0 e^{i2\pi k_0 \cdot r} + \phi_{g_1} e^{i2\pi k_{g_1} \cdot r} + \phi_{g_2} e^{i2\pi k_{g_2} \cdot r} + \dots$$


2 beam condition; $s = 0$ and $g' = g$ $I = A^2 + B^2 - 2AB \sin 2\pi g x$

Intensity of image fluctuates with periodicity $d = 1/|g|$

Lattice fringes – Periodicity depends on lattice plane spacing
– No relation to atom positions in the unit cell or structure

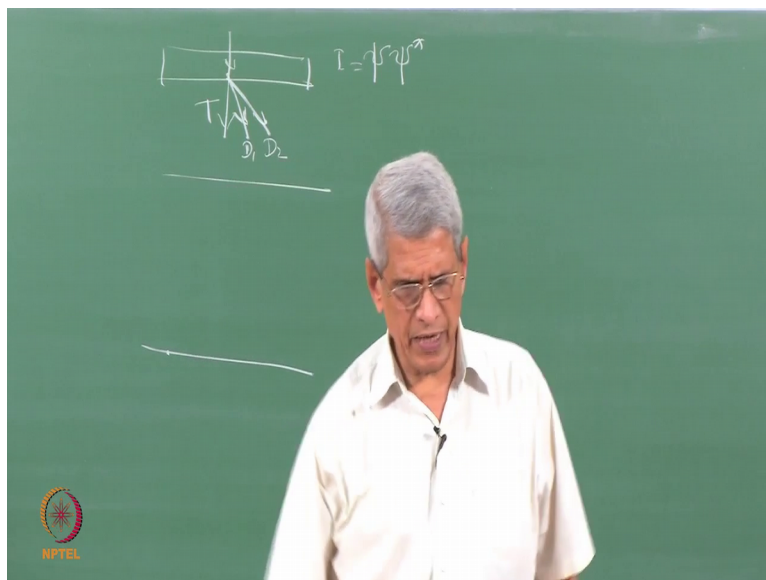
Ideal HRTEM condition

λ < interatomic spacing = point to point resolution



Then what we did essentially was that we try to find out at any point on that image, what is going to be the contribution from the various beams. That is the beams which I have scattered that is from the sampled as the beam enters into the sample, it is getting this is transmitted beam and their beams which are diffracted in different directions $D_1 D_2$ we want write it all these beams ok they come together and form an image.

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So, what we try to do is essentially is this term tells what is going to be the amplitude of the transmitted wave and what is that as a troublesome distance and reaches here at this point, at that point what is the phase which it is going to generate.

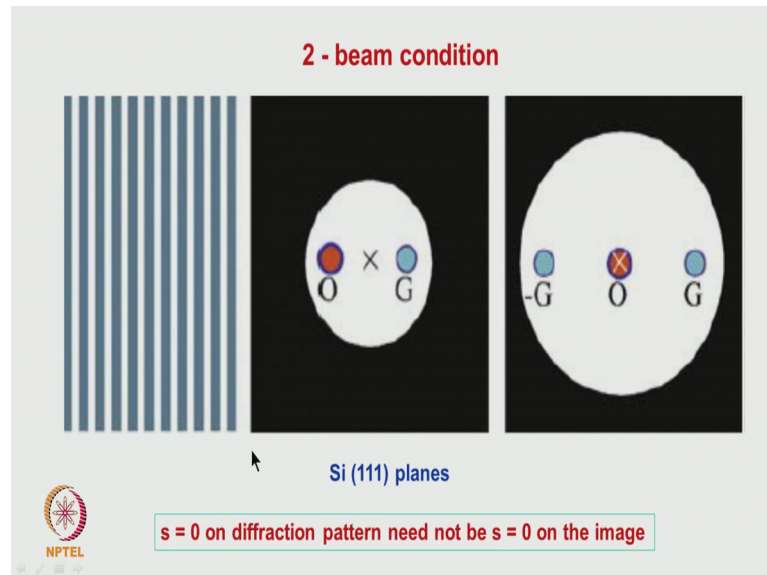
So, all these wave are allowed to again join together interfere, this interference pattern is what is giving rise to the diffraction. Then we consider the case where is essentially a two beam condition where only the transmitted beam and only one of the diffracted beam is there. In this case what happens is that intensity if you consider is essentially fluctuating with respect to g , where g is the reciprocal lattice spacing. But what is essentially important is that this is the amplitude of the wave and the intensity is nothing but I equals $\psi \psi^*$.

So, this term itself is a complex term, the phase factor which is there in this term they cancel each other. So, in the intensity there phase information about that sampled is lost. Though we get some intensity fluctuations that can give formation about the periodicity or the lattice spacing in some directions, but how atoms are arranged in that plane that information is totally loss this is, but even then this is one an ideal high resolution electron microscopy condition which we have ok.

As I mentioned earlier if λ is assumed to be smaller than the inter particle spacing, then the point to point resolution is decided by the Rayleigh's criterion if all the lens

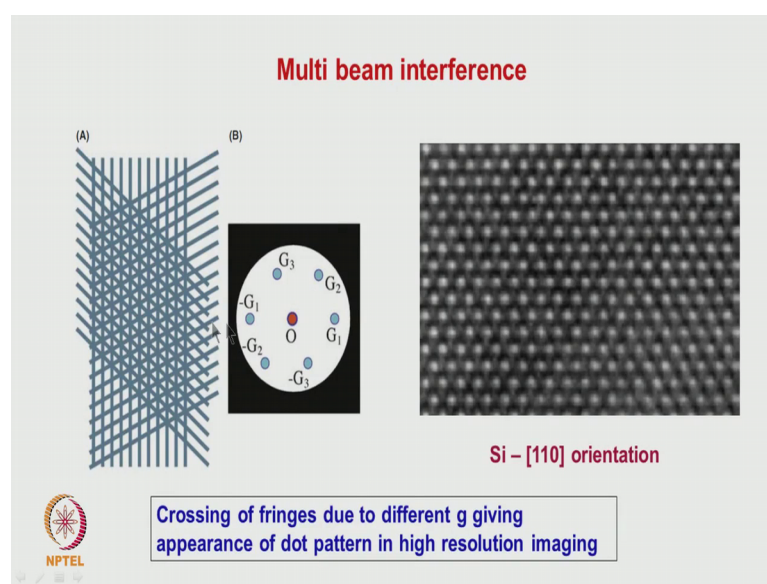
aberrations are not there, then wavelength of the radius sides there resolution then we should be able to resolve the atoms in an ideal condition.

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But what is the reality before we go into that we will just we considered the case where in a two beam condition, when two spots are considered this gives rise to a fringe contrast. This is typically what be obtained we have obtained in a (Refer Time: 04:02) which is using two beam conditions ok.

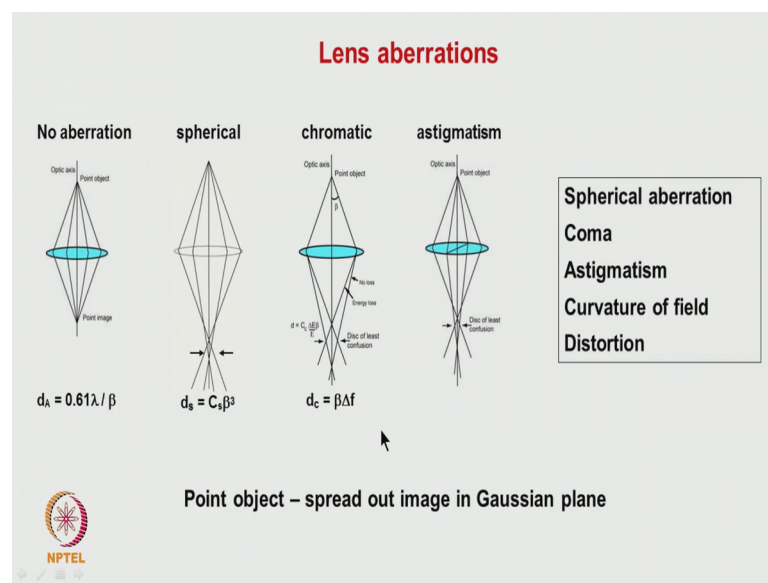
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If we use multiple beams then fringes due to each of the beams we will be getting, it actually this fringe space if you look at it the spacing that is that planes on which the maximum or minimum intensity occurs, they are perpendicular to their diffraction vector.

If many spots if we use to create a lattice fringes then this if intersecting fringes we will give rise to duct contrast and this duct contrast we will appear like an atomic resolution, but though this does not truly representation atomic resolution, which we have discussed in detail in the previous classes.

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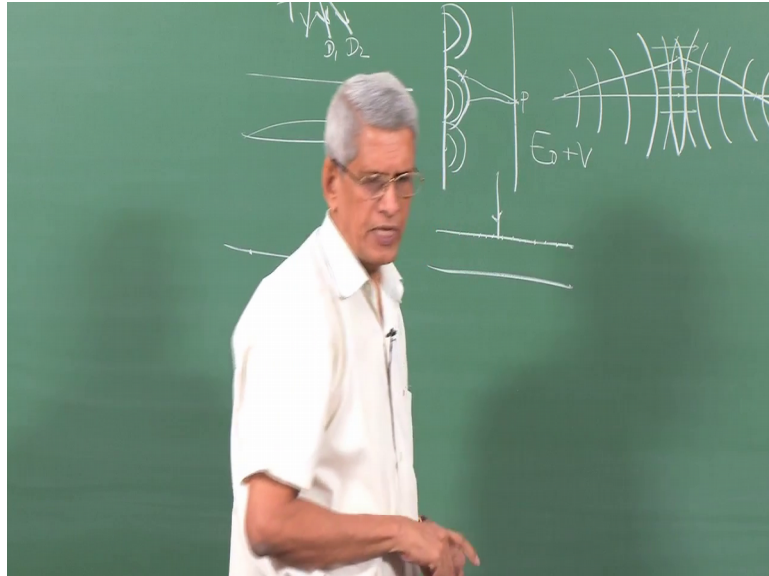


But what is the reality in a microscope? The lenses have for aberrations associated with it, in an ideal lens we should have no aberration and in such a case for are point object we should get a point image. What is the spherical aberration do for an point object, we do not get a point image we get a spread in the intensity; that means, that there is a variation in the intensity from the centre to the optic axis to the directions, this is due to spherical aberration, chromatic aberration, astigmatism all of them give rise to the sort of spread. So, the point to point get resolution get degraded considerably, this is one of the things.

