

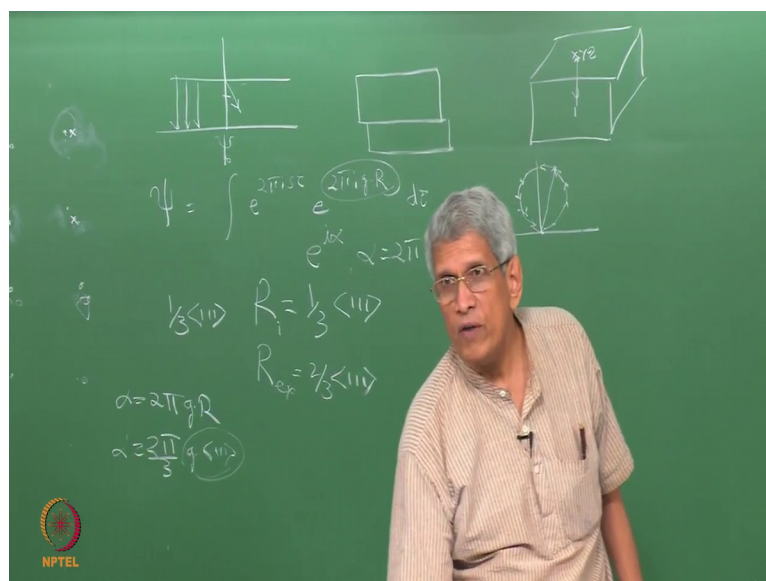
Electron Diffraction and Imaging
Prof. Sundararaman M
Department of Metallurgical and Materials Engineering
Indian Institute of Technology, Madras

Lecture – 20
Contrast from Planar Defects

Welcome you all to this course on electron diffraction and imaging. In the last class we looked at the kinematical and dynamical theory for contrast.

That is, essentially looked at how the intensity of the or the beam at every point on the back of the sample will be changing. That is what we are mapping as the image. You have doubt? That is as the electron beam passes through the sample. Diffraction phenomenon is occurring because of which at every point you concentrate only on the concentrated beam.

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So, suppose diffraction is taking place at this point, intensity of the transmitted beam amplitude, if you look at it will depend upon how the scattering is taking place as the beam passes through, that will decide. And the square of that is going to give the intensity, correct? So, essentially from region to region if you look at the back of that sample, there is going to be a variation in amplitude of the wave which is going to be there. That is what this manifest will try to magnify it and that comes as the image in the image plane. Correct? That is how we get the image, is it clear? Then we looked at how

the dynamical theory especially the concept of extinction distance makes a lot of difference in the variation in contrast when the thickness of the sample varies. All those aspects we considered, but that is all for a perfect crystal.

Today what we will do it is that, we look at various types of defects. Because in many classes I have told what all the types of the defects which we can have in single crystals, what all the type of defects which we can have in polycrystalline material. How contrast arises in defect? That is what we will look at it in the next one or 2 class. When wanted to look at contrast from defects the defects itself we can classify into 2 categories. One is like the defects which produce a strain field around the that is one type of a defect. Give me an example.

Student: Dislocations.

Dislocations, and second phase particle precipitation. Suppose bending of the crystal is there in some regions, that is also going to introduce variation in strain in the material. So, these are all the type of defects which introduced strain field around the, correct?

Then the other type of defect is that defect which brings about the change in the lattices, shift in the lattices. What all the types of defects which we can? I say that defects without strain fields that is what I had put it up, this could be some planar defects. What are the types of defects which we can have?

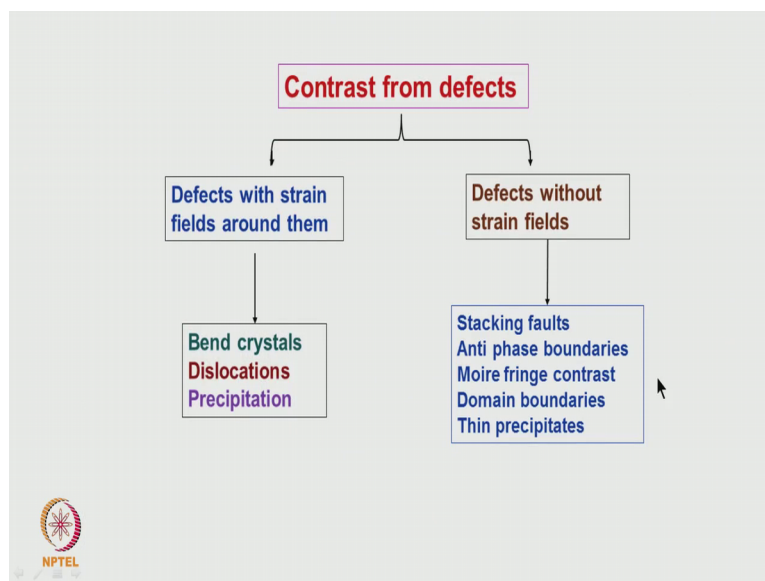
Student: Stacking faults.

Stacking faults, yes right. Then anti phase boundaries, all interfaces. Then domain boundaries even thin precipitates they can bring about some shift, yes.

Student: Bend crystal is also.

Bend crystalline is that suppose we prepare a sample, TEM sample normally there are many methods which are being used. The most frequently used technique or conveniently used technique is that jetting, jetting.

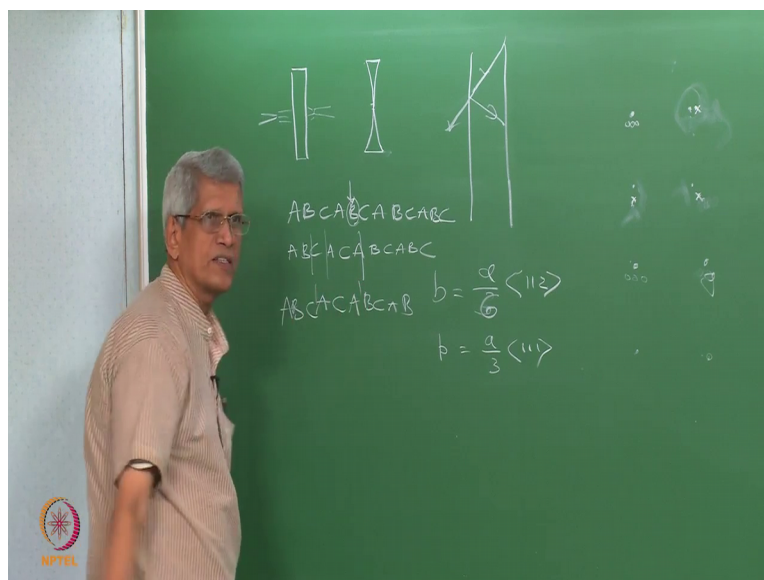
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Student: Jet polishing.

Jet polishing, there what you are trying to do what it is that, you have a samples in which from 2 nozzles ok.

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Jet is coming and falling onto the sample right. The sample gets thinned finally, this is how the sample becomes, which maybe a hold which is coming at this point. Closer to the hold you have thin regions are there right. When this jet falls itself when the sample becomes extremely thin, even a small flow of the jet can bring about some bending in the

introduced deformation in the material. That will introduce the unit cells which should be perfectly flat you find that that is a slight bending of the unit cell is taking place. That is with respect to any particular origin if you choose, the unit cell orientation has shifted. That is also can be considered as a sort of strain. So, it is clear?

So, these are all the types of defects which we can have. We will look at how contrast arises from various defects in the microscope. To understand this contrast the first thing which you should know is about, what is the type of defect which we have. And on the basis of if we know about the type of defect then we can find out what all conditions under which the defects will become visible, what is the condition under which the defect will not will not be visible. On that basis we can formulate some rules for observing this defects right. That is what is being followed to identify defects in the sample, is it clear?

So, if you remember the last we talked about both the kinematical condition. How the intensity of each of the diffracted spot will be affected, right?

