Electron Diffraction and Imaging

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

Lecture – 16
Double Diffraction and CBED

Welcome you all to this course on diffraction and imaging. So, far in the last few classes what I was trying to tell you about the different modes of diffraction correct, there is one using a parallel beam another using an divergent beam, and another I mentioned that on a convergent beam we can have this diffraction. So, if you consider the parallel beam diffraction for different type of structures Bravais Lattices you consider that there are some structure factor consideration right, what is the basis for this structure factor consideration.

Student: Atom positions.

Atom positions other than the with respect to the beam one is the beam is parallel and another is that kinematical condition is the one which is working right; that means, that only one scattering event as the beam passes through undergoes that is the first thing we have considered. But what normally happens in a material with the electron beam that is valid only for x-rays. X-ray essentially it is a single scattering mostly whereas, in electron diffraction multiple scattering can take place. We will consider the effect of that later, that will have some effect on this structure factor consideration.

And another thing which we also have looked at is that this extension rules we are looked at it for Bravais Lattices correct then we have looked for when there is a glide, when there is a screw axis for those conditions also there are some extension conditions are there, correct. That I had mentioned on that I given on that table and also mentioned that for different types of glides for specific you know how the intensity of the diffraction parts will be affected some spots will become systematically absent. That means, that using this kinematic condition of diffraction itself we can get information about the some information about the space group symmetry also correct because when that extension rules are being followed it tells about what is the type of a screw axis is present or what is the type of glide is present is always related to this symmetry correct.

Then lattice parameter we can determine correct from looking at the right, but though the lattice parameter is not accurate from that you get some idea of the unit cell dimension, then one more information is that when we wanted to find out the complete symmetry of the crystal only problem which comes in a kinematical condition is that whether the crystal has got a center of symmetry or not cannot be distinguished. Because if at whether a crystal has got a center of symmetry or not if we have any reflection 1 on 1 - 1 bar, 1 bar, 1 bar will be also always be present whether the atom is there in the crystal structure or not that is immaterial this is called as the Friedel law. So, that is one condition which is going to be because of that we will not be able to get complete information about all the complete spaced groups because in a normal diffraction pattern what information we will get is essentially what is called as a lave group that is (Refer Time: 04:25) lave groups only we will be getting that information that is the main drawback of that diffraction.

This we considered it for a different types of Bravais Lattices, then we know that in the unit cell atoms can occupy different positions in the lattice right some specific positions different type of an atom can occupy. If atom occupy different type of positions what is the consequence of that atom occupying different positions the reflections which are not permitted by structure factor rules, they appear as faint and the intensity of the reflection is nothing but if 2 atoms are there a and b then it will be f of A difference f of B with some factor it will come, if 2 atoms are there in lattice 2 different types of atoms each has different structure pattern.

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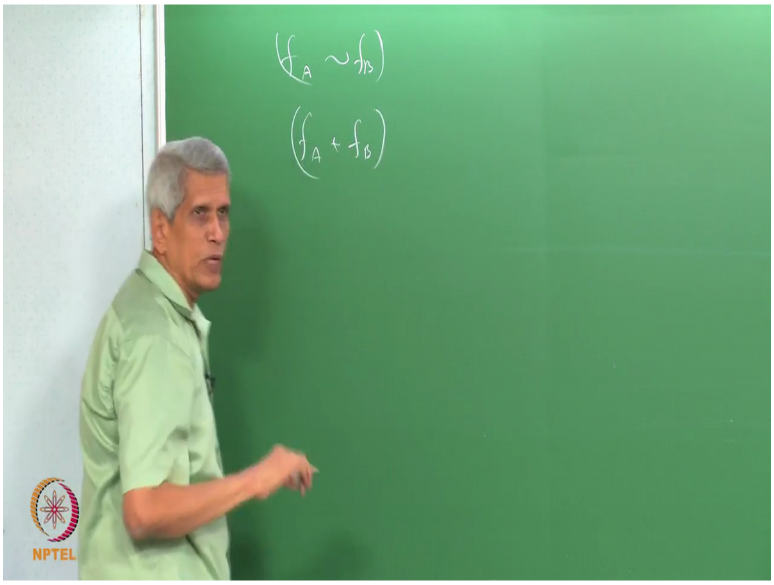

The fundamental reflections are one where it will be f A plus f B what this amplitude will turn out to be some factor which come correct intensity will be squared of this with some prefactor will come which depends upon number of atoms which are going to be in the lattice correct is it right? Because c c it will have the factor rule before will come right b c c a of factor 2 will come is it not number of atoms in the unit cell also will come is it clear hm.