So, these are all the aberrations all these things which we considered, we will come to it a little bit later, but what is essentially going to happen is that when this sort of a situation arises if you have two points the object from which the raise are coming, they will be a since there is a spread in the beam in the image plane, they will be

unnecessarily interference of these beams giving rise to artifacts will be there so that also adds to complexity in the analysis.

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So, in a normal microscope with lens aberration, in the last class how we considered is essentially that incident wave we considered read as a spherical wave. This is because whenever we take of a wave phenomena and diffraction which is occurring the hygiene principle has to be used. The hygiene principle as it says that the even if it is a plane wave which is going to be there from every point on the wave.

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In CTEM, with lens aberrations

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

Wave propagator $p(R) \equiv \frac{-i}{R\lambda} e^{ikR}$

Lens distortions $q'_{\text{lens}}(x, y) = e^{-ik(x^2+y^2)/f} * F \left[e^{-iW(\Delta k)} \right]$

Specimen $q_i(x, y) = e^{-i\sigma \phi_i(x, y) - \mu(x, y)}$ Phase object

You have a spherical wavelet which is getting emanating from these points from each of this point the spherical wavelets. If we consider that any particular point p here there is going to be a contribution from the various regions of this point from those spherical surface and that is how we can find out what is going to be the amplitude at this particular point when the wave propagates.

So, this essentially gives that has this spherical wave propagates at any particular point what is going to be there amplitude that is given by the incident wave amplitude, in to e to the power of $i k R$ by R . What is the wave propagating? That the wave propagates there is the one which tells that from here to here from all this points there is a contribution going to come to this way here, but each of this raise from here to here or from here to here they travel at different distance so, the path length is different. So, they introduce surface. So, this gives rise to modifies the amplitude of the wave which reaches each point and this is called as the wave propagator, this is one term which will be coming into the picture.

Another what happens is that the lens itself when we consider it, we know that we draw the lens right this has spherical lens. The lens itself what is the action of the lens for a point object it forms an point image; that means, that essentially if we consider the spherical wavelets which are coming like this, this spherical wavelets has to change the direction and then it will be broad back to they are focus at this point. That means, that the waves which are traveling in this direction there is a phase shift which has to be that lens what it does a differential phase shift which introduces to the beam which is coming there.

So, that it will be that is what this phase shift is given by this term. In addition to it the raise which travel along the optic axis and the wave which travel like this and when they reach there, that is spherical aberration is going to focus this ray to a particular point the ray which comes here it is focus to an another point ok that also introduces an additional phase shift and that is given by this term.

This term essentially is given an reciprocal space this $W \Delta k$ this is called as the d local registration 10, and since it is in reciprocal space we have to take a Fourier transform I have to get it in $d l$ space. So, that is who we get that lens this is the total lens distortion. So, so for what we have considered is an incident wave which is coming and

this propagating and it is heating that sample. So, how do we define that sample? For high resolution microscopy the way we defined that sample as the sampled acts as a one which changes the phase of the incident wave as it passes through. There is no other change which takes place and the phase change which introduces depends upon what is the sort of potential it sees it, as it passes through that sample that is. If this is the thickness of that sample as the beam enters we have atoms which are sitting at different points on the sample surface there is potential which is associated with these point.

So, it has to pass through this potential which it is going to do is change introduce a phase shift. That phase shift is because the electron (Refer Time: 11:01) has an energy if you assume that E_0 , as it enter some potential with it is V so it going to bring about the small change in their in their kinetic energy of the electron or the k of that electron. This has it passes through different thicknesses we can integrate the total phase shift which it comes and that is what essentially this gives and this term is essentially and absorption when it comes.

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Weak phase approximation


Specimen is so thin that potential ϕ and μ are small

$$f(x, y) = [1 - i\sigma\phi(x, y)][1 - \mu(x, y)]$$

$$f(x, y) = [1 - i\sigma\phi(x, y) - \mu(x, y)]$$

$$Q(\Delta k_x, \Delta k_y) = F\{f(x, y)\} = F[1 - i\sigma\phi(x, y) - \mu(x, y)]$$

$$Q_i(\Delta k_x, \Delta k_y) = \delta(\Delta k_x, \Delta k_y) - F[\mu(x, y)] - i\sigma F[\phi(x, y)]$$

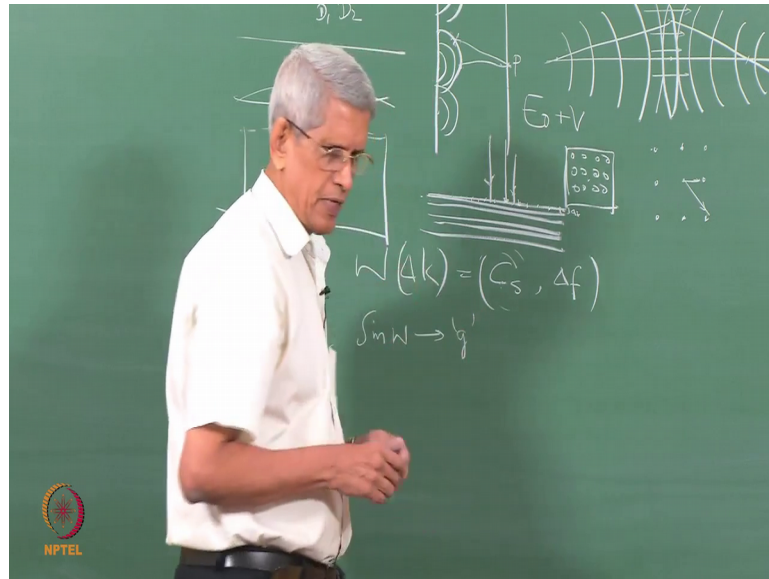


NPTEL

So, this is the term which is what is going to be the depression there is the phase shift and this is the absorption term this is how we described a sample. This is called as the sample is called as a phase object if we what we considered; then what we did was that we made another approximation that the thickness of the sample is small μ is also small absorption and there is potential ϕ are the phase shift ϕ is small.

So, that we can expand it (Refer Time: 12:00) power of this one in terms of a series expansion then finally, that f of x y we will turn out to be. What essentially means that this term says is that essentially as the beam passes through that sample, if it is passing on a position where an atom is there or if it passes in between the potential with its easy to going to different.

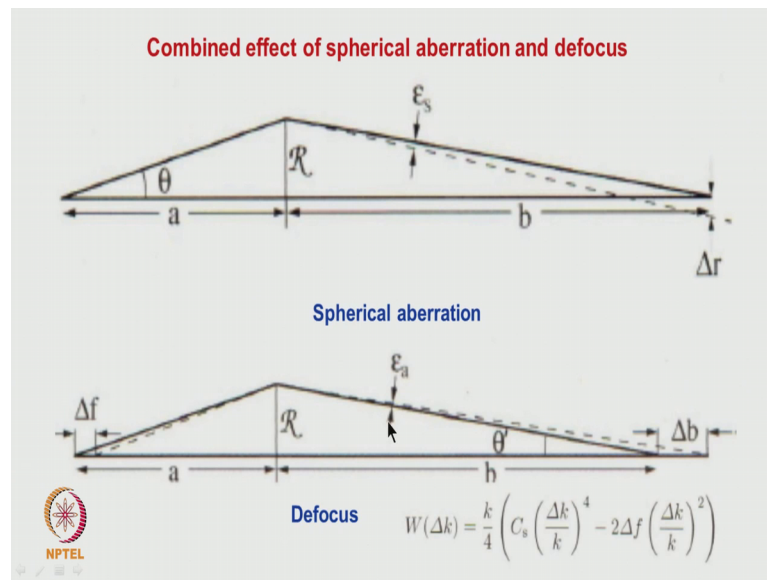
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So, as a function of x and y on that sample surface like if you look at it this is of the atoms are seeing, and the beam direction in this case we will be perpendicular to it if that electron beam is falling here or falling here, there is going to be a variation in the phase shift which is going to be introduced from point to point as the beam comes out on the other side ok.

So, both in absorption as well as the phase shift and generally it is easier to work in a reciprocal space.

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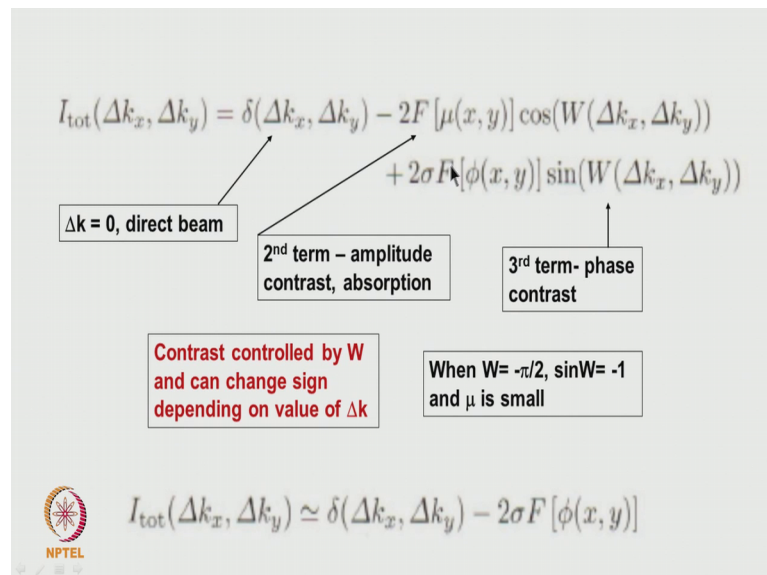
So, if you do that we can take a Fourier transform of this and this is what the essentially the Fourier transform gives it before why. So, this is how that time is described both in real space as well as in the Fourier space how it will be described. Here instead of one it becomes delta function. Let us then we looked at what is the combined effect of spherical aberration and defocus. As I mentioned earlier what does the spherical aberration do as the beam which is closer to the optic axis that is focused at a point, the ray which is traveling for example, in the case of a microscope the diffracted rays we will be is away from the making an angle with respect to a optic axis, assume that they come like this and this is the end of that is lens that is the outermost radius of the lens from which it is scattered refracted.