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Contrast from defects

When a defect is present in the sample and it produces a small displacement R_d from the normal lattice position, then $\Delta k \cdot R_{imp}$ becomes $(g+s) \cdot (R_l + R_u + R_d)$

$$\Delta k \cdot R_{imp} = g \cdot R_d + s \cdot R_l$$

$$\psi_g = F_g \int \exp 2\pi i (s \cdot R_l + g \cdot R_d) dz$$

Integration over $t/2$ to $-t/2$

$$\Delta k \cdot R_{imp} = g \cdot R_d + sz$$

when variation in z direction is only considered

Perfect crystal with deviation s	Crystal with defect
$\frac{d\phi_g}{dz} = \frac{\pi i}{\xi_g} \phi_0 e^{-2\pi i s z} + \frac{\pi i}{\xi_0} \phi_g$	$\frac{d\phi_g}{dz} = \frac{\pi i}{\xi_0} \phi_g + \frac{\pi i}{\xi_g} \phi_0 \exp [-2\pi i (s z + g \cdot R)]$
$\frac{d\phi_0}{dz} = \frac{\pi i}{\xi_0} \phi_0 + \frac{\pi i}{\xi_g} \phi_g e^{2\pi i s z}$	$\frac{d\phi_0}{dz} = \frac{\pi i}{\xi_0} \phi_0 + \frac{\pi i}{\xi_g} \phi_g \exp [+2\pi i (s z + g \cdot R)]$

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So, that is essentially governed by $\Delta k \cdot R_{imp}$. Which represents the position of each atomic point in the unit cell. This value equals whether an integer or not, correct? When we substitute this value Δk equals g plus s and the defect itself can be written as position of each of the unit cell represented by a point which is called as R_1 . Plus the position of atoms within the unit cell which is given by R_u plus deviation defect is R_d .

If we substitute this and these things and solve this then you will find that this is the sort of an expression which we are getting it, correct? On that basis and finally, this has to be summed over the whole volume which we are eliminating or with respect z that is, at each point if you try to calculate how the intensity is going to be there that is a full volume is being covered, right. And then variation in intensity will come. And summation can also be changed into an integration you know that. That is essentially what is being done.

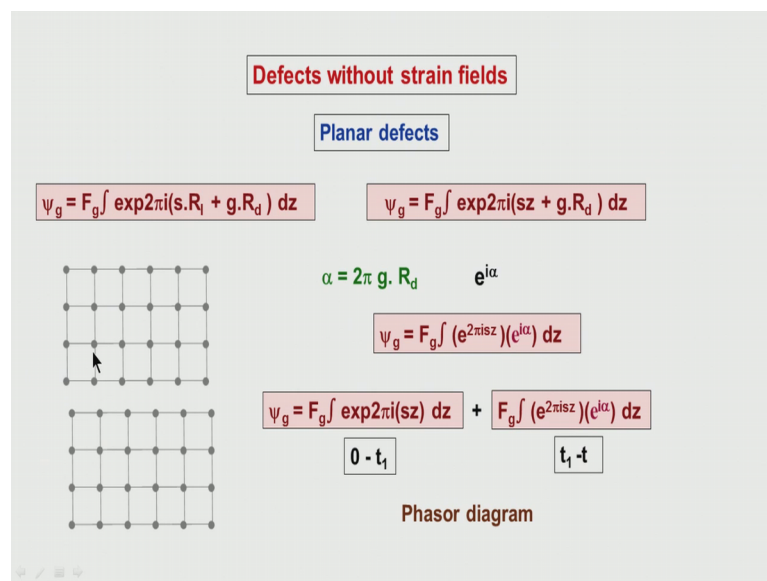
And then we define that deviation which the defects introduces in the lattice is essentially what we called as the deviation parameter s which is only along the z direction which exists, correct? So, then this expression will turn out to be $s z$ plus $\mathbf{g} \cdot \mathbf{R}_d$ where \mathbf{g} is the diffraction vector which you are using for imaging the sample. And \mathbf{R}_d is the defect vector. And then we mentioned that this vector, this product becomes 0 then it will behave like a perfect crystal. And if the product is going to be different some value then that will introduce some phase shift in the overall amplitude. This we considered on the basis of our kinematical condition using the phasor diagram, right. No that is what we will be employing it here to look at some of the intensity.

Now, when there is a deviation, not deviation this is with respect to kinematical theory. Under dynamical theory what we considered is that the electron beam interacts strongly with a material and that is a fact. Especially at Bragg condition the both the diffracted beam as well as that transmitted beam contribute to each other. In such a condition, if we write a plane wave we can represent the electron, as it enters into the sample it interacts with the periodicity of the lattice that is a potential which is going to be there, plus the wave also can be represented as a contribution coming from the various diffracted beam, this is how we considered it.

And then we solve the Schrodinger equation. We get an equation of these type which couples how the diffraction amplitude, that is the beam amplitude varies as a function of depth. Which depends upon if now you can see that it depends upon both the amplitude of the transmitted beam as well as the diffracted beam at every depth at the sample, correct? This couple equation when it has been solved, we are able to get the amplitude of that transmitted beam and the diffracted beam at the foil. And on that basis only we could explain the fringe contrast which occurs in the case of a wedge sample that is, right.

Then also I mentioned that if it contains a defect then what is essentially going to happen is that, s_z which is going to be there this will be modified by this term also will come the defect term also. So, this is how the equation will change, correct? Then the solution to this equation has to be found. So, using this also that is either using phasor amplitude diagram which is for kinematical condition or using dynamical theory both of them could be used get information about how the intensity of the diffracted and the transmitted beam varies at different points. Both in the perfect crystal as well as in the a regions which contains the defect ok.

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Let us consider the case because we I mentioned that we will talk about first a planar defect we will take that as an example. And as we discussed as the type of the defects are anti phase boundaries. Then stacking faults interfaces between different regions all these things are there. How what sort of a contrast which they will exhibit that is what we look at it. This is how the amplitude which we are trying to explain. What is important is that now you look at this sample suppose, a defect is there at midway which has shifted atom by some distance. So, essentially what we are considering it is I am just showing the external form of the lattice ok.

This lattice is being now shifted by some distance p in the x direction you assume. Then when this has been shifted the waves which are coming here and when they are scattered and when they reach here there is going to be an additional amplitude which will be

created to this. That is essentially what we are trying to look at here. What is this? Which it is going, how we can find out this R_d , is what it is? Is the defect position right.

So, suppose this the perfect position of the atom which is going to be there. R_d equals t then we can write α equal to $2\pi \mathbf{g} \cdot \mathbf{r}$ it will turn out to be, right. This α itself we can, right. It in the this term can be explained $e^{i\alpha}$ to the power of $i\alpha$ we can write it if we do that now the $\psi(\mathbf{g})$ becomes 2 times one due to the deviation, is this clear? Because essentially 2 term integral $\int \psi(\mathbf{g}) e^{i\mathbf{g} \cdot \mathbf{R}} d\mathbf{R}$, right. This \mathbf{R} we assumed to be some translation which has been given to the lattice from the original position which is there on all the layers of the top. So, if you do that and So, this term itself can be written as what we are trying to do it is into $d\mathbf{z} e^{i\alpha}$. So, α will be equal to $2\pi \mathbf{g} \cdot \mathbf{R}_d$. Depending upon the value of \mathbf{R} which we choose the value of \mathbf{R} is decided by the nature of the defect that decides what is the vector. So, here we have chosen a some arbitrary distance where that lattice is just displaced in the x direction.

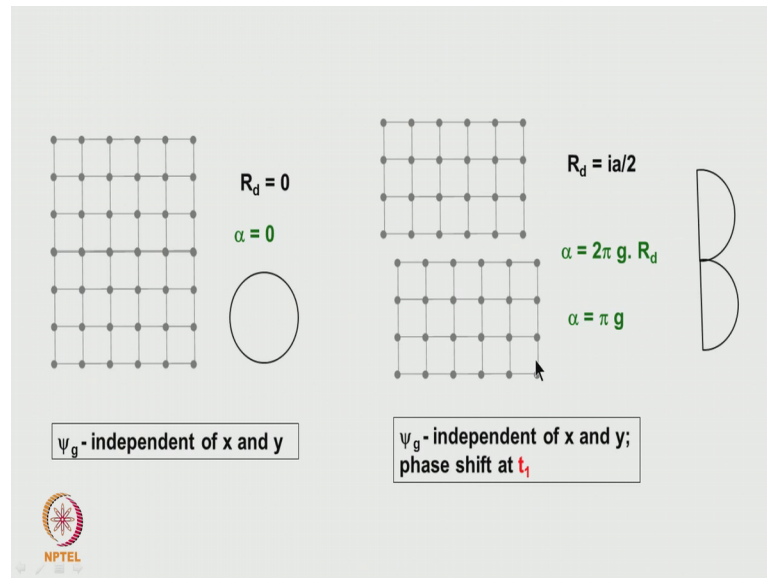
Then to find out the intensity what we have to do it is that, first there is going to be a we have to take the amplitude which is going to be there, from up to this particular point defect is there. Then beyond that if it introduces some variation in the amplitude because everywhere there is phase shift has been introduced. So, if we add both of them together we will be getting what is going to be the amplitude at the end at every point, you understand that?