Suppose a phase transformation takes place from one structure which is FCC, it goes into a structure which is primitive simple cubic, that simple cubic from FCC to simple cubic then what is going to happen essentially is that in the diffraction pattern where which are not allowed by structure factor consideration.

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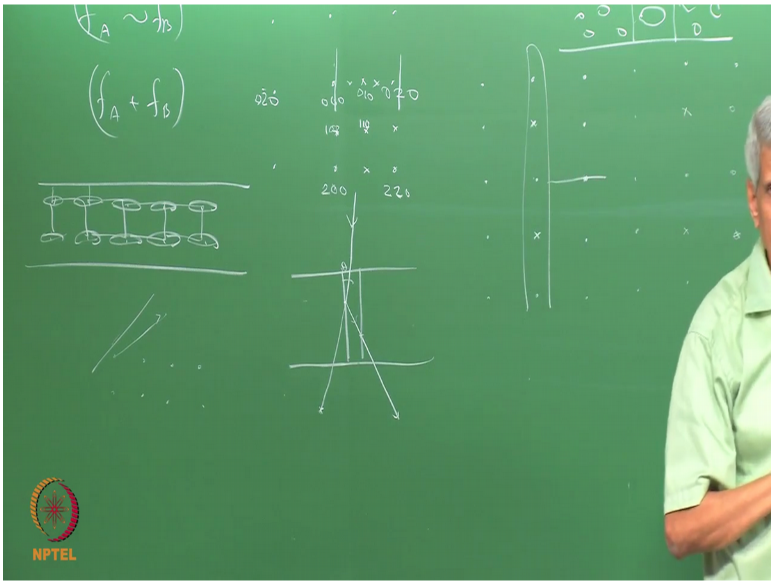

For example suppose if we take a 001 zone this is how the pattern will appear right correct, this is how the reflections are there. Suppose it goes into an ordered lattice like an a I 3 a l then what is going to happen is that because these are all the positions this corresponds to 0 1 0 this is 1 0 0 which are not permitted by structure factor consideration for FCC correct. When it goes into an ordered lattice these positions also we will be getting then 1 1 0 which is not permitted in all these positions we will be getting some intensity, but the intensity of this spots will be very small compared to that of this one this is what I had in one of the assignment as due to work also what will be the order of difference which it will come that is clear right.

Then if it is ordered the lattice is the sample is completely ordered this is the sort of a diffraction pattern you will get it; that means, that in addition to a fundamental reflections you get super lattice reflections also. This is a case where the lattice parameter of the disorder lattice and the lattice parameter of the ordered lattice are the same correct. Suppose it goes from a disordered lattice into an ordered lattice if it has got a different lattice parameter then what it will happen then it will have a pattern which is corresponding to the ordered lattice with fundamental and super lattice reflection which will be there which will also appear in the diffraction pattern, correct.

Because from the region which we are taking if it contains both the matrix there is suppose that is a you assume that there is a sample in which a precipitate is also there in these region ok.

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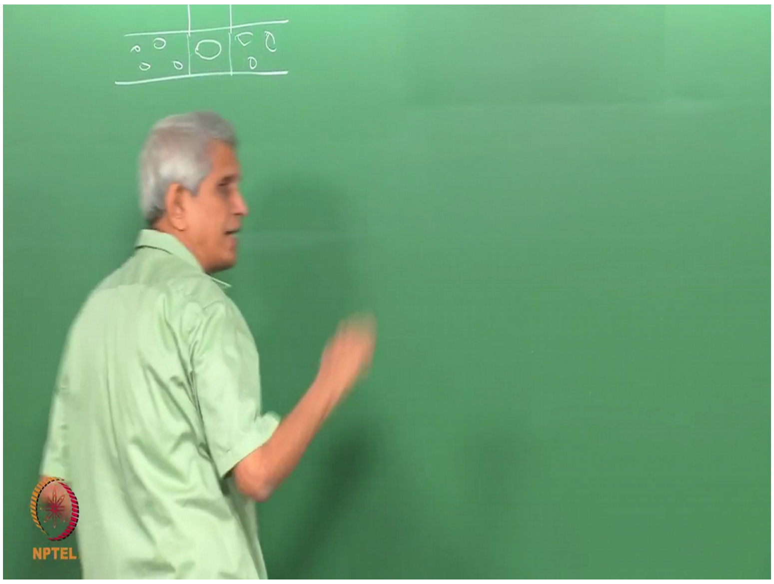

This is the beam size which we choose. So, this means that matrix and the precipitate both of them will give raise to diffraction correct. Depending upon what sort of orientation relationship between axis between the matrix that is the disorder and the ordered lattice or you can call it as any a second phase particle that relationship will be exhibited in the diffraction pattern also correct.