Then this comes to a focus at this particular point; that means, that the ray should in principal as further geometrical optics all the rays is focus to a particular point in the image, but that does not took a some rise or broad to a focus in earlier because of this there is a spread which is going to come. What is going to be the case when we consider small defocus if you introduce? The effect of the defocus is essentially going to be that the ray instead of being brought close to the optic axis it is deviated away from the optic axis, but the dependency here it is going to be epsilon is theta to a power of 3, here it is going to be theta. So, the net displacement or the net a the size of the object for a point object in the Gaussian plane we will be given by this particular formula, which depends

upon delta k. Delta k is nothing but g the diffraction vector and then Cs there is spherical aberration coefficient of the lens and delta f is the defocus.

These are all the for some particular value of defocus for a specific value of theta this term can turn out to be 0, but we know that even a diffraction takes place when we orient it for perfect shown axis condition, we get a lot of diffraction spots all diffraction spots are going to come and all having an equal intensity and each may be at different distances from the center. So, when they pass through that lens this delta k is also going to be different, because of each these w will be changing with respect to the g vector.

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The slide displays the following equation for total intensity:

$$I_{\text{tot}}(\Delta k_x, \Delta k_y) = \delta(\Delta k_x, \Delta k_y) - 2F[\mu(x, y)] \cos(W(\Delta k_x, \Delta k_y)) + 2\sigma F[\phi(x, y)] \sin(W(\Delta k_x, \Delta k_y))$$

Annotations on the slide include:

- $\Delta k = 0$, direct beam (pointing to the first term)
- 2nd term – amplitude contrast, absorption (pointing to the second term)
- 3rd term – phase contrast (pointing to the third term)
- Contrast controlled by W and can change sign depending on value of Δk (pointing to the second term)
- When $W = -\pi/2$, $\sin W = -1$ and μ is small (pointing to the third term)

At the bottom, the NPTEL logo is shown next to the simplified equation:

$$I_{\text{tot}}(\Delta k_x, \Delta k_y) \simeq \delta(\Delta k_x, \Delta k_y) - 2\sigma F[\phi(x, y)]$$

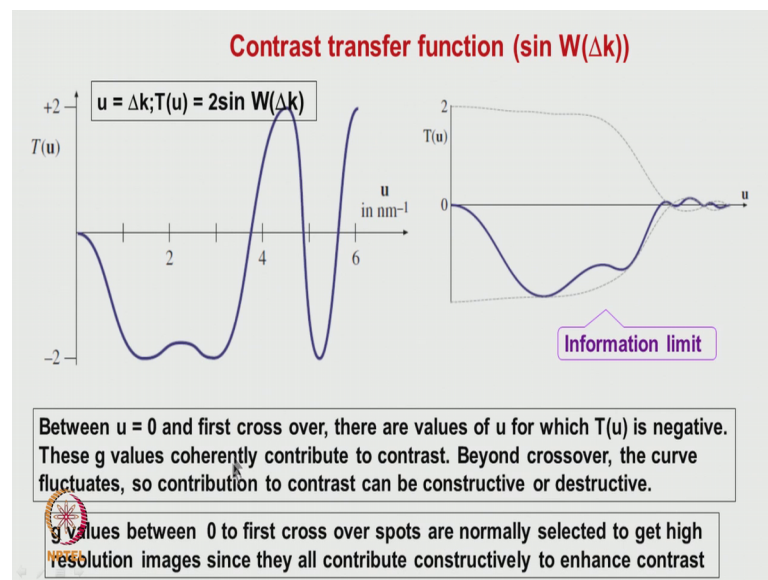
So, as I mentioned now the intensity of the spot if you have to consider it the object function which we have described that has to be that will be modified by this factor that W a to the power of phi W into delta k x minus delta k y this term.

So, this if we will what essentially is going to happen is that this first term corresponds to a direct beam, the second term essentially corresponds to amplitude contrast and absorption and the third term which is the phase contrast term. Now if you look at it when we use many beams to get a fridge contrast the W is going to change, but what is essentially important is that the value of W can go from positive to negative depending upon what is the value of g which we choose it, if the value is between 0 and minus 1 all the beams we will essentially with respect to this, it is going to give rise to subtraction of

this one; that means, that they are going to add and then constructive interference we will take place that essentially means, that we are going to get a contrast enhancement ok.

Suppose the different beams introduced different values for this one plus and minus, then these terms can cancel each other and finally, no contrast may be seen. Should to get the best contrast in a high resolution microscopy, for all the values of g which we use to interfere they should and enhance the contrast ok.

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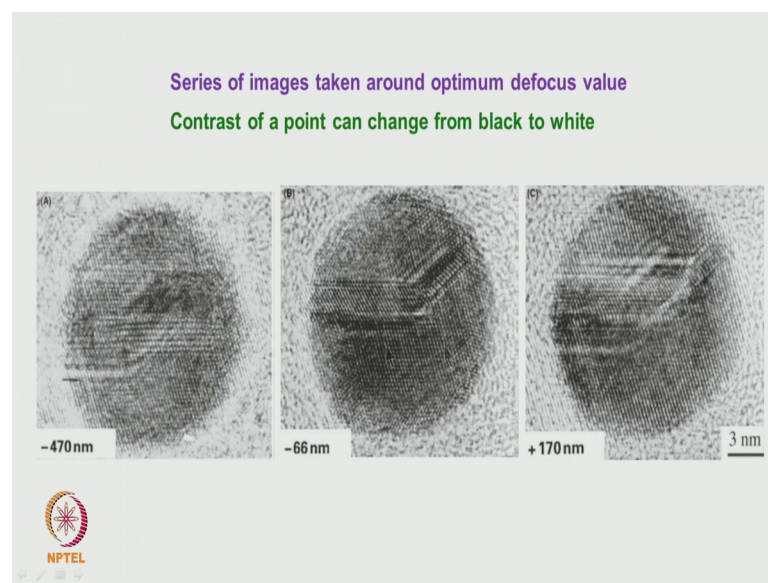
This how we can decide is using this term the W we have drive the name we have shown that expression and this expression itself if you tried to plot it as a function of Δk are the g for various C_s and defocus value of the lens, then this is the sort of a this term this is for a specific defocus value which correspond to what is called as defocus which has been defined earlier a in the last class ok.

Now, we can see that for most of the values from here to here essentially the signed W value turns out to be nearly that same and its all negative; that means, that this will add to announcement of the contrast, this is for a lens with an abera only a spherical aberration and defocus which we consider. But there are many causes of aberration like that aperture can give rise to a phase shift then a sample drift, drift in that image that can also add to it. Then chromatic most important part of is that chromatic aberration can also give rise to a defocus. So, the effect of all these the annual functions is that in this particular case if you consider it, this is going to fluctuate between some values, but what

is essentially going to happen is that the fluctuation essentially stops and comes to a 0 this is called as the information limit.

So, beyond this particular one higher values of in a g does not contribute to the contrast in the high resolution image that is what the essential it is being given mention. This I showed some pictures to tell that how with a different defocus values for a microscope with a C_s value, how the image contrast is changing we can see between this and this we can see that there is a change in contrast here again there is a change in contrast.

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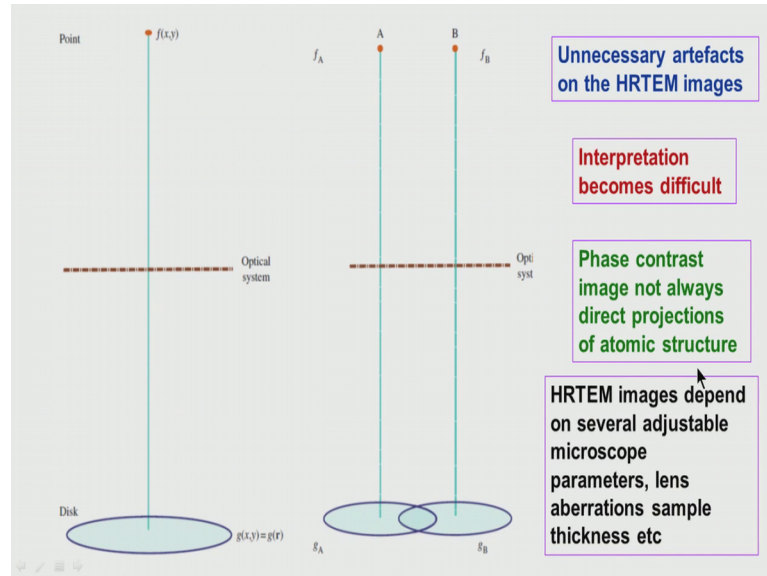


Finally, how does this contrast change come it is because if you have a point object as I had mentioned earlier what the optical system does; it is there is a spread in the image which is going to take place. But if you have two points are there very close to each other which I have just resolved by the beam, but in the image space we find that there is going to be a in the reference that is overlap of this disc when this disc overlap this gives rise to some contrast variations ok.

So, the actual contrast variation is not corresponding to each of this points, it is some sort of an artifacts which can come because of all this affects interpreting the high resolution images in a qualitative I just looking at the image, is going to be very difficult. So, we have to do some to get a quantitative information image simulation has to be carried out to interpret the results. So, that is what essentially is says that unnecessarily contrast comes, interpretation becomes difficult. Phase contrast image is not always projection of

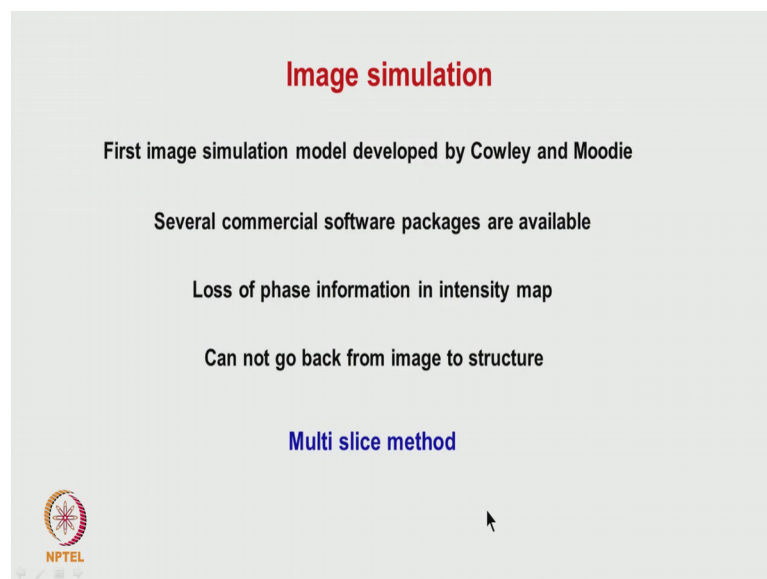
direct projection of atomic structure and another if that a (Refer Time: 21:42) images depends upon several adjustable.