See if we have to find out the amplitude. How we are finding out the amplitude? What is going to be the amplitude up to this point? We can calculate it using this expression. Here what is the value of there is no defect which is present. So, \mathbf{R} will become 0 right. So, this is what essentially is going to be up to 0 to you take this the thickness to be t_1 up to this we have done it. Now what we do it is that beyond this there is a phase shift which is introduced. So, what will be the amplitude when the beam introduce here it is going to be this value this from t_1 to t we have to do that the total sum is going to give what is going to be the amplitude at the end, correct?

So, this same thing can be represented in the case of a phasor diagram. The phasor diagram what we are trying to do essentially is that we know \mathbf{g} at we as we go along the beam in these direction the position of \mathbf{R} is changing. So, that the phase factor is going to change through the amplitude remains that same. Then what we are trying to do

essentially is that to find out the net amplitude like this it will be going like this. If there is not absorption it will be rotating here like this, this is the way the and if at some particular point at some particular depth we have reached from here to here. So, this vector gives what is going to be the net amplitude, correct? This is what the phasor diagram does it, that way we can also do it.

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Now, I am considering a case where the translation which we have introduced is 0. Then what will happen? Then essentially the phasor diagram will be like a circle which it will be propagating this value of α will turn out to be 0. Then the ψ_g if we look at it is a perfect crystal it is independent of the x and y position. Whether I calculate it at this particular point or this particular point with respect to different x y and the same because the x and y is define and this region, right. This will be x and y will be you take perpendicular to it this is the z of the sample which we consider it ok.

Now, let us take that case where this is the particular case where, with respect to this up top layer at this point the layer is shifted by a distance a by 2. If this is shifted by a by 2, what will happen to this value α will become? π into g ; that means, that if up to this particular point if the amplitude of the phase you assume that it has reached up to this particular point. Then this introduces a phase shift of π by g means that now for the next one from here when it comes instead of going it from here to here it will go from here to here in the opposite direction, now it will again retrace it like this. And now on this point

suppose at some particular point here I wanted to find out from here to some particular point I will have to look at what is going to be the net amplitude that is how we have to do this calculation as far as the phasor diagram is concerned, is this clear? How this phasor diagram can be used to find out the amplitude ok.

Suppose we assume that the vector which we are using this is simple cubic lattice which you have considered. The vector g equals 1, 0, 0 then what will happen to α value will become π , right. Is it not? If α becomes π this introduces a phase shift which is reverse of this. Now suppose the vector which I use g to image the defect equals to 0, 0 then what will happen to α ?

Student: 2π .

Becomes 2π , when α becomes 2π what will happen to this then again it will go as if it is a perfect lattice. So, even though there is a defect is there depending upon the g vector which you use it that is specifically depended upon the fault vector that decides for some g vector, you find that in this particular case the amplitude can become reversal of it. In the other case the amplitude becomes.

Student: Sir in the phasor, there is no direct like, there is no direction ray.

No the direction is there this is way the direction I had marked you have to mark it.

Student: Like not a lattice direction, right. There is no.

No it is essentially it is we are not looking at the lattice each the lattice, what it does it is it introduces some phase shift to the wave which is scattered in the direction.

Student: Sir g could be any,

which one?

Student: it could be a translation in any direction,

No g is a g is a reciprocal lattice vector.

Student: yes

diffraction in the.

Student: any diffraction.

Any diffraction by.

Student: sir if it is a 1, 1 0 the long.

You tell me if it is a going to 1, 1 0 then what will become g.

Student: we need to when you take mod of g .

Yeah see here that value which you have to take it is this $R d$ which you are taking it is in whichever unit is you take it see, π is in radiant. So, here when we write it this one is for a by 2 this specific case. Otherwise what you have to take it is that g into $g \cdot g \cdot R d$, d has to be a dimensional as quantity correct

Student: yes.

Thats what we will be doing it we here we are considering as a specific case where 1, 0, 0 because the essentially is going to be a know.

Student: yes

1, 0, 0 also i. So, i into i will becomes 1.

Student: yes

So, that is why otherwise we have to take the pro this one.

Student: dot product.

Dot product ok.

Student: yes

Thats a general case this, clear?

Then when you do this we find that it introduces some phase shift, correct? This is as far as a vector which is essentially at some particular depth from the sample surface which we have considered. It can So happen that this fault itself could be explained with respect to the sample. If the fault is inclined like this in this direction the t is also going to. So,

different points you will have. So, what will happen is that some places they will all add together some places they will subtract. So, you will have a variation in intensity will come. Essentially it will give rise to a fringe contrast that is, if some regions amplitude all add together some places they subtract and become 0 then you take the square of it. So, as a function distance when you do it, it is going to give rise to a fringe contrast that is how all planar defects give rise to a fringe contrast, is it clear?

Now, let us take another case. Suppose one crystal is sitting on top of another crystal, the lattice parameter is that same. That also case happens that is you have a matrix in which a precipitate is there the precipitate has also got the same precipitate structure as that of the matrix you can assume like α' and α . Or if we consider simple cubic lattice in which we have another lattice with a slight lattice parameter difference we can consider that.

Suppose it is such that at from here to here when we consider it there is perfect matching of the lattice because a slight misfit is there. In between the separation between the planes are going to change continuously. At some particular point here it becomes midway. So, now, if we calculate that amplitude, what is happening is the vector with respect to x y position? Is continuously changing. So, this will give rise to variation in the phase and finally, when we look at the amplitude and the intensity, the intensity will be the here it will add together at point because you do not see the defect and that this midpoint it is an phase difference of π it will become intensity will become 0. Here again it will become though the lattice separation is large, now we are able to get a spacing of the amplitudes the fringe spacing which is much larger than that.

Student: (())

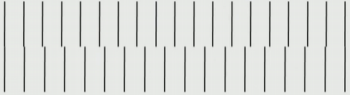
And from that from this now we can find out what is the separation between the 2 lattices we can calculate if we measure this fringe spacing.

Student: the lattice

yeah, what the difference between them that value.

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Crystals with two different lattice parameters



Translational Moiré fringes


$$g_{tm} = g_2 - g_1$$

α Changing with x and y

ψ_g – varying with of x and y

$$d_{tm} = \frac{1}{g_{tm}} = \frac{1}{g_2 - g_1} = \frac{\frac{1}{g_2} \cdot \frac{1}{g_1}}{\frac{1}{g_1} - \frac{1}{g_2}} = \frac{d_2 d_1}{d_1 - d_2} = \frac{d_1}{1 - \frac{d_2}{d_1}}$$

Rotational Moiré fringes



$$d_{rm} = \frac{1}{g_{rm}} = \frac{1}{2g \sin \beta/2} = \frac{d}{2 \sin \beta/2}$$

$$d_{gm} = \frac{d_1 d_2}{\left((d_1 - d_2)^2 + d_1 d_2 \beta^2 \right)^{1/2}}$$

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So, if we know the value of one of them then we can find out which one all this things could be done, is it clear? This sort of fringes which are coming are what we call it as a moiré fringe. This moiré fringe could be seen easily with our eye. I do not know whether you have noticed moiré fringes. The simplest thing which you can take it is, grids are there no? Not this grids even on the road side that [FL] for the window you put the grids no very fine mesh is there. If 2 meshes of different sizes are there. Mesh size you keep one on top of the other you look at it, then you will find that there will be a this I think if you go to any of this science museums here they will show this is for kids one of these things. And if you rotate both with one grid with respect to another if you rotate it you will get a different type of a fringe pattern you will be getting it. This is nothing but a moiré fringe pattern because with the light which we are using it. Because this essentially a combination of monochromatic wavelength which we use it, with that we will be getting as a sort of a contrast ok.

And here.

Student: (())

What will be the effect of this one suppose this is an one dimensional lattice which is going to be there. What will be the effect of this on the diffraction pattern?