Suppose it another case which can happen is that, this sort of precipitate which are there this precipitates could be distributed randomly in the sample. Suppose the precipitates are randomly distributed when we say randomly distributed what it means mathematically what means suppose you have to define there is no special coherence no special correlation right, spatially if it try to correlate from one particle to another how they are distributed we find that the distances are random correct that is what it can happen.

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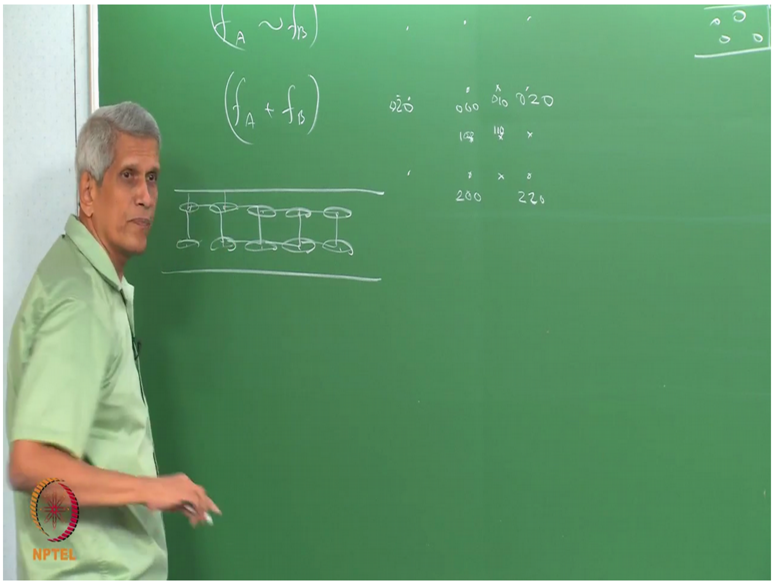

Suppose we consider a case where the second phase particles are correlated in space, the correlation which it can happen is like we assume that so; that means, that all have the same size assume and all are at some distance. So, this is spatial correlation is there right now what can you think about this one this distribution. Now it is an another lattice with a large lattice parameter within one lattice your precipitates form an another lattice right now I can say that this is what the unit cell of this one know this can always happen then how will it be reflected in the diffraction pattern. So, you should get spots which should be inverse of this in the reciprocal space. So, additional reflections will come suppose same particles are randomly distributed you get only fundamental and super lattice reflections.

Suppose you assume that in this particular case these are about 4 times the distance of the lattice parameter of the matrix then how it will be reflected in addition to it you will have one will come one will come some additional reflections will come this sort of situation occurs quiet often ok where do you face this sort of a situation in which type of samples you give me an example.

Student: Super.

Other than that super alloys this sort of periodic lattices which can come.

Student: Multilayer films.

Multilayer films exactly. So, multilayer films you have the periodicity with which the film repeats itself correct, there you will be seeing one a lattice which is corresponding to each of the sample structure which is periodic in itself in addition to it at a regular interval the thickness the film changes from one phase to another phase correct there also you will be getting this sort of diffraction pattern you understand that. Why I am telling is that, when you do an analysis you should know when you get the diffraction pattern what all the possible reasons why such a pattern appears always it may not happen that you get a very simple pattern if a sample is a multilayer type of a sample this is the sort of a problem which we will enter.

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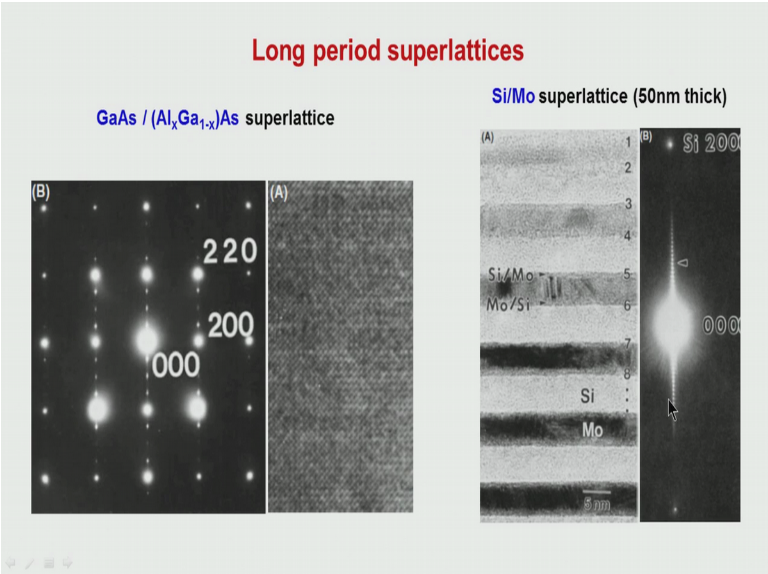