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This spread depends upon several adjustable parameters; lens aberrations, sample thickness all and then convergence of the beam there are so many factors independence on ok.

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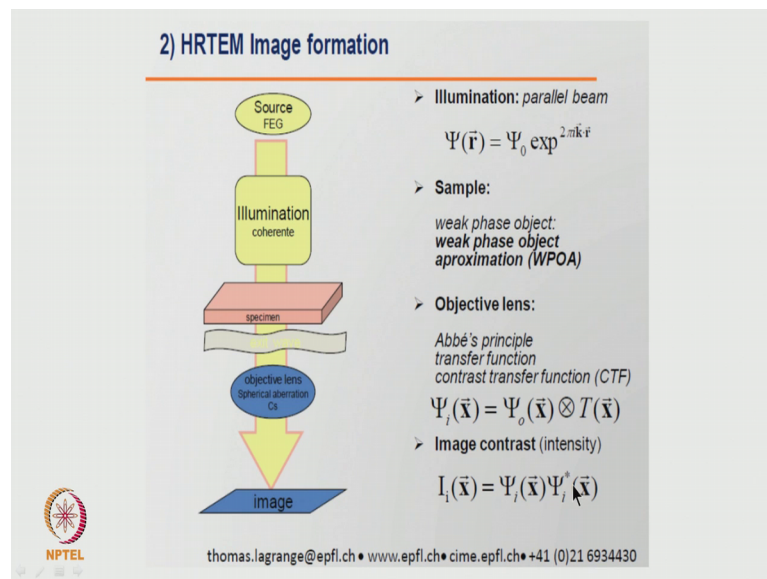


So, the image simulation is must. The first image simulation model was developed by Cowley and Moodie and they published it in 1957 itself. Now several commercial

software packages are available to do this simulation, but these are all like black boxes. So, when you are using any of these packages if you have more than one package it is better to check whether the data which is information which is given by one package, has the some consistency if you try to do with other packages, each box on a different principal and different way in which these packages are operating. As I mentioned that the major problem in getting from this high resolution dotted contrast which we get the position of atoms in the units is, because the phase information has been lost when the intensity mapping is taking place. So that means that from the intensity we cannot go back from image to the structure.

So, to get some information about it what we have to do is that we have to assume some model of the structure if we have some prior idea, and then do some what is called as a technique which is called a multi slides method to find out what is going to be the phase amplitude.

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So, in this particular slide which is taken from Thomas Lagrange's presentation, essentially these source and all these cases the source has to be FEG. So, if you take a field emission gun source what we can do it is there is beam spread could be reduced considerably; that means that the chromatic aberration could from the source could be reduced. If the objective lens currents are stabilized all the fluctuations are reduced then the contribution to defocus from that could be reduced considerably to a chromatic

aberration and then what about if the sample is taken as very thin specimen, then also the contribution to chromatic aberration from the beam as it passes through the sample that could also be reduced because of inelastic scattering, ok.

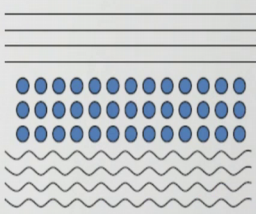
Here what is being shown is that uniform illumination, which is coherent and which is falling on to the specimen. And as it comes out and these electrons source even though the electrons which are coming we consider as wave it supply in wave and we see that the as if the wave is getting scattered. The objective lens because of spherical aberration it adds to it distortion and finally, in the image when this ψ ψ^* we take that image intensity there are some fluctuation, that is what essentially given how mathematically each of these operations results in the change in intensity, ok.

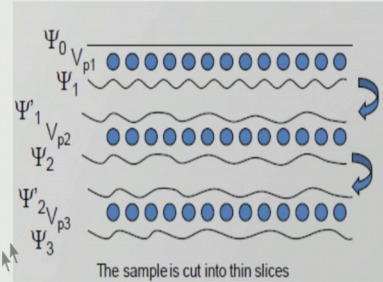
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$f(x, y) = [1 - i\sigma\phi(x, y) - \mu(x, y)]$


WPOA

Multi-slice calculation:
Calculation of the exit wave function for complex structures:





The sample is cut into thin slices



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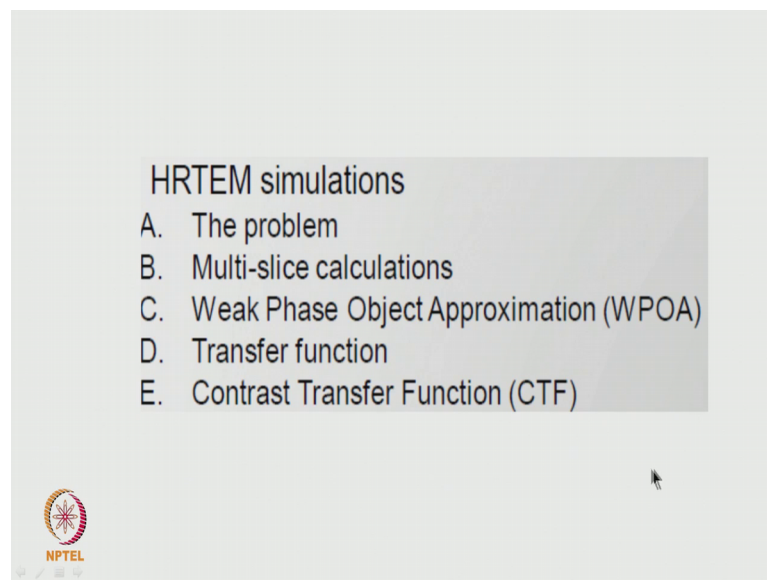
What is done in multi slice calculation let us just going little bit detail. First be assume that sample to be essentially a weak phase object approximation, that is what essentially is being done; that means, that the sample can be considered like a these are all the positions of atoms are you can consider are position are some potential variance you can. As the plane wave comes and enters as it comes out of the sample surface we can see that the wave fronts have changed because the beam passes through that sample, there is variation in the phase shifts are being introduced ok.

This calculation how exactly it is done is that you assume that the plane wave is coming and corresponding to this there is a potential which is their going to fluctuate the as

function of position, and as it interacts with this and its going to modify the wave was it comes out of this thin small thickness of that sample. Then this has to be propagated from here to here and which propagates it reaches here with some wave functions ψ_1 and again the potential operates on it. It modifies this that ψ_2 again a propagate and factor as I mentioned earlier has to take and this how. So, this way we have to take it for the various thicknesses.

And finally, we get what is going to be the exit wave this is called as the exit wave function that is at the back of that sample, how as a function of x and y the wave the wave function is changing ok.

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In the HRTEM this ones, so this is the multi slices calculation which we have to do and for that we beam approximation, then now once this has been done we have to take the transfer function and the contrast function of that sample also has to be added on it, but this entire for a perfect way of doing it is taking a block wave approach.

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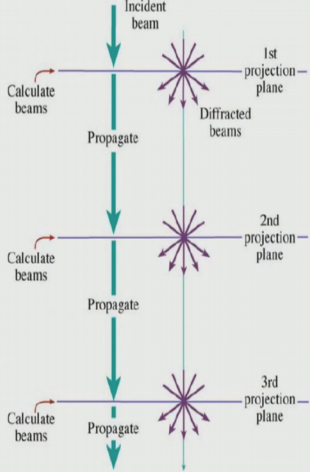
Models based on electron scattering, diffraction, optics

- The reciprocal-space formalism.
- The FFT formalism.
- The real-space approach.
- The Bloch-wave approach.



I will just mention a briefly about real space formalism, but others you can see in that text.

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Reciprocal lattice approach

- ψ describes the *electron wave*.
- P is the propagation of the electron wave in free space: the *microscope*.
- Q is the phase grating: the *specimen*.

$$\psi_{n+1}(\mathbf{k}) = [\psi_n(\mathbf{k})P_{n+1}(\mathbf{k})] \otimes Q_{n+1}(\mathbf{k})$$

Real space approach

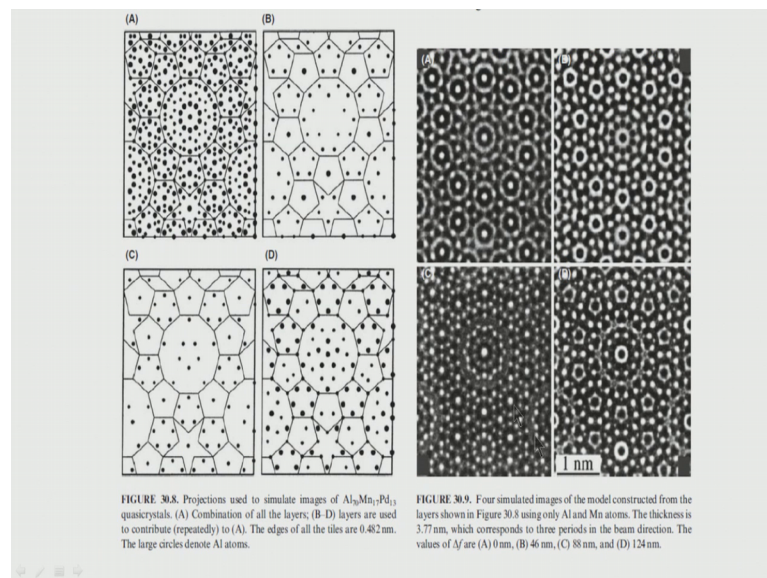
$$\psi_{n+1}(\mathbf{r}) = [\psi_n(\mathbf{r}) \otimes P_{n+1}(\mathbf{r})]q_{n+1}(\mathbf{r})$$

So, as I mentioned earlier that incident beam as it context, it passes through the sample there are many diffracted beams this propagates and the as it reaches here we get the new the wave function is going to be different, the again it propagates this is what we have cal done earlier. So, essentially what happens if that in this case that psi describes the electron wave, P represents the propagation of the electron wave in free space that is in

the microscope or in the sample also from each layer or some particular thickness, d is a of that sample is taken into a small slice and then from each of these slice δ is a defect correspond to unit cell we can represent in item one layer, and then we calculate what is going to be the exist wave at the back of this and then propagated from here to here to reach the front of it that is how this calculations are done ok.