Student: So, where the this if it is a maximum you will have.

No. So, when the misfit is there suppose this a central spot is there you get one spot corresponding to the top layer. The bottom layer has got a lattice spacing which is small inverse of it will be in this one. So, you will be getting one more reflection corresponding to that, correct?

Student: no, we didn't got sir.

See, what does the g vector depend on?

Student : g vector lattice.

Lattice spacing of the planes in that directions. Suppose we have a crystal like this, for this crystal there is a particular here the spacing is large. So, because of that the g vector will be small. So, I will just mark this is origin and this is the g , corresponding to a top lattice.

Student : this in a spots for the above part and.

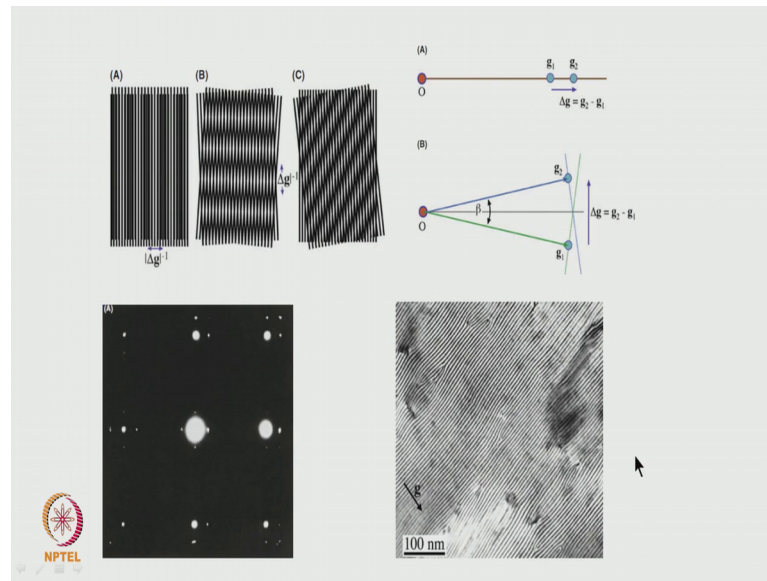
Below part will come, because the beam is because these are all parallel to each other that is one right.

Student: sir where are we seeing this fringe pattern.

Where are we seeing this fringe pattern is now when you have to take the image. What you do it is that, you put aperture around this point. Because this separations are very small. So, when you put an aperture these 2 beams they are monochromatic beams these beams are going to interfere. And when they interfere they will give raise to a beam pattern, interference pattern is nothing but a beam pattern know. So, here that is what I am just showing it is that this is difference.

Essentially these are all simple this. So, the separation between them is the real spacing will be $1/g$. This you can calculate this is how it will turn out to be d_1 and d_2 are the spacing these things you have to work it out. Similar thing which can happen with rotational moire fringe also that is where if the it is displaced it is slightly rotated then also will be getting a fringe spacing corresponding to that. What I will try to do it is I will show examples now you see that, when this is a fringe.

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Student: rotated when the point will go up or something?

Yeah it will go this is with respect to what we have shown it with respect to 1 I will come back to the where it is zone axis the beam is falling then when. So, many planes are diffracting what it will happen, is this clear? Ok.

Now, you see that it is slightly rotated how the fringe pattern is changing. For this you do not require anything else. What you do it is, you know what has been done here? It is only lines with 2 different spacing have been drawn. And if you look at it actually tell lines with 2 different spacing starting from here it has been done when we look with our eye it appears a fringe pattern we are seeing it nothing else. This you can draw a general line on a piece of paper and look at it you will observe this you just superimpose one on top of the other this pattern you will get it. And what is essentially important here is that suppose we tilt the sample then when the beam comes the effective the diffraction planes may change the separations will change depending upon this fringe spacing can shift here and there. So, that is an indication that this is not a lattice fringes because, when you do high resolution microscopy you see some fringes. Those fringes essentially correspond to separation between the atoms because there are not 2 lattices it is only one particular lattice at which we are looking at it whereas, if a moire fringe is there the moire fringe pattern a spacing can change .

And if you see here this is a diffraction pattern which is taken. For a beam which passing along a simple cubic lattice you assumed to passing along 0, 0, 1 then, yes.

Student: sir is exactly in that moire fringe the distances of the planes changing right in the.

Yeah.

Student : So, then basically how I will get only one point that point will be over?

Lecturer: no, no this what actually here you see it more point how it comes. Suppose I assume that here there is an another one ok.

This is g t and this one will be I will corresponding to a bottom crystal g b. Similarly you will be getting one here and another one will come, right. This will be g t and this will be some value of g will come this is how this should come, right. The 2 patterns super imposed one on top of the other.

Student: it will be a one single point because the spacing is like linearly changing, right? Like the adjacent is equal then spacing of the top.

It is from 2 different crystals.

Student: yes sir.

As far as for the moire fringe is concerned only there is going to be a.

Student: there will be 2 spacing right.

Because when we calculate that intensity down along it is going to be, but the same beam can give rise to as it passes through a parallel beam it will give a diffraction pattern from the top layer, a diffraction pattern from the bottom layer. Both are independently which is coming from the close by, but when calculate the.

Student: spacing at the bottom layer is one spacing right.

Lecturer: 2 different spacing no that is not changing, but when those lattices are kept close to each other at some distance you find that some lattice will match at some periodic interval that is all diffraction is taking place at each lattice separately. So, this

phenomenon will give rise to a diffraction spot like this which are separated. When we put an aperture around it an interference fringe contrast is essentially from the top layer the beam which comes and when it sees the bottom layer, the amplitude of the wave which is coming is going to change it. So, the net amplitude this is something like considering an interference essentially.

And this is the type of a pattern which we should get if I remove all these g_1 and g_2 and these things, essentially we should have that the inner pattern square corresponds to the top lattice and the outer pattern diffraction pattern correspond to a bottom lattice. But you know that, when this is a strong diffraction in x_1 axis the diffraction beam also contribute to scattering, correct? In the forward; that means, that the diffraction beam is now acting as a particular point as an incident beam right. So, then I can do what I can do it is with this as the point.

Student: (())

Another pattern which is corresponding to this one. So, points spots will come like this know now, if you draw a pattern like this which you should do like this as an exercise, you will get like this. You see that here, here, here, here, here patterns will appear no.

Student : So, basically you are saying the bottom has the diffracted beam as the incident.

Incident beam that is what it is going to happen because, the scattering is very strong here each is a very strong beam. The reason is that the reason is very simple if the scattered beam intensity is very small, when it acts as direct beam for diffraction the intensity of the diffracted beam will become much, much smaller, but that is not what is going to happen in normal diffraction because both the transmitted and the diffracted beam has got equal intensity, because of this we will be getting a pattern like. So, whenever you get a diffraction pattern like this sort of thing, there no need to be alarmed you know that it is happening because from the top to bottom there is some relationship and lattice parameters are changing.

Student: then for the bottom lattice what will you say is the incident beam direction?

Which one.

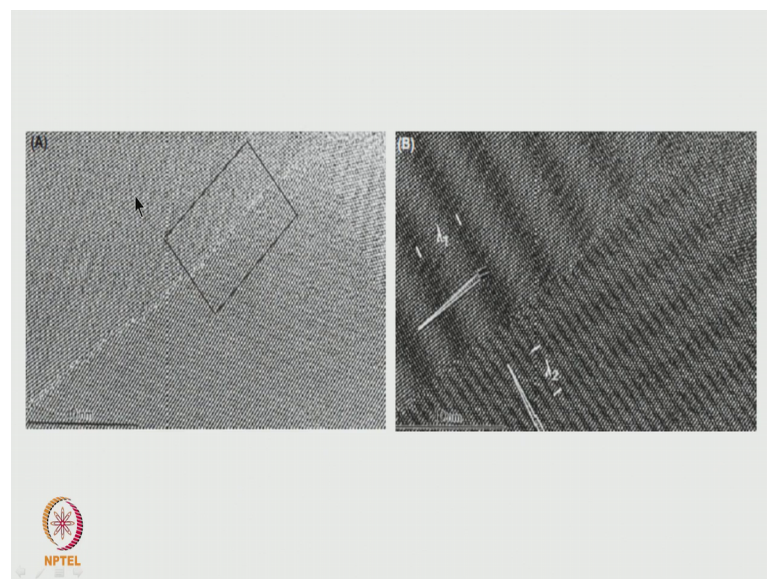
Student: like multiple you know.