You see this is gallium arsenate aluminum gas arsenate as a super lattice layer it is being formed. In this if you see this is way the structure should appear for the gallium (Refer Time: 13:59), but you find that there are more reflections are coming in addition to it these reflections are coming because it is a multi layered film, where the thickness of the film is 4 times that of the lattice parameter of that structure this is how this is high resolution picture it is all taken from the literature. If you look carefully there is a slight variation in contrast here is there, this using an another technique called as a c contrast it could be observed that I will talk about it towards the end of the lecture last few lectures I will do out with that that modern new techniques of imaging in electron microscopy.

Similarly, here you can see that silicon molybdenum super lattice structure, you see that here it is silicon and molybdenum layer it is alternating with the thickness of 15 nanometer thick and you see that diffraction pattern. If you see there are very close parts are there and the separation between the spots looking at the diffraction pattern immediately you can talk about what is going to be the thickness of the multilayer. So, multilayer thickness could be measured very accurately from the diffraction pattern; because this we also know that whenever we look at complex like acoustic wave if you look at it the wave how it propagates like when I speak this can be when we synthesize it are going to a frequency spectrum.

In a frequency spectrum it tells clearly what all the frequencies at which the sound is coming right, similarly what we are doing it is that multilayer the thickness of the film may be varying from one to the other small variations will be there it could always be there, but what all the frequencies with which it gets repeated, is in the diffraction pattern it makes it very clear. So, analyzing the diffraction pattern we can always get information about lot of information about the structure of the multilayers is it clear this is one important aspect. This is all with respect to a parallel beam you understand that what we are talking about it is all if the parallel beam we are trying to look at kind a diffraction and essentially we assume that it is a kinematical condition so, that depending upon the Bravais Lattice we will be getting the extension the some spots will be not visible, on that basis we can talk about what sort of crystal structure which the material has right.

Generally when the electron beam enters into the sample we know that electron since it is charged particle it interacts very strongly with the sample; what will be the consequence of this strong interaction is that multiple scattering can take place what we assumed earlier when we derived a formula for diffraction we assumed that.

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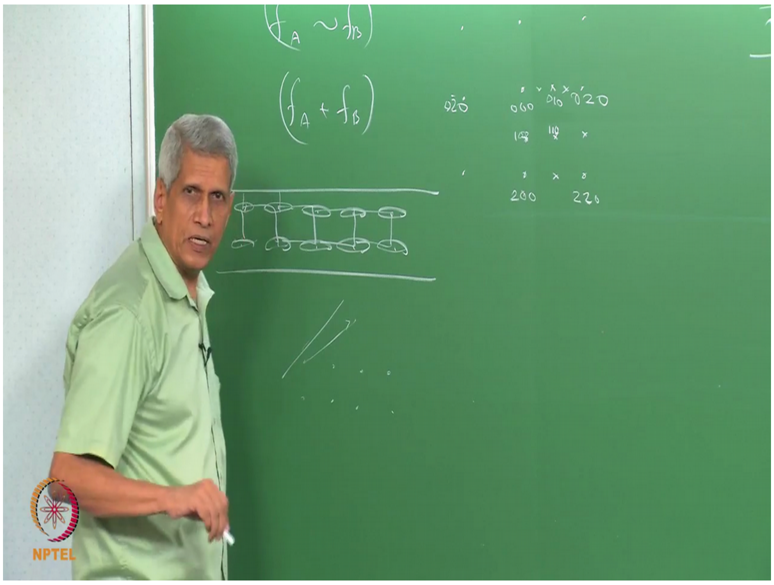

Suppose atoms are situated here and a plane wave front wave is entering into the sample, that is from every atom position it is getting scattered, it is only that one scattering which we are considering it.