And Q is the specimen itself is in this case is considered something like a phase greeting that is the Q represents the phase getting. So, you have very layer when we have to calculate this essentially a convolution of the various terms which we are taking it and here it is essentially in the reciprocal space we are doing it, but the same function. In a real space approach also we can do it both methods are possible in this particular one ok.

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What is beings for a quasi crystal various positions of atoms and various planes is being shown three planes, which are shown and the calculations are done to find out how the end of each one of now them the fourth simulated images for this models are being shown we can make out that this shows the fivefold symmetry.

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Image simulation

Exit wave function

- at the specimen exit surface,
- at the back-focal plane of the objective lens (i.e., the diffraction pattern),
- at the image plane.

Main steps

- evaluating the scattering from a single slice of specimen with thickness Δz ,
- repeating the steps of the multislice calculation to achieve a specimen thickness t ,
- modifying the phase and amplitude of the exit surface wavefunction by the characteristics of the microscope.

Do the iteration changing small changes to atom position in structure till the computed image matches with the experimental one. This is normally carried out to match few through focus images taken around Scherzer defocus

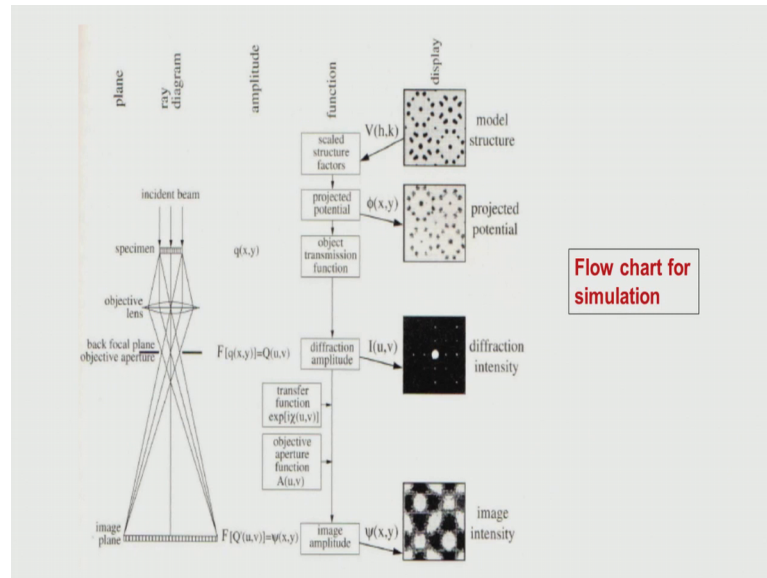
So, in short if you summarize what do you do in image simulation, the first thing which we have to find out is that exit wave function at the back of that sample. Because the beam is a perfect plane wave which is coming into this one and the plane wave passes through that sample and then what is going to be the wave function at the exit one.

At the back focal plane of the objective lens the diffraction pattern we have to consider and at that image plane this exit wave how it is going to be modified that is because of the destruction and the diffraction both of them we will give rise to. So, what all the various steps which are required one is evaluating the scattering from a single slice the multi slice calculation, and each slice after that exit wave has been calculated all of it to propagate and reach the next slice, and then find out what is going to be the exit you at the back of it and then all of it to propagate then calculate till we reach the back of that sampled, then the this process modifies both the phase and the amplitude at the exit wave function, ok.

Then this iteration how we go about it this will give rise to some image and this a simulated image which we can compare with the experimental observation, because here when we take that all the various factors which we are taking as a function envelop function those function should correspond to the microscope parameters. If matching is not perfect maybe in the model of the atom which we have chosen some modifications some changes in the atomic structure of the sample has to be incorporated, by doing that

and again repeating this process we do till we get a perfect matching of that image and then we say that this is what is the structure of the sample for this particular set of particular conditions under which the image has been taken, ok.

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This is exactly what is being shown for a microscopy in this schematic flow chart of that simulation which is normally used, this is the model structure which we use it this is a projected potential for that model structure, ok.

Then the object transmission function and the diffraction be get it, then we put the transfer function of the lens objective aperture function and all these things when we do this is what that image which we get it. In this way of image simulation that way we went about is we assuming a model structure and then incorporate all the aberrations and try to get a matching of the simulated image with the actual image which we have observe, and then they try to find out which is the structure which is the best matching and we say that this is what the structure of the specimen should be for this image, ok.

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Limitations of HRTEM

- True lattice image only at Scherzer defocus
- Atomic resolution is nothing but intersecting lattice fringes
- Delocalisation of atom positions
- Position contrast can not be related to atoms
- Absence of atom position in columns can not be identified
- Light atoms can not be identified in the presence of heavy atoms
- Limited or zero tilt
- Simulation of images have to be done
- Planar defects and nucleation stages seen clearly
- Local crystal structure, orientation, symmetry, lattice parameter

NPTEL

Truly not an atomic resolution

There are some limitations associated within the true lattice image you observe only at Scherzer defocus for other conditions also closer to it, there are some images which we get it. If you wanted to do a good to find out the structure correctly, taking this effect of the microscope you know and how it is going to affect the image far away from the defocus, for all those conditions we do an image matching and so that the model structure which we develop is able to explain the intensity contrast which we obtain for different defocus values.

Then about delocalization of atom positions all these aspects which I had mentioned already. But what essential one should understand is that just the picture if you look at it is not an atomic resolution picture. So, we have to do that image simulation is some must to get the correct information. There is another thing which is also being done which is we call it as an image processing.

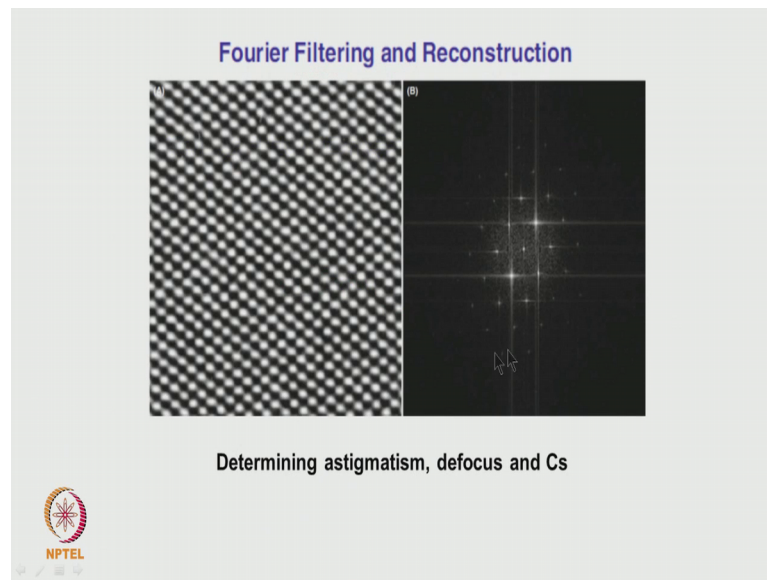
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Image processing what is being done is that we do not record that high resolution images, we instead what we do is collect the data now either using a c c d, then that data can be quantified and that to you know that the range is very dynamic in c c d very large dynamic range is there. So, a linear quantification is possible linear data collection, then what we can do it is that using many other image processing softwares, we can remove the effects of various aspects of it.

Like if the noise is there we can remove how if we remove the noise how it is going to take place. Suppose a drift is there we know this is the drift. So, if you do a correction for that drift how the image we will appear that we also we can try to do we eliminate the various effects and try to find out how the image we will appear in the absence of all of this, and then to a comparison with that image simulated that is what essential.

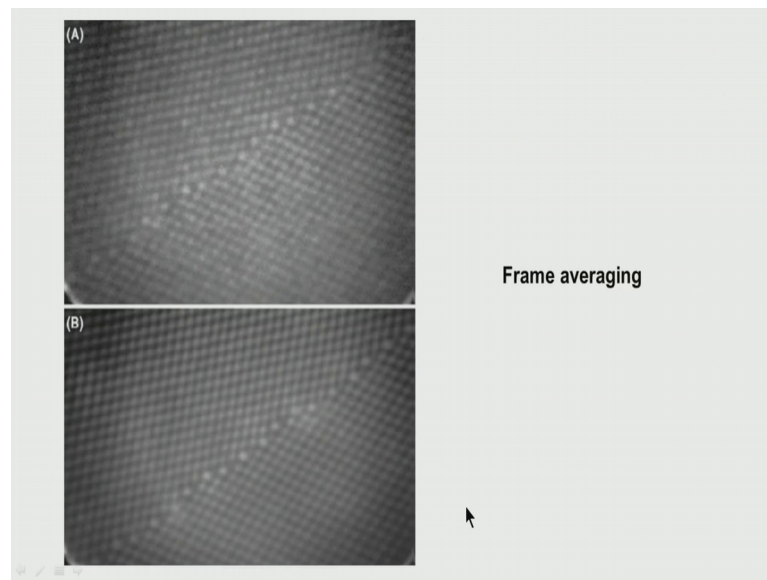
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This has some advantage also like for example, this is a what happened this is an image which has been collected for a small region we can choose, and do an f f t. So, this gives rise to a pattern which is like a diffraction pattern. Here if you look at it this taking essentially is due to the artifact of this f f t, we can choose and remove many of these artifacts and then try to join all from this particular region we can choose that spot, and then try to reconstruct back that image and try to compare how it looks like there that is a processed image ok.

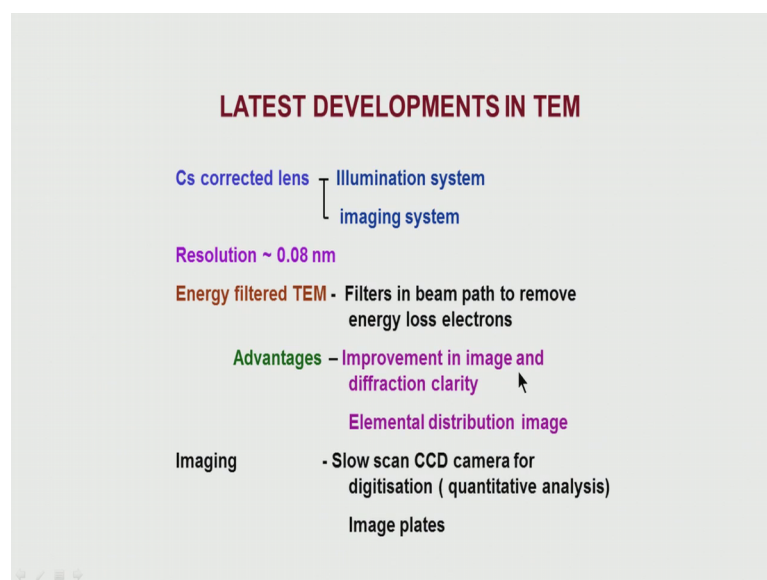
In this process we can get information about what is astigmatism defocus Cs all these effects also what is that affect on that actually image which you obtain we can get that information and that can also be eliminated from the image which you have obtained.