No incident beam direction has not changed.

Student : So, the diffraction beam is the incident beam, right. The top layer if the diffraction beam is going to.

No that can happen even in the top layer also. See, multiple scattering when it takes place you assume that see this is a diffraction you assume that it is only a one type of a lattice. This is 0, 0 this is g . This can act as a that is and the beam is falling like this, it is in this So now, this can act as a point and again raise to a diffraction. When that happens we can assume that with respect to this as a center you can plot it, but these points will be matching this, but that will not happen in this case when there is a slight shift you understand that that is how you are able to get subsidiary spots which are going to be there. Even before the that one of the first observations of dislocations was that using this moire fringes where dislocations are there, you can see that these regions like the way we draw planes to show h dislocation you can see this sort of an effect.

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But this should not be extended too much, because there are hazards associated with it just qualitatively trying to extend it. But if one works out properly one can find out whether defect is there or not.

Another example which I will take it is this is a high resolution micrograph. Taken from a region where a boundary is there. Suppose I wanted to find out whether there is any

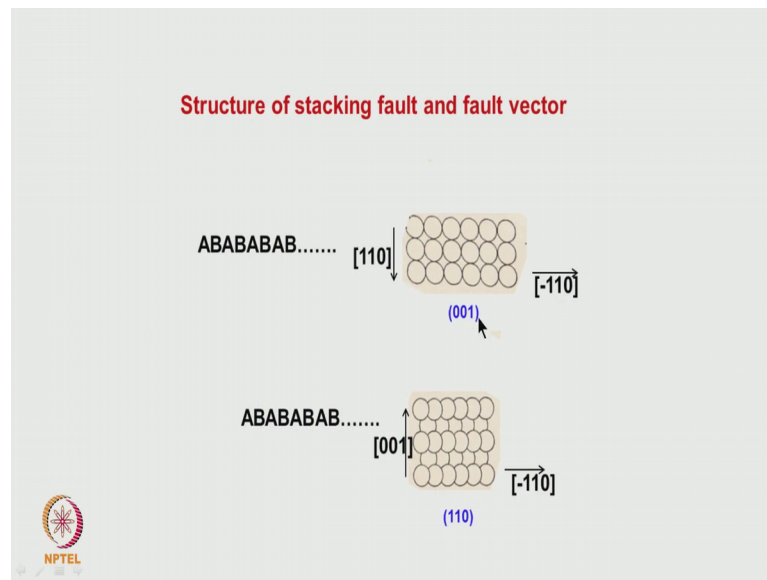
defect is present, what is the difference between orientation between these boundaries and all, what is the way in which I can do it?

Student: this is basically that moire,

No, no this pattern essentially is a just a normal pattern from a one crystal it is like a it is from an aluminum. Suppose I take that is this region itself is an aluminum it is giving a pattern. Suppose some defect is present in that region there will be a slight rotation like dislocation is there close to a dislocation core the planes might have rotated. Top and the bottom there may be because of compressive and tensile strains there is a small variation in the lattice parameter, but that do not get reflected in the conventional high resolution microscopy. What do we do? I just generate the same lattice I take the unit cell slightly expand a little bit, the same pattern I can take it expand it and super impose on top of that, I will be seeing a moire fringe pattern know, correct? Because I said the moire fringe pattern is a visualize session effect you see it.

Now, you see this is how the pattern will change. Now looking at the moire fringe pattern the spacing at which they are coming we know how much is the deviation which we had given. Now you can calculate back precisely what is going to be the deviation , is it clear? See, that is because in this pattern if there is a dislocation is going to be there somewhere here some planes are slightly deviated from it, you cannot even make out because it is difficult. But if you expand a lattice and put it there small deviation, now you can generate a moire fringe pattern and enhance the contrast, So that now you are able to see it. You understand that this is one technique which has been employed by scientist when this high resolution microscopy became quiet prominent, is it clear? There are many methods in which it could be done, and just wanted to tell these are all the way in which the result which you get it. You can manipulate it to get a lot of information from the sample, but one should be aware of it. Because moire fringe patterns are always seen in inter scopy ok.

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Now, we will come back to stacking fault. What is the stacking fault? In FCC let us take that case, it is the easiest one which has been very studied crystallographically as well as in microscopy also. What is the sort of a defect which it introduces, introduction of fault. What it does shifting of an atom layer, but what is the fault vector.

Student : in f f c.

Yeah in FCC.

Student : always 6 bar 1 to

Student: 1 by 6 1, 1 partial.

That is a partial that dislocation partial that is not the fault vector.

Student: 1, 1, 0.

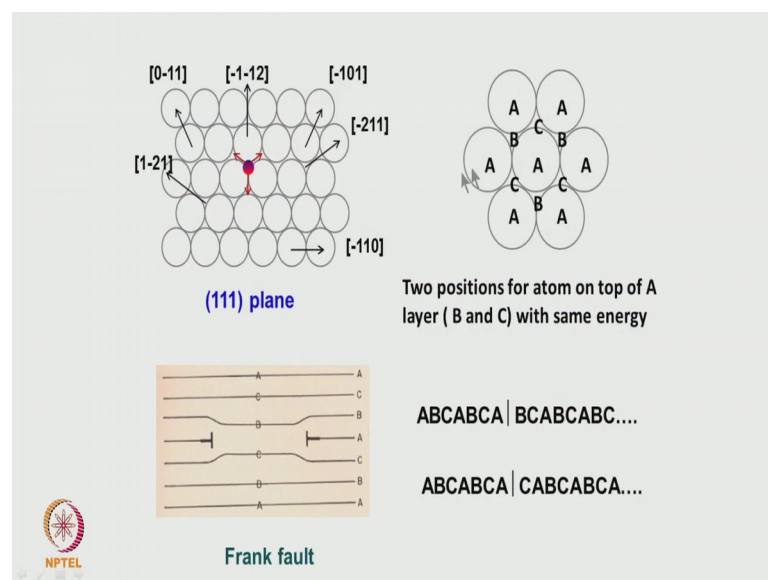
Fault vector is 1 by 3, 1, 1, that is, in an FCC along 1, 1, 1 direction if we consider it. 3 layers a b and c layers are kept on top of one of each other. Suppose I remove one layer what essentially I have done it I have created a stacking fault, correct? So, if that layer has been removed now what has happened to the what is the distance which we have made a modification one third of that distance, correct? In an extrinsic fault what we do we remove we modify 2 layers.

So, for an intrinsic stacking fault R will be $\frac{1}{3}[111]$ and we have to choose the appropriate depending upon which plane and which direction this will change. This is for an intrinsic or extrinsic will be $\frac{2}{3}[111]$ this is going to be the fault vector and this intrinsic and extrinsic stacking faults could be created by Frank dislocation or it could be created by Shockley partials, correct? When Shockley partials create.

It is going to be a $\frac{1}{6}[112]$ type is the Burgers vector of the dislocation. If it is the Frank dislocation which creates then the Burgers vector of the dislocation will be $\frac{1}{3}[111]$. I think these things you have studied if any of you are not studied I think I will explain now.

Student: we just heard the names Shockley and Frank.

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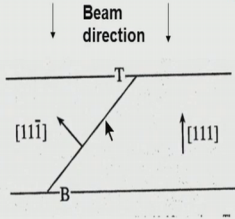
Yeah you are not. Now you look at this one. This is an A layer, on top of which it is hexagonal arrangement in FCC, right. $\frac{1}{3}[111]$ plane. In these there are some gaps which are there. In this hold next layer of an atom can come or the next layer of an atom can come on this hold. The same type of an atom cannot sit here and here on a hard sphere model because that spacing does not permit. So, this A layer if this is the position which B layer occupies and then similar gap will come and the next layer of the atoms if you put it comes to these positions then we call it as the C layer position. So, the stacking sequences essentially becomes a b c, a b c, ok.