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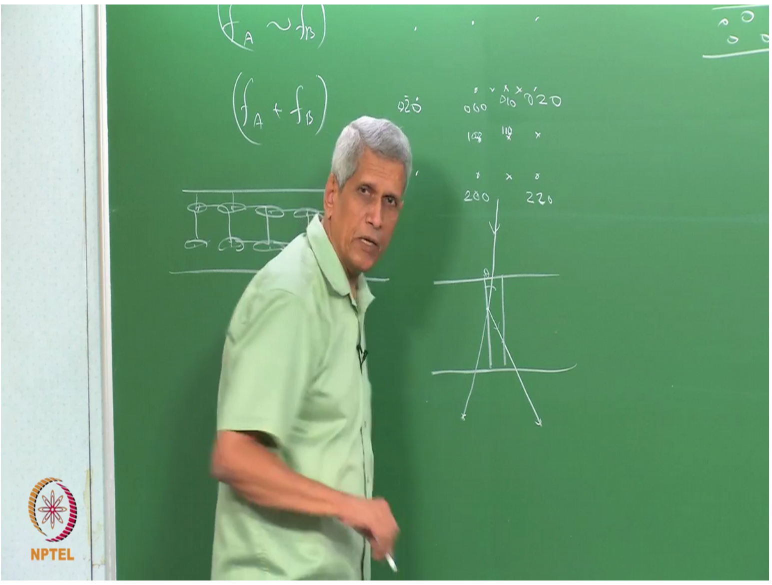

So, in the case of an electron beam what will happen is that suppose you assume that this is the sample and these are the planes we know that in the electron diffraction the Bragg angle is very small. Suppose the electron beam enters like this then from here it can be scattered in this direction it should come like this, this is the diffraction assume that this is angle satisfies the Bragg angle. So, this should be the diffracted the spot this should be the spot. Now, as it enters here from here also plus if a scattering takes place what happens as if the incident beam is in this direction a scattering is taking place from here also right.

Now, like this from so many places if it considered. So, the spot which this corresponds to it is essentially is also acting like an another independent source and giving rise to an another diffraction pattern is it not? What will be the consequence of such a diffraction is that especially in no symmetry elements, the reflections which are not allowed by kinematical conditions those reflections will become present in the diffraction pattern.

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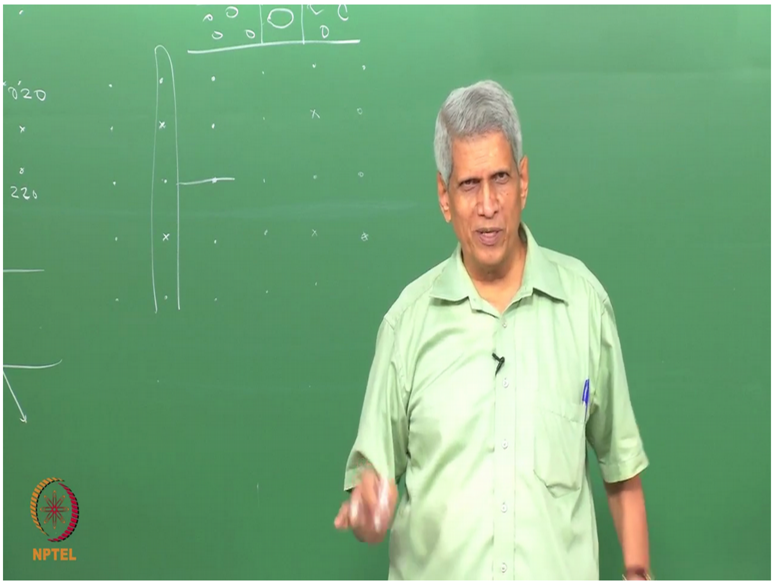

In a example which we can consider is that this is I am just drawing with respect to f, this is with respect to a diffraction pattern which you get in titanium. These 2 reflections by structure factor consideration this will be essentially 0 0 0 1 reflection which are not permitted like if this is the direction in which beam is coming, this acts as a center we have various diffractions are taking place you get you have got this pattern.

Suppose now this point the beam coming in this direction also acts as a another one under diffraction takes place; that means, that this as the center of the beam another diffraction pattern will come. Suppose I draw that diffraction pattern that means, you can draw it 2 ways; that means, that now this as the one I had the pattern, but actually the pattern has to r center if a diffraction pattern comes you know that this reflection should be present correct for this as that means, that this as the center also one reflection has to come here. So, where it should be absent now you find that a reflection comes.

This is a consequence of double diffraction this is called this is a consequence of dynamical theory. Dynamical theory this is a consequence of multiple scattering multiple scattering for which the kinematical condition is not valid then dynamical theory has to be applied that I will come to it later maybe after the diffraction is over will go into the what the dynamical theory and what all ways in which effects the intensity of that contrast because that is the one which correctly explains all the fine structures of the contrast which we observe both in the diffraction as well as in the image.