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There is another in fact, which happens that suppose we take just grab on image there is then this is how it looks like. If we use a video camera we can grab that image many times from that same area and we can do a frame averaging. Now you can see that this has led to an enhancement in the contrast of that image. So, these are all the various things which are possible using image processing, ok.

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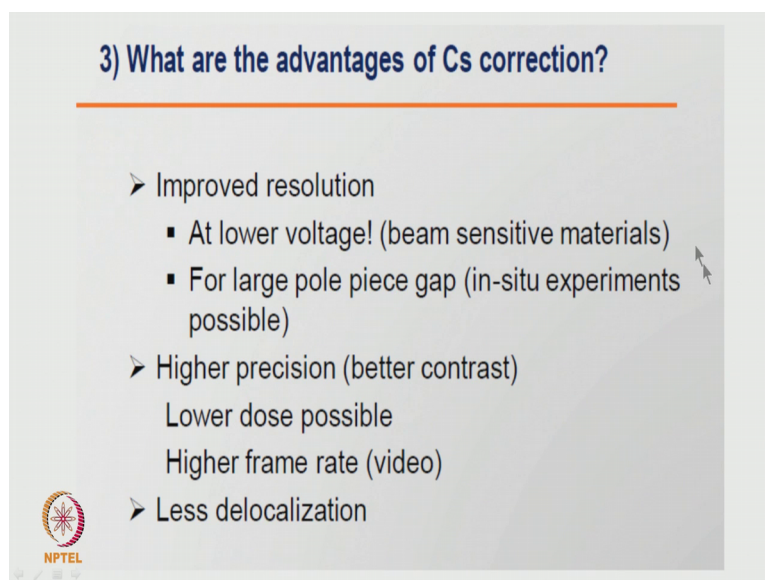
Having talked about all this the other aspects of it which we thought that we mentioned that the Cs is one, that is spherical aberration of a lens which cannot be coming because

we have to live with it because all the lenses which we use in an electron microscope are convex lenses.

So, for us spherical convex lenses the spherical aberration is already limited. If you have to reduce the spherical aberration you have to reduce the pole out pole be gap between the pole piece; that means, that reducing the gap between the pole piece means that the tilt everything you have to compromising on that what is the other way. So, since the development of the microscope if we will have been trying to look at it, how can we correct for the Cs. We know that in optical lens system using a combination of convex and convex lenses, we can correct for spherical aberration that is using lenses with different refractive indexed or convex combination of convex or plane of convex, plane or convex, concave all this lenses could be joined together to get lenses their all aberrations have been corrected and can this be done in the microscope.


Since beginning of this century such systems have been developed with which now the resolution of the order of 0.0 here its written nanometer up to 5 nanometer is in principle as possible and has been achieved in that microscope like energy filtered microscope this I had already talked about the earlier.

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3) What are the advantages of Cs correction?

- Improved resolution
 - At lower voltage! (beam sensitive materials)
 - For large pole piece gap (in-situ experiments possible)
- Higher precision (better contrast)
 - Lower dose possible
 - Higher frame rate (video)
- Less delocalization

 NPTEL

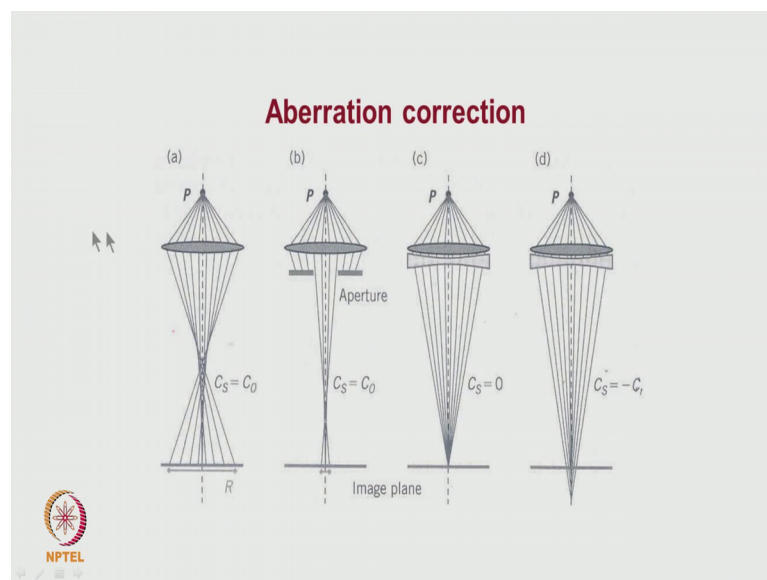
So, what is the advantage of Cs correction? That is Cs essentially is spherical aberration is corrected or not only the spherical aberration can be corrected now the spherical

aberration can be made negative also, that has also got some advantages. What is the advantage of doing the sort of correction?

Since it is done external to the lens that is we have a if this is a lens system, there is another series of lens systems which are being put which do all these corrections get computer control system; that means, that as far as the original lens is concerned the pole piece gap is quite high. So, that we can have a time sample and we tilted it, and then with high that when C_s is corrected we know that the factor $w \Delta k$, which we wrote it this is the delocalization factor.

If C_s become small this depends upon the two terms C_s and Δf ; if C_s become small are we make it 0 then this delocalization could be reduced that also to made zero similarly as C_s is being made small the Δf also defocusing is also necessary not necessary, because the defocusing is the one which we use it to compensate for the spherical aberration so that sum range of Δk values we have for this $\sin \omega$ for the various g vectors, they always constructively interfere to give rise to enhancement in contrast the image ok.

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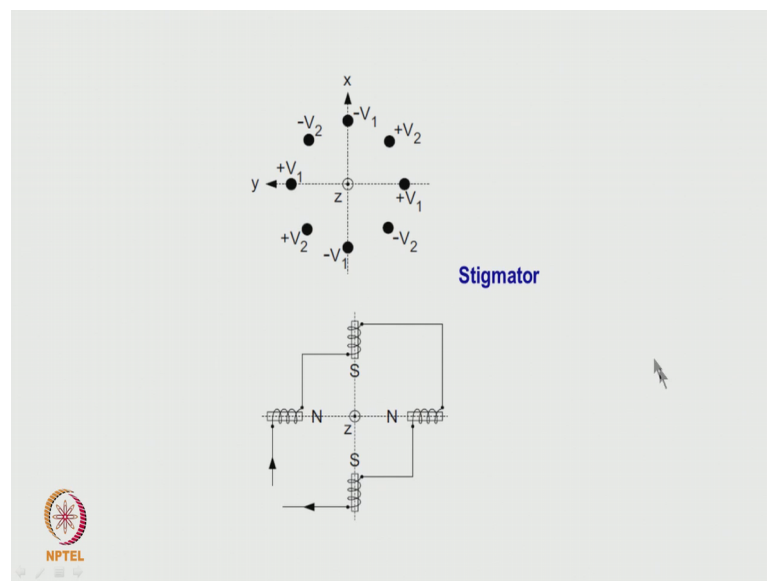


A schematic diagram which I am showing it here is using a convex lens, which has a spherical aberration some value. So, because of this at the Gaussian plane we get some image and then there is a disc of least confusion whether the size of the image reduces. How to reduce the effect of this spherical aberration? We put an aperture so that the of x

is beam is reduced, then the spherical aberration could be reduced considerably. The other way we can do it is said if we can include a convex lens, which essentially what it does it is depending upon the lens choosing a lens of a particular value particular size and focal length ok.

We can make this beams which are far away from it also bend a little away from it. So, that all are focus so that for a point object we get a point image. Or this value can be that such that the (Refer Time: 41:01) aberration becomes it is more like a concave lens it behaves. So, that we also we can reduce, we can make the spherical aberration the negative. So, this what we can see here is that essentially the rays which are coming far away from the optic axis only they have to be bent a little bit ok how can this be achieved in a microscope.

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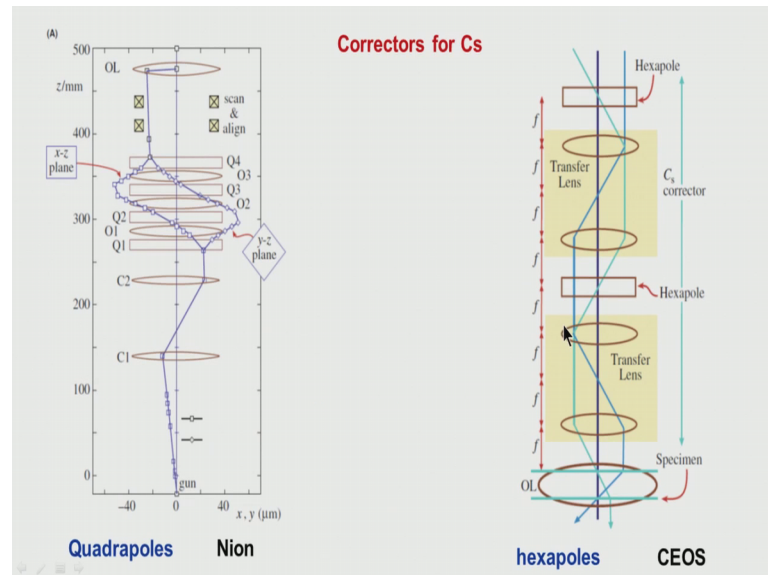


This we have discussed earlier when we talked about lens aberration, that if we use a stigmator, stigmator is nothing but the either quadrapole lens system which is being used.