Suppose from here to here, what is the vector? This vector is nothing but or from this vector will be in this direction is going to be a by $\frac{1}{6}\sqrt{3}$, $\frac{1}{6}\sqrt{3}$. From here to here because you can see from here I had just marked the direction from here to here this vector this you can calculate it. If a dislocation with these burgers vector moves then what it does is that it moves the atom which are there in b position to a c position. So, when a dislocation moves it moves all atoms on the layers above also right. So, the c position will be moved to the next position, like that this layers will be shifted; that means, that instead of b atom layer coming, now after a atom layer it is a c layer comes. This if you write it as a stacking sequence it will turn out to be a b c, a b c, a b c. Suppose this b layers is shifted then becomes a b c, a b layer becomes c, c layers becomes a, b, c, a b c.

Now, if you look at this, this layer essentially is now is a stacking fault which is created. By shifting a layer stacking fault could be created. What all the other ways in which the same type of a fault which could be created is that by instead of moving this dislocation. Suppose I remove this b layer, then what it will happen? On top of a layer c layer will collapse then it becomes a b c, a c a, b c a b c now also the same type of the fault created, but if I remove a layer, that is equivalent to a distance which is going to be a by $\frac{1}{3}\sqrt{3}$, $\frac{1}{3}\sqrt{3}$, $\frac{1}{3}\sqrt{3}$ as if that is what the burgers vector of the frank dislocation is. So, either having a frank dislocation or a this one, but the same type of a fault is the same, but 2 dislocate, but 2 types of dislocations could generate the same type of a stacking fault. By identifying the stacking fault we will not be able to make out what is the dislocation which has caused it. Only when we analyze the dislocations which are bounding the stacking fault then we can tell which type of a dislocation caused is stacking fault to occur in the sample, is it clear? Ok

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Stacking faults



$$\psi_g = F_g \int \exp 2\pi i (sz) dz + F_g \int (e^{2\pi i s z}) (e^{i\alpha}) dz$$

$$0 - t_1 \quad t_1 - t$$

$$I_g \propto \frac{1}{s^2} \{A - B \cos(2\pi s t')\}$$

For stacking faults in fcc lattice, $R = 1/3\langle 111 \rangle$. Invisibility criterion is $\alpha = 2\pi g \cdot R$
 $\alpha = 0$ or $2\pi n$, SF fringes are invisible; For $\alpha \neq 2\pi n/3$; fringes are visible

In this case (figure shown above), stacking fault in fcc lattice is inclined wrt foil. Beam is along $[111]$ direction. Fault is lying on $[11\bar{1}]$ plane. Fault vector is $1/3[11\bar{1}]$. This fault will be invisible for $g = 2\bar{2}0$ and $g = 1\bar{1}1$.

Problem: Stacking faults are imaged with 200 , 020 , $02\bar{2}$, 311 and $1\bar{1}1$. Find out the g vectors for which fault is invisible and those for which the image is visible

Now, suppose such a fault line is inclined like this. And the fault vector is always in these direction. Now you see that when the fault is inclined up to this it is there is phase shift which will introduce because of right.

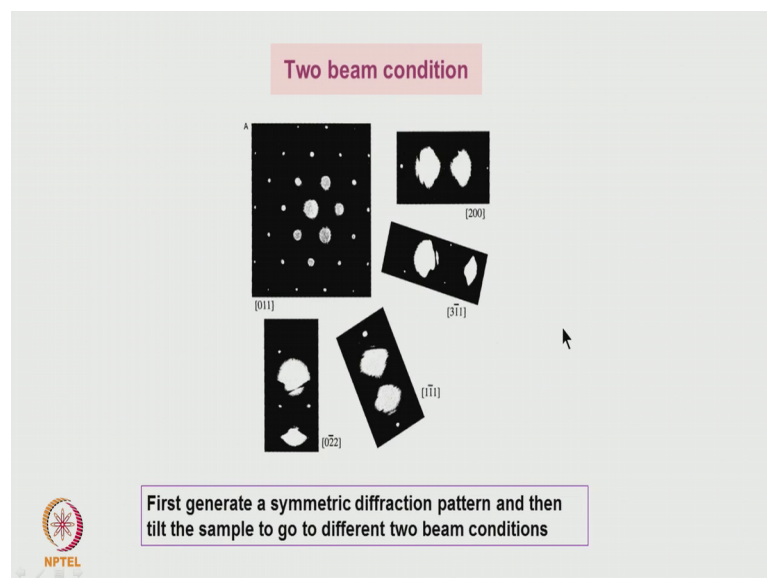
This phase shift is essentially is that as we have written in that expression α equals $2\pi g \cdot R d$. What is $R d$? R turns out to be $1/3$. $1/3$ by 3 , 1 , 1 , 1 is the fault vector. So, the dot you take it. So, α will be equal to $2/3$ into $g \cdot d$ this is what it is essentially is going to be. Suppose this term turns out to be 3 then α will become 2π , if g becomes ok.

If these 2 are perpendicular to each other then it will become 0, then also α becomes 0. So, these are all the conditions under which the fault will become invisible α becomes zero; that means, that under those condition the stacking faults will not be seen, but in other condition for other g vectors you will be seeing the faults. When we see that fault, then since we know the α is constant with respect to the g value you substitute this now we can try to find what is going to be the intensity. This is under basis of a dynamical condition when this is a kinematical condition of expression. Which I mentioned dynamical condition when we do it because here what has to be done is this is for a particular value of x and y . Because if you look at that sample if I see a sample like this, if I write x , y and z , this is x and y , z is going to vary like this in the sample thickness right. So, that is how we are trying to find out the intensity which is going to be at the

bottom of this sample at every point. This we have to do it for varying x and y and then they it will give some variation in contrast.

And if you see this the dynamical theory what the expression which it gives is that I_g equals $1/s^2$ that is the intensity is proportional to the deviation from the Bragg condition square of inversely proportional to the square of deviation from the Bragg condition. And another is that it is fluctuating with respect to s , correct? s into t inverse what values they can choose. They can choose value which is equal to this whole term can become $\pi/2$ depending upon that intensities will be fluctuating. So, when the intensity fluctuates as a function of t for a constant s then what essentially we are going to get it is a fringe contrast ok.

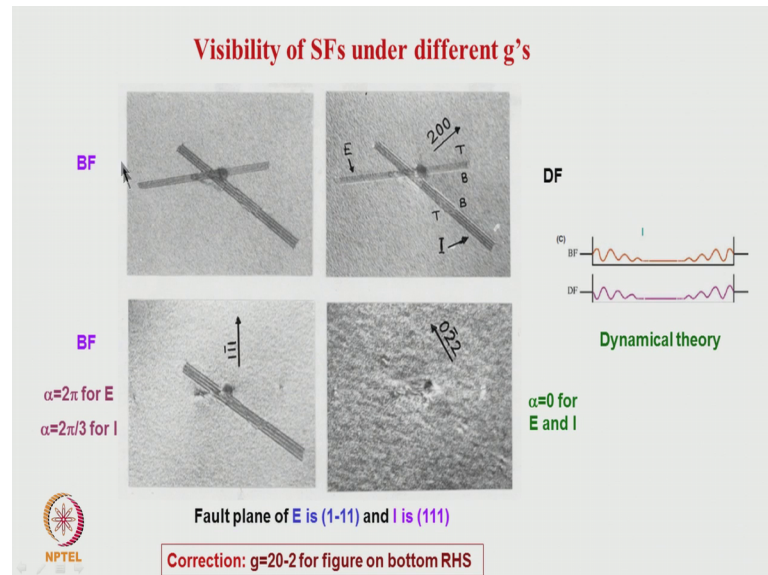
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This exactly what is happening. That is, suppose we wanted to find out the fault vector. What we have to do is, the only one g we cannot find out the fault vector for any. So, we should know at least 2 vectors for which the stacking faults becomes invisible. If we know those 2 vectors for which it becomes invisible then we take the cross product of 2 vectors we will be able to find out the fault vector, right. That is what the vector algebra tells that is essentially what is being used here. So, if we have to choose few different g s the way in which we can do it is a you go to a zone axis pattern diffraction pattern you get different spots corresponding to that. Then go to a 2 by tilting the sample in the same

region we can go to a 2 beam condition. In that 2 beam condition we try to image the defects using bright field as dark field reflection, both the things are being done.