Student: (Refer Time: 21:54). This will not lead to precipitatory.

No, no this does not lead to kikuchi pattern this is what essentially it is given, how to find out that this spot suppose we suspect that the reflection which is appearing as a plane reflection it maybe there whether it is a double diffraction or not what we do essentially is that by rotating perpendicular to that is if I take this row. If I rotate the sample perpendicular to around an axis in this one then what it will happen is that, this is the plane know you assume this plane if this is the axis around this axis if I rotate does the plane the plane rotates. But still with respect to a beam this giving rise to diffraction then what will happen is that when you rotate from the symmetry when it changes, these reflections will vanish that is one that fine details of it which there is no point in going into this, but I wanted to tell that this is one of the pitfall which happens when other than cubic structures which we go.

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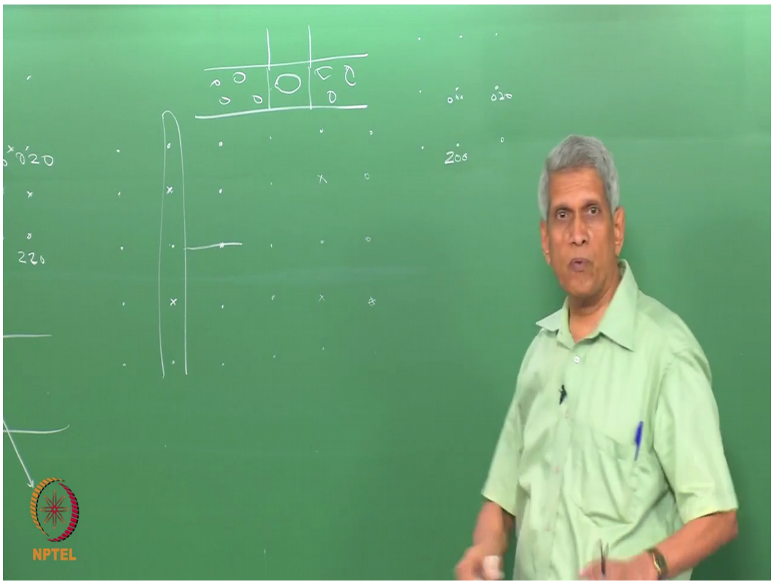

Cubic structures what we are fortunate about it is that if you look at the diffraction pattern on a cubic structure like FCC, BCC. So, if this is the diffraction pattern if I take it this is the spot which appear correct. If suppose I take this as the diffraction pattern also the sail spottle the spots will superimposed that is what it happens, but for those symmetry material the especially non primitive one, this we can see it in the case of silicon also I will just show an example.

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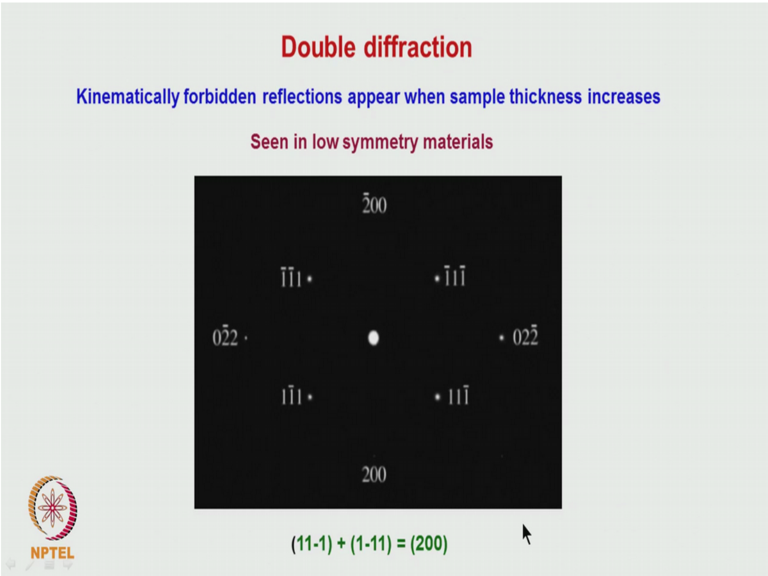

I do not know whether the spots are visible, here what it happens is that if I consider this 2 spots 1 1 1 bar and 1 1 bar 1.