Then what is happens is that there field will be from here to here, from here to here, here to here like this that field is going to vary. The effect of this field is going to be only the rays which are away from the optic axis they are going to be deflected, but whereas, the rays which are going to be on that optic axis they are now getting affected; that means, that by controlling the voltages which are being applied to these various ones the effect

of we can introduce different amount of deflection to different beams, which are half that axis this same stigmator is used to correct for astigmatism in their microscope.

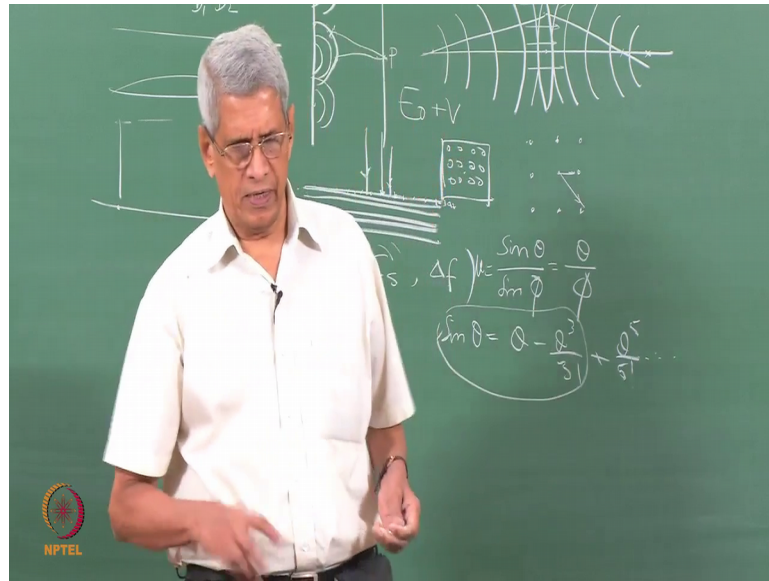
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Now that same type of stigmator which are used this could be either quadrapole lenses are this could be a hexapole, there are two types of lens system which has been made for neuron company what they have made it is essentially using some a normal lenses and quadrapole they could make the spherical aberration almost 0, they are same thing which could be done this was that see was Germany this was developed, ok.

Here also what they have it is a some 3 Hexapole 2 Hexapole lenses and somewhere they call it as a transfer lens which is being used with these what is essentially is being done nice that the spherical aberration is corrected, also that in addition to spherical aberration off axis rate they give rise to a the body is that aberration which is called as the comma. Both comma and the spherical aberration which is being corrected this correction is as we said why this spherical aberration itself comes because in the formula for the refractive index.

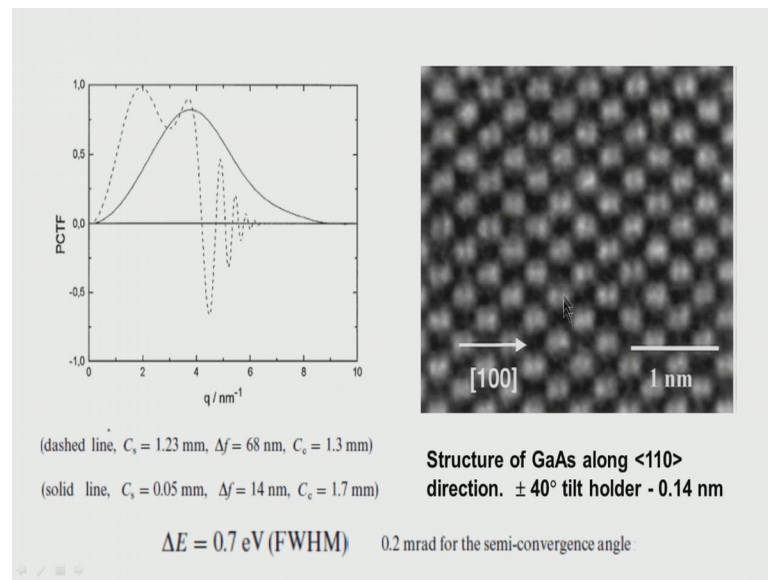
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We use that sign there refractive index μ equals $\sin \theta$ by $\sin \phi$ if we take it, these values for paraxial rays where we assume that the θ is and ϕ or so small that this can be written as θ by ϕ . But actually $\sin \theta$ is written as θ minus θ^3 by 3 factorial plus θ^5 by 5 factorial, this is how the series expansion we will go.

So, when we correct for the spherical aberration essentially this the third order correction is corrected very easily with these lenses, but this lens system it some build the introduced some corrections all these things are corrected and finally, we get one with very small spherical aberration values here.

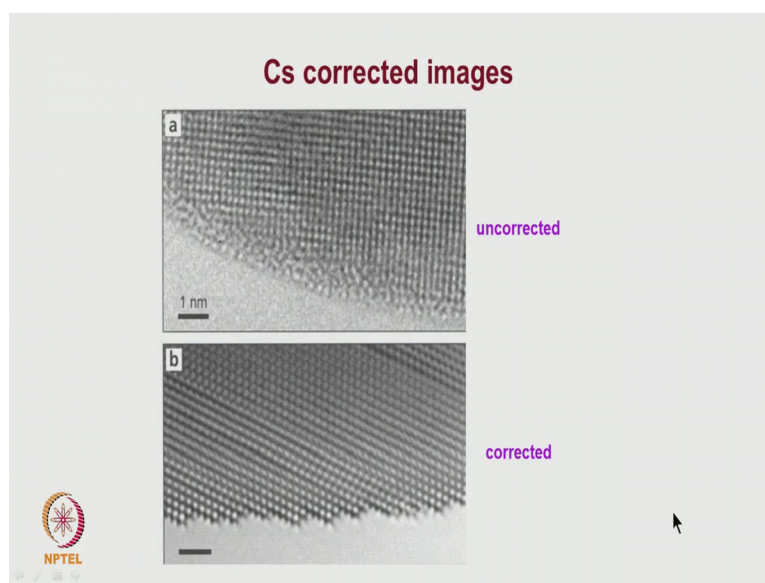
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What is being shown is that transfer function for a microscope which is an uncorrected one, and that is where the spherical aberration coefficient C_s is 1.23 mm and this solid length correspond to 1.4 which this spherical aberration has been corrected that is a corrected lens, and for which the C_s turns out to be 0.05 mm we can make out that how drastically testing, then that is defocus also changes that C_c value essential remaining the same and the energy of the radiation which is used.

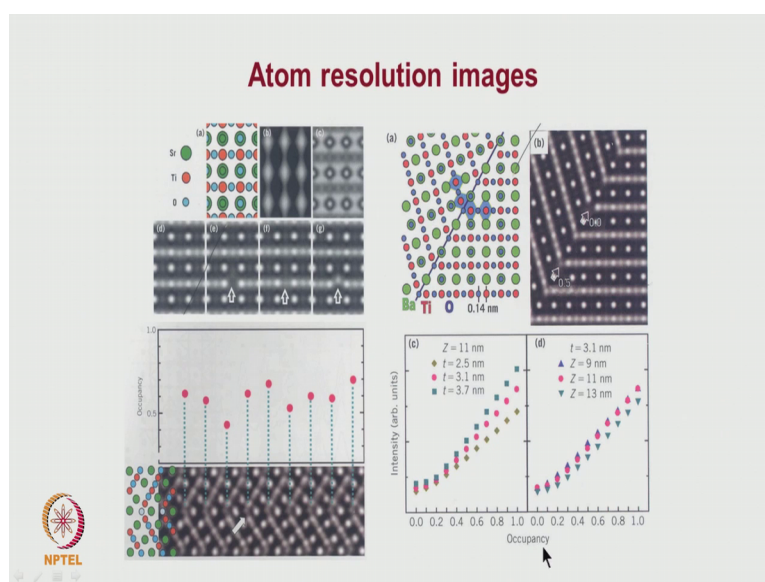
So, these one of the first microscope which I earlier microscope is there constructed with which further a gallium arsenide structure along 110 planes the separation between them, they could see it this aberration is essentially 0.14 nanometer . Now represent a microscope which have come with which the separations of the order of 0.05 nanometer between this dumbbells could be seen and this was done in a microscope if a microscope which has say plus minus 40 degree tilt sample hold that.

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What is the effect of making the deam delocalization? Because edge of it the fresnel fringes appear the effect of these Fresnel fringes essentially going to be that blurring of the image which takes place here ok.

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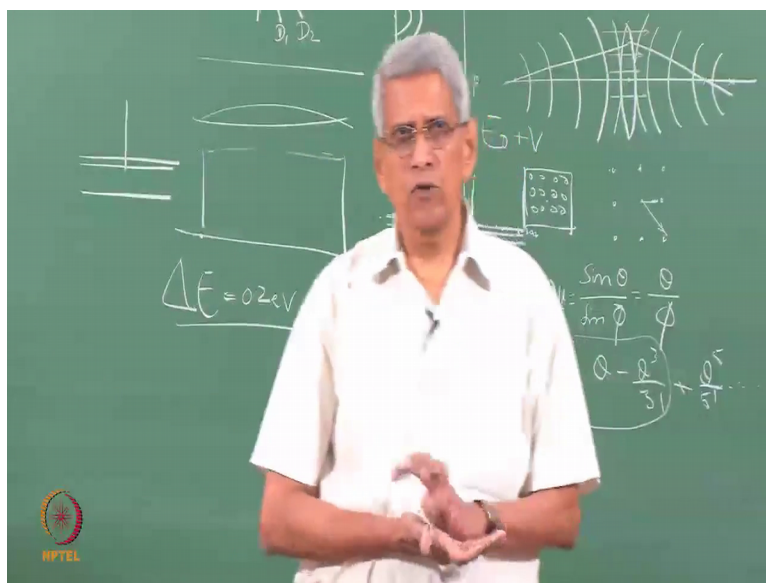


When Cs is character tried up to the end this is for gold, we can see that the atom positions could be seen very clearly. And the another is in many of this images, as I mentioned earlier this is one way in which high resolution could be obtained, the other mode in which we can do it is in a scanning transmission mode. In a scanning

transmission mode what we do is that we make that beam scan on the surface of the sample.

If we can make the size of the beam as small as possible, but to make the size of the beam as small as possible all the aberrations of the condenser lenses, have to be corrected. Using this sort of characters we can make the beam size has small as now about 0.1 nanometer this one then if the sample is sufficiently thin ok.