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If we do that, then we will be getting fringes for various reflections. And one example I will show you is here you see the this is a bright field where it is image with a g which is 2, 0, 0. This is a dark field which is image of the same stacking faults, which are imaged with g 2, 0, 0 this is a transmitted beam that is a bright field and a dark field are the same. Now you can make out that here if you look at the top at the bottom of the fringe have got the same intensity, but the fringe is there, correct? You look here the fringe is asymmetric the top is one is bright we know which is top which is bottom that has to be found out there are many methods by which, and this is one thing which happens. And now the same area I image it with a reflection 1, 1 bar 1 that is I go to a 2 beam condition where the central beam is there, the diffracted beam is the planes 1, 1, 1 bar planes are the only ones which satisfies the Bragg condition. Then under that condition when we image it I find that this is this dislocation is this stacking fault is absent. We are able to see only one stacking fault, correct? .

Now, I go to a g which is 2, 0, 2 bar that is I slightly tilt the sample, So that now the planes which are satisfying Bragg condition is 2, 0, 2 bar planes. When they satisfy the Bragg condition now you find that both the faults are invisible. What is the consequence of this? Suppose you do microscopy, your beam is such that the orientation

is such that it satisfies this invisibility criterion, you will be seeing no faults in this. But that is why looking at only one direction like looking at you people only from this angle, I do not get complete information about it. You know this information is used in common practice in our society where exactly it is being used?

Where do you do this? For important personalities when they take photograph, they take both the front and side view. So, very important persons in society, right. 2 views are required because only when you match them you can get the complete information about the person. So, more than one is required. So, that is true even in microscopy otherwise you will be getting all wrong information, is it clear? Now this is vanishing with respect because here it is a mistake that is why I had just written it here. Then using this dynamical theory of diffraction when the contrast has been calculated. That part of it I am just not talking about it because that is beyond the scope of this class it requires the whole dynamical theory it has to be taught in our one semester if that has to be done.

Now, you see that the variation in the intensity both the top and the bottom it has that same for the dark field you see that there is an inversion of contrast which is taking place. So, this theory is able to So, the dynamical theory is able to predict this correctly. And we know that what all the vectors for which this fringes become absent ok.

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This is a stacking fault is nothing but planar defect, correct? The similar planar defect which we can no before we go. Suppose one stacking fault is there, another stacking fault

forms on top of that, then what is going to be the both the fault vectors? Together it is twice that know. So, it will become 2 by 3 1, 1, 1. If that is the vector which we use it when we look for the intensity of the fringes the fringe contrast will change, because that is going to bring about a variation in the amplitude of the wave, correct? For the same position at which we are trying to calculate it So you can.

Suppose 3 faults are coming on top of it then what happens to R ? R becomes 1, 1, 1; that means, a it is a perfect translation vector. Perfect translation vector should not give raise to any variation. Now you see that here in between that is why there are some regions you find that if you look carefully very faint fringe contrast could be seen; that means, that it is an overlapping stacking faults are there depending upon that how many layers are overlapping we get fringe contrast. This also does occur in microscopy when you look at deformed samples yes.

Student : sir is this stacking fault address to y 3 1, 1, 1?

Yeah.

Student: we are adding intrinsic to that together.

Yeah.

Student: becoming 2 y 3 they have a differentiate between these two.

Which one.

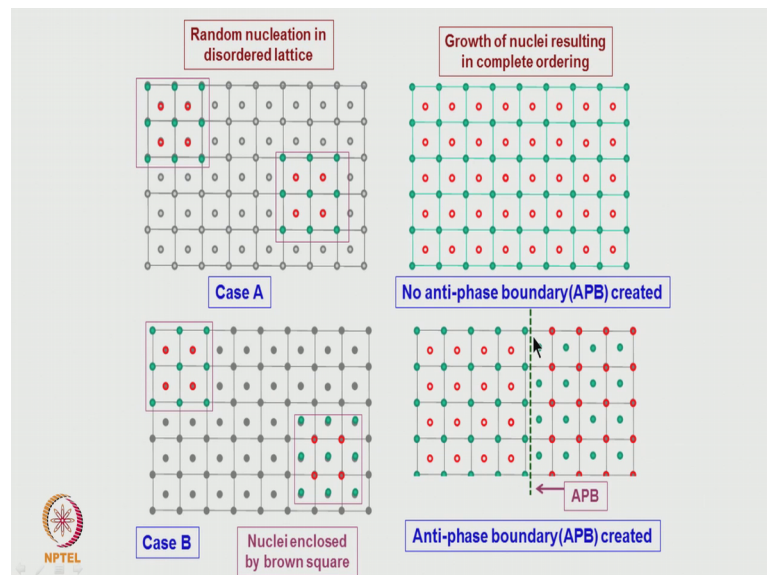
Student: extrinsic stacking faults or intrinsic to overlap.

The intrinsic and extrinsic fault for which there are some protocols which has been developed on the basis of a contrast with which we can do that. And the burgess vector of the dislocation also has to be looked into it there are. So, many things into it is not in one way. Now those part of it I am just talking about only simple others I am just explaining it, but not going into the detail. If you look into the book edington practical transmission electron microscopy there all the procedures are mentioned for identifying various types of defects. That is what we used to use, but essentially you can understand that the fringe contrast is going to change, correct? Because what is going to happen is that the dislocations will be bounding this stacking fault no, that stacking fault also will change

depending upon whether it is an overlapping stacking fault or whether it is going to be an extrinsic stacking fault ok.

There are many cases when you find that in many complex alloys using $g \cdot b$ you may not be able to identify uniquely the fault vectors. In such cases you have to do computer simulation of the images also has to be done. When you have to do the computer simulation of the images we should know the full dynamical theory of contrast very well that are softwares which are written, which are available like a package called as a $e m s$ package with which one can do that. Now from stacking fault we have talked about it.

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Let us talk about anti phase boundaries. What is an anti phase boundary? You are studied anti phase boundary, all of you know what anti phase boundary is. So, anti phase boundary is essentially like from one crystal to another crystal when they form a group. If from one region to another region the position of the lattice remains the same lattice position, but the atoms which occupy it they change that position. So, if we go from here to here since the specific atoms changes, this introduces of fault vector one in these direction is essentially from here to here if it comes. So, since it is changing the fault vector is going to be ok.

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APBs form during transformation from disordered state to ordered state

APBs are called translational orientation variants. The translational symmetry lost during disorder to order transformation appear as APBs.

These boundaries are called anti-phase domain boundaries (APD)

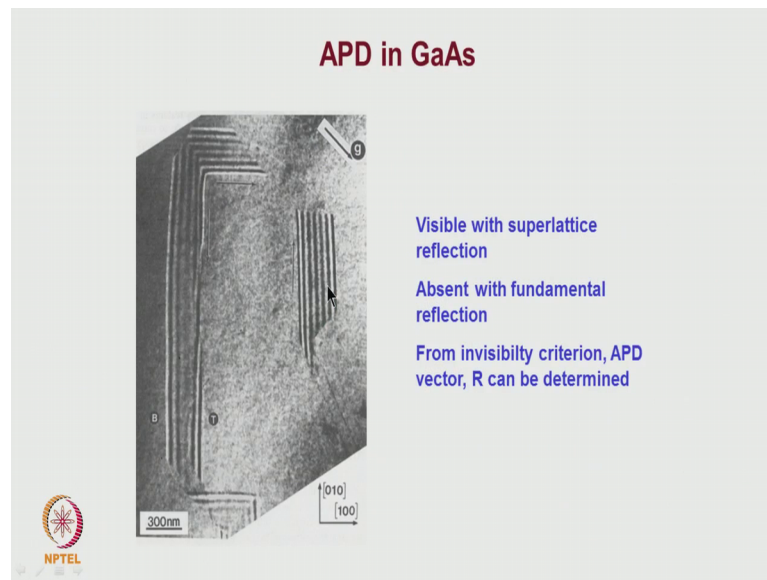
Exercise:

A defect, imaged in electron microscope, exhibits fringe contrast. The crystal structure of the disordered material is fcc. This defect disappears with $g = [220]$ and $g = [200]$. What is the R vector of the defect and what is your comment regarding the nature of the defect.