If any one of them if I consider as a second resource it is equivalent to if I add these 2 in any reciprocal lattice section if we consider it if we add vector addition of 2 parts id we take the another spot should come, but normally what happens is that when double diffraction takes place by kinematical condition those spots are not allowed, but when you do it those spots will appear that is one way another way to look at it that is what essentially what I written, that is because that happens in silicon or diamond if you look along 0 0 1 axis, because there is a screw axis along the body diagonal. Now we have atoms at 0 0 position, then at one fourth position along also atom is there half position that is 0 0 half also had planes contains atoms 0 0 3 by fourth also atoms are there, then to a one plane comes; that means, that 4 planes are there correct.

So, the fundamental reflection has to be 0 0 4, 0 0 2 should become one if it is the same type of an atom which repeats like in the case of carbon or silicon or germanium or tin in all those cases they should vanish, but by double diffraction spots do appear. When such spots are there when you index it you should also know that what is the why such spots are appeared in the along the body diagonal at one-fourth, one-fourth, there is a carbon atom is there; that means, that if we look along the 0 0 1 direction that zeroth plane plane is there then 0 0 1 fourth there is a one another plane which contains atom then at 0 0 half another plane which is atom is there then 0 0 3 by fourth an atom is there then one which comes at 0 0 1 right all.

That means 4 planes are there where we have no atoms right. So, now, if you look for the reciprocal lattice if you try to consider draw it, then the fundamental reflections will come at 0 0 4. 0 0 2 comes exactly half way between these two. So, that reflection should be absent by selection rule structure factor rules, but they do appear because of double diffraction, that is if we take a sample and if the sample is extremely the a white strape of the sample.

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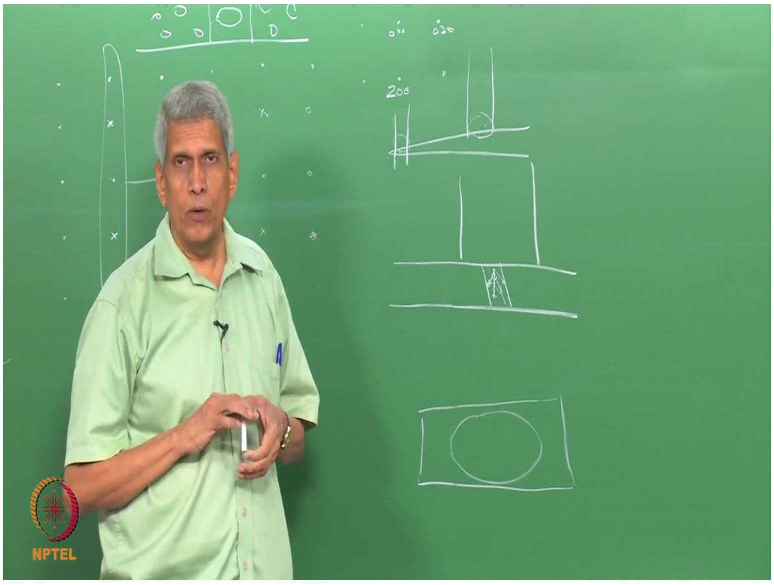

Like we have a sample like this, and the thickness is very small in this region. If I take a diffraction from in these region from these region, when I take a diffraction I may not see the double diffraction. If I take it from this region the probability of diffraction increases that is because from these region whenever a multiple scattering this also we can consider it in a probability.

Suppose scattering is taking place an atom from one particular position, you assume the scattering for the probability is p 1 as the scattered beam goes further probability of it to be scattered again is going to be another p one. So, what is the probability that twice it is gets scattered p 1 into p 1 p 1 squared it will be correct and whereas, for one scattering it is p 1. So, you can see that the. So, intensity if you take it, it is going to be square of it. So, it will get doubled reduced considerable; when the thickness when the thickness of the sample becomes large the probability of multiple scattering increases. So, you will be this is another way you can verify it that is if you see that is if you suspect that you could be a double diffraction you come close to the edge of the file and try to look for a diffraction pattern, that way we can identify it that whether it is a whether some spots are coming due to diffraction pattern or not is it clear.

Student: (Refer Time: 28:35).

Finally, when we do an analysis in a microscope we should make sure that whatever is the information which we come is the true information otherwise if some spot like this extra spot comes then the whole analysis of the crystal structure will be some other way we will be looking at it right. So, that should not occur that is why I am telling you all these things. So, this also one has to take it into consideration. What will be the consequence of it how it effects in the image part of it when I talk about image I will talk, but in the diffraction at least this much one should remember.