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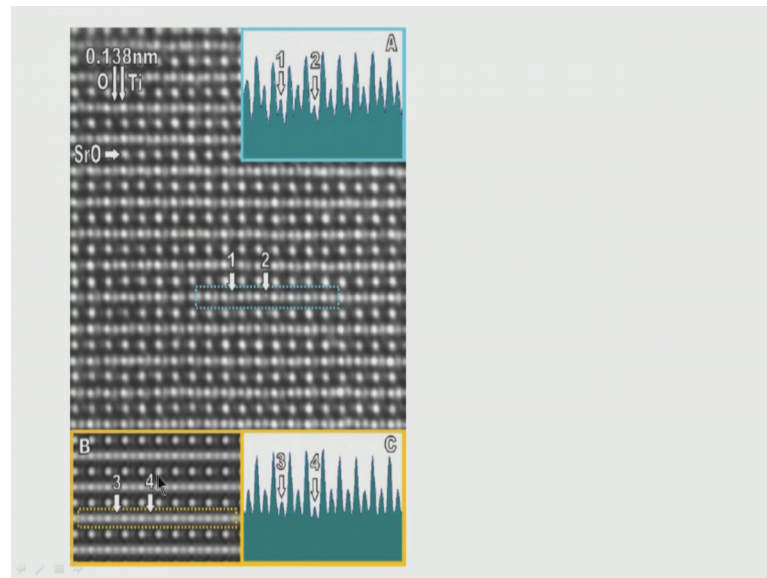


Beam of one nanometer size if it falls on to it if the same is a very thin sample if you use it; the spread is going to be small. So, essentially as the beam passes through that sample at various points, we will be able to find out depending upon whether it fall on falls on that column of atoms are whether with it is in between the intensity of the electrons which come out will be different. So, it gives a true 2D projection of the column structures, here what is being done is that this is for a strontium titanate, this sort of structures the intensity has been calculated. Suppose what it happens is that along some of this column one of this column some atom positions atoms are missing. So, if atoms are missing then the it the contribution to scattering from those regions could be different because of that we find that some region you see that there is a almost 0 they shows that there are some atoms are missing on this column.

This sort of information also we can obtain not only that suppose an atom is displaced from particular lattice side, what is the displacement this sort of displacement also could

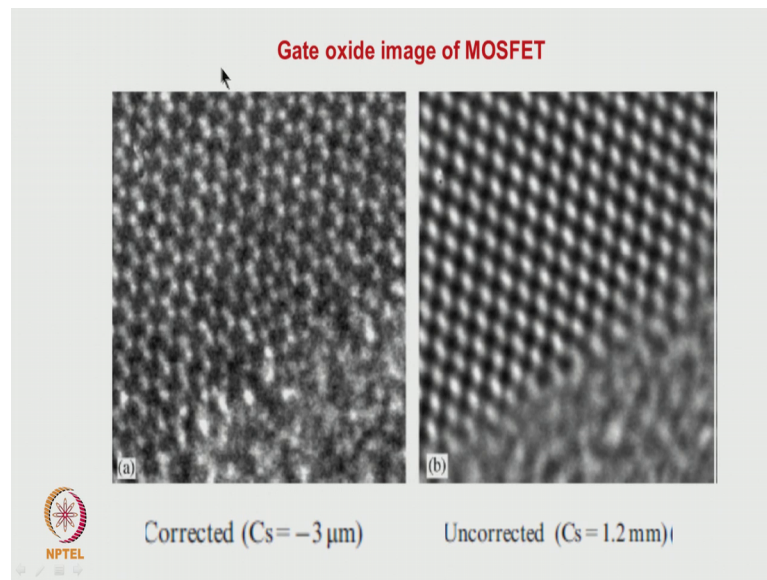
be measured, this is because the resolution with which the spatial resolution with which we can measure is of the order of a few picometers then become it restless there is what essentially it is because of this in a strontium titanate, we know that because of a slight shift a tetragonal distortion comes titanium atom and that is what it gives rise to the piezoelectricity, ok.

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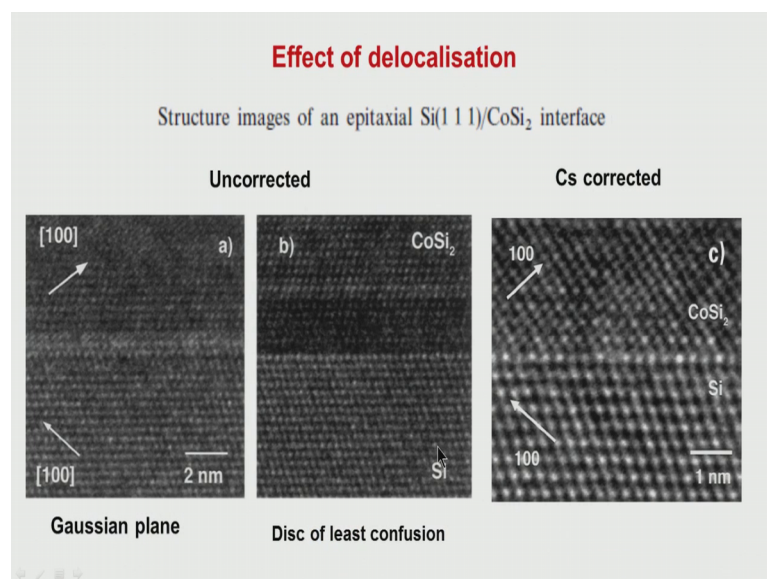
These are some few examples which we have and not only that we can find out also that how it is going to be the quantify what is going to be there intensity along each of these columns, all this information which we can get it ok.

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This is another classic example in which they gate a oxide image of Mosfet this is with an uncorrected microscope, here we can see that one side is an amorphous this side is a silicon that is crystalline one. If we see here we can we are not able to see the sharp image of this number when we use a corrected microscope with the C_s which is see that minus 3 micrum it, a then we can see the atomic resolution right up to the end of that amorphous region even in the amorphous region we can see that there is a clarity.

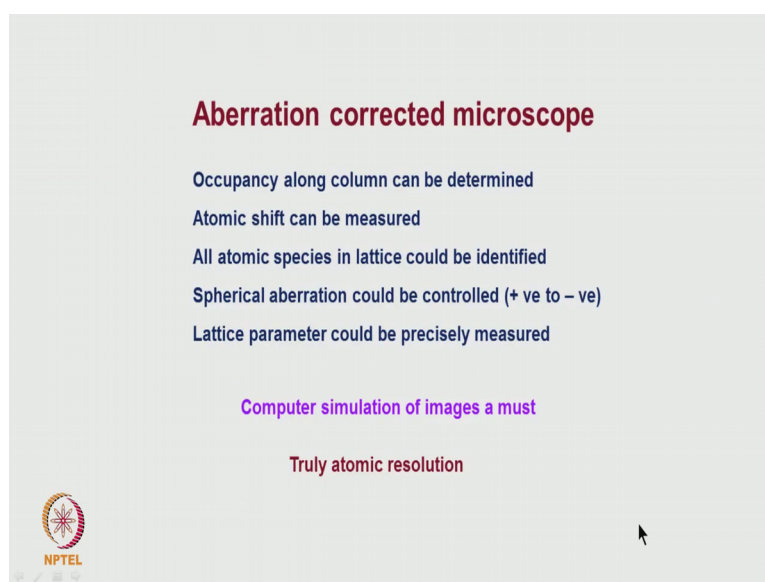
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This is another example in which the effect of delocalization; how the delocalization disturbs that atomic resolution contrast are the lattice resolution contrast. This is one where that images as a Gaussian plane and on unconnected one this on a multilayer sample are that silicon with CoSi₂ interface ok.

Here at the using the disk of least confusion if you try to find out sorry then you see that that image cannot be seen very clearly in this region when we uses E_s corrected microscope it becomes very clear that we can see all the atom positions can be seen very clearly this is a real advantage of a high resolution microscopy are Cs corrected microscopy you can do.

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So, what all the advantages occupancy along the column can be determined. Suppose depending upon how much of atoms are going to be along each of the column that information can be and if atoms are shifted from their normal position, what is the shift that of the order of less than 10 picometer that would be measured, then using negative spherical aberration coefficient the transfer function for the different atomic numbers ok.

They changed because normally what happens is that when we take a microscope in a conventional microscope a high resolution image, the contribution to scattering comes mostly from the high said elements the lowest said elementary effect is not seen that clearly what the essentially happens is that if you use a negative spherical aberration then we can modify that contrast so that corresponding to all the elements because this

strontium titanate is an example, where you can see that the contribution from strontium the contribution from titanium, contribution from oxygen, all of them could be seen very clearly in this images.

And another is when we are able to find out the atom positions very precisely then the lattice parameter could also be determined very accurately, but for getting all this information image simulation is a must because even under this, but for doing this sort of a work what we do require essentially is a field emission gun. A microscope which is fitted with a field emission gun is required, because that gives source with a very high spatial coherence and even if there is a the beam is not perfectly parallel, still we get highly coherent beam a another one is that the spread of the energy spread of the beam is very small in the case of a field emission gun, compared to thermionic are 1 a b six filaments ok.

In such cases especially in a if you one because if you can reduce the energy spread still further in an FEG, the advantage will be that they chromatic aberration could be reduced that is even if we correct all the spherical aberration and make it 0, now the whatever is the spread or delocalization which is occurring in the image is coming due to chromatic aberration. So, if you have to make it small we have to use some filters, when such filters have been added the spread in energy can be brought down to ΔE to about something like 0.2 electron volt.

So finally, what would like to say that with a corrected microscopes we get truly atomic resolution, but to do all this calculations we have to assume some model of sampled for an ideal condition it is a perfect cell or if some defects are present when the defects are there how the defects are going to modify. What does the defects do the defects change the atoms from there lattice position to some displacement occurs this displacement can we calculate a modeled using some elastic constants of the material and how it will take place around dislocations all these works is good. So, to interpret the results we should have good idea about what is happening within those samples, and also about the material behavior the material properties those understanding are also very much necessary to get good correlation between high resolutions that images and the structure of the models.

So, using the present day microscopes what we can do is that we are not modelling an ideal structure we can get a structure material which contains defects that is a defective structure how it looks like. And what sort of contrast that we will give rise to or when we get a microstructure that is the atomic resolution from a sample from that we can find out how atoms are displaced, from the lattice sites that is essentially we get information about those defective structures that is possible in the present day microscopes.

I will stop here now.

Thank you.