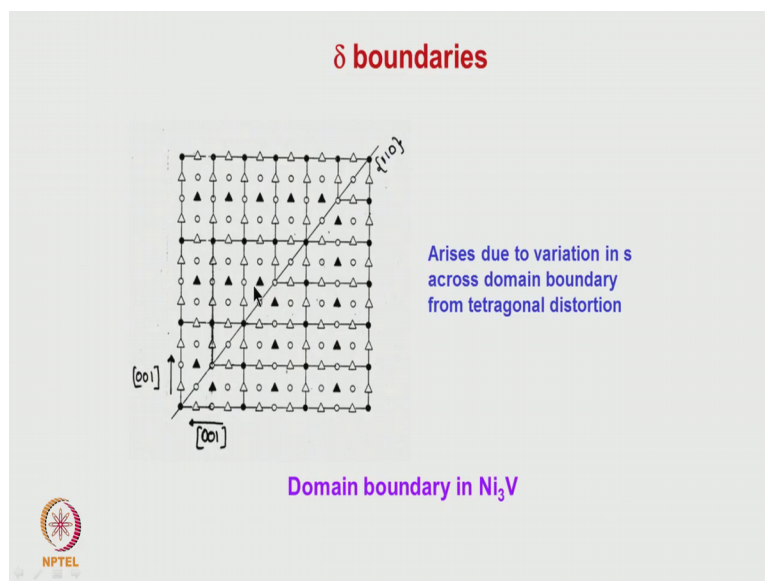
In this particular $1, 1, 0$ or $1, 0, 0$ that depends upon the type of crystal lattices which we are considering it. What will be the effect of this fault vector, as I mentioned there earlier the first itself that if we introduce the shift which is t by 2, midway if we between the periodicity of the lattice from one lattice to another. That will give rise to for $1, 0, 0$ type of a reflection the amplitude will become 0. For $2, 0, 0$ type of reflection the amplitude will that is essentially for fundamental reflections. You will not be able to see the faults, but if you image with the with the super lattice reflections you will be able to see this. That is very, this also gives rise to essentially a type of fringe contrast exactly like a stacking fault.

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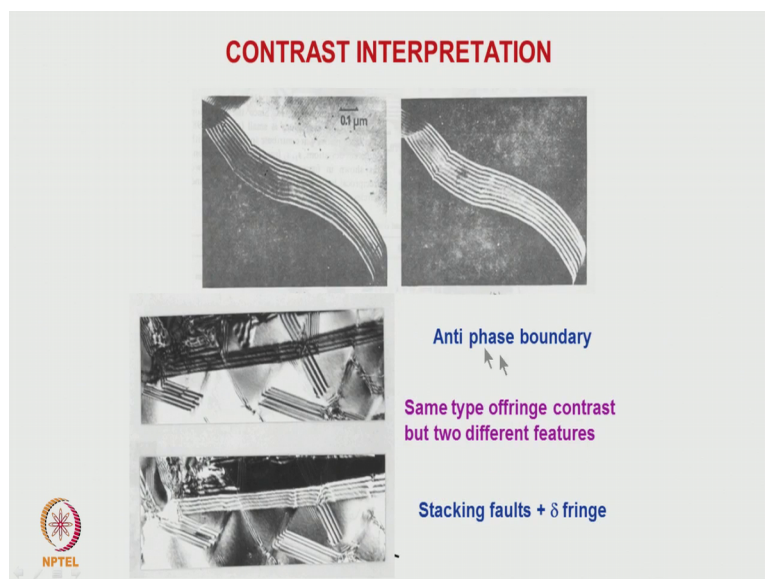
But what essentially the difference between the how it is when the intensity has been calculated for the fault for the stacking, for the stacking faults between bright field and dark field the fringes are asymmetric top and the bottom. In one case it is asymmetric the same type of a fault dark or bright in the other case one is dark and one is bright. In the case of anti phase boundary first the vectors which we use are going to be different because there it is some g vectors which we can find it, those g vectors may not give rise to a stacking fault like here. If we take 1, 1, 1 then FCC type of a lattice if 1, 1, 1 is a fundamental reflection you will not see, but in FCC 1, 1, 1 reflection if you do it in quiet often you will be finding the fault. So, that is one way to rule and another is that if we take 2 vectors for this faults becomes invisible we can try to identify what the fault vector is because that 2 g vectors which we were taken cross product of you will give you it is used to find out the magnitude of the fault vector, is it clear? And another is that intensity both in the bright field and dark field it becomes symmetric. All these things are given in the book Edington, but what I wanted to tell is that there are So all planar faults give rise to a fringe pattern they look quite similar. So, when you look at the fringe pattern now you have to identify whether it is a stacking fault whether it is an anti phase boundary.

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So, this is like here if you see it these are 2 type of lattices which are being shown. 1, 1, 0 is the interface between them and in these the c direction is here c direction is here. This is like a twin related generally in this sort of lattices the c by a ratio need to be exactly is since c by a ratio can be away from one. So, if that is the case that gives raise to from one region to another region from here, if the c is like this when we come here if c by a ratio is different this will give it a small variation in s . So, as I mentioned in that formula for i g the variation in s also k gives raise to a fringe.

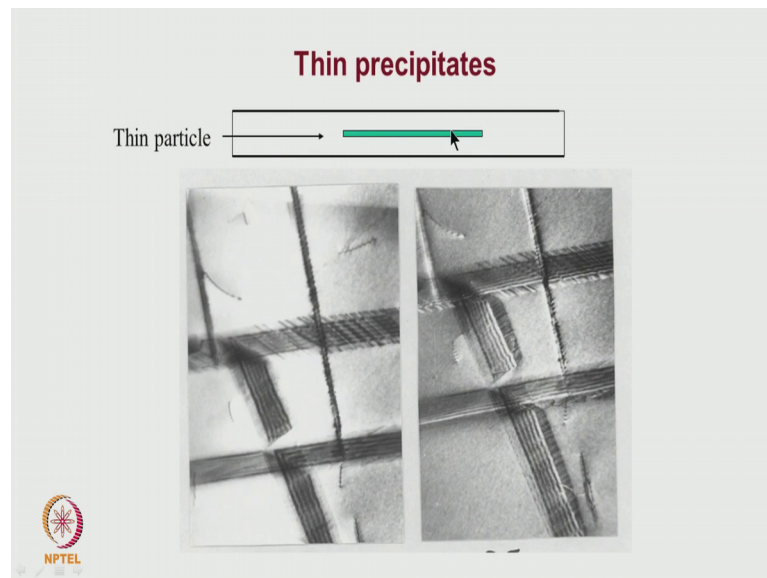
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This will give rise to now you see that when a domain boundary is there between 2 domains there is a fringe contrast which is coming here. This also looks like a stacking fault contrast. And like this example if you take, it here this is a boundary which is a domain boundary, this is a stacking fault. We could differentiate this because we try to do a detailed analysis to find out which is the stacking fault, right. Otherwise can you make out from this one to this one, which is which looking at it you itself unless and until you do an analysis you will not be able to identify it. So, just doing microscopy that is what I want to tell is that in an electron microscope because of dynamical interaction of electron especially the interference of the electron beam which is giving rise to a contrast. Unless you understand what the interaction is and how they can give rise to contrast this has been all done and given in some books also unless if you have to simulate it you should know the theory much better. There are many situations where you have to all this simulation as well ok.

This is essentially a thin precipitate if I take it. The precipitate also may be it one or 2 layers.

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That precipitate, what it is does is that the beam which is enters here to a beam which comes down. It may introducing only a small phase shift. If such phase shift is introduced that will manifest itself as a fringe contrast, this is one case which comes from a precipitate here also you get a fringe contrast. So, there are various reasons why

you get the fringe contrast. So, all fringes are due to some type of a defect, but which type of a defect if you have to identify it you have to do a detailed analysis. At least for defects like stacking faults if you know crystallography if you take FCC you know what all the types of faults stacking fault which it can form what is the fault vector you know.

Similarly, if you know an ordered lattice immediately you can find out which what all the vectors which are going to be the anti phase boundary vectors like, anti phase boundary vectors are like, whatever the crystallography which you have studied there are some symmetry operations which are there, right. Symmetry elements when it goes from one lattice to another lattice and this symmetry operations are it could be a translational symmetry, rotational symmetry, mirror symmetry all are there. When from one lattice to another when the space group symmetry changes; that means, that some symmetry elements will be lost from the other lattice. All those symmetry elements which are lost they appear as defects in the ordered lattice, that is translational symmetry elements will appear as anti phase boundary the which are lost and the rotational ones which are lost they will appear as domain boundary. And all of them will give rise to these are all planar faults. So, they give rise to essentially a fringe contrast the next part is imaging strain. That we will do it in the next class. Will stop here.