And now you can imagine various types of cases in your sampled as the beam passes through the way the second phase particles are situated with respect to as the beam passes through whether there is a what sort of correlation it has special correlation it exists depending upon that, at least I feel that you got an idea all this things can give rise to extra reflections in the diffraction pattern otherwise you will be thinking that why this particles are coming correct is it clear. Now suppose the beam is entering in the sample from here then since the thickness is very small, then what will be the consequence there is that essentially the beam is the parallel beam only a kinematical condition right and what is the probability of incoherence scattering taking place.

Student: (Refer Time: 30:20).

It is very less; suppose the beam is entering here what is the probability of incoherence scattering taking place is large; that means that this parallel beam give raise to a diffraction pattern which you normally observe like this correct that is what you get it. In addition to it that is if I draw it a magnified views at some particular region you assume that from here and incoherence scattering is taking place; that means, that some energy is lost by the incidental electron then this electron has different energy with which it is coming in all these directions correct? This is an that is incoherently scattered electron, but when these planes are there it can again coherently gets scattered.

If it gets coherently scattered will be getting giving getting a diffraction pattern correct that pattern which we get it in this we call it as a kukuchi pattern that is because only the beam which is coming in these direction undergoes scattering; the when we the beam which is travelling in all other directions they come onto the screen and generate a uniform intensity background correct. In that university background suddenly you find that and the in some direction the beam is undergoing diffraction those appear as dark lines at the center and away from it an excess line is come which I have explained in the last class.

Student: Sir why do we need like divergent this parallel.

Which one?

Student: This, given in a parallel beam.

No the beam is parallel; that incident beam is parallel the parallel beam is falling onto it as the beam falls onto it there are at some positions the incident electron beam is losing some energy by plasmon scattering. When it loses some energy has lost that energy that happens randomly. So, there is no correlation from one to other; now in addition to the coherent beam which is coming from different positions in the sample like this now there are incoherent electron beam is coming. This incoherent electron beam is scattered in all the directions. So, the maximum intensity will be in this direction and as the angle theta increases the intensity reduces.

So, now we have the same diffraction planes is there which is there for the parallel beam for some angle theta this planes satisfies Bragg angle. So, this incoherently scat suppose the sample you assume that it is a amorphous material, then what it will happen is that you will get a overall dark diffuse background will come; that background is going to come even when the sample is crystalline because intensity is, but only from these regions the diffraction is taking place. So, in addition to the normal diffraction pattern which you get it like this, you will be getting some patterns which gives rise to.

Student: Sir, but you said, but for kikuchi pattern we need like divergent or convergent beam right.

That is from this point how is the beam coming it is a divergent beam correct. That is what I wanted to tell though the parallel though the parallel beam we are incidentally initially putting on that sample the beam which is responsible for kikuchi pattern to occur is essentially a divergent beam you understand that emanating from this point that is what I said is this clear ok.

Student: In kikuchi and diffractions called both (Refer Time: 35:00) in the back focal plane.

Which one?

Student: Kikuchi band and diffraction spot.

Yeah.

Student: Both form in the back focal.

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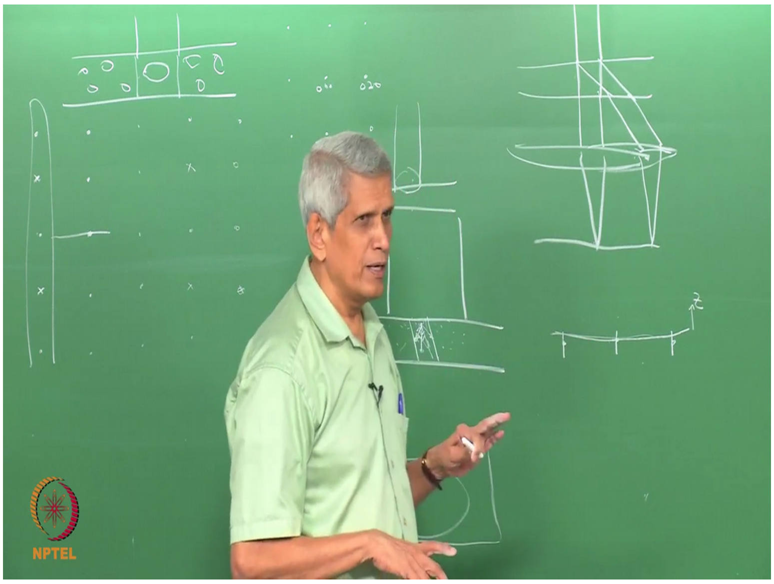

See what as the lens do? There is the beam which are all it is like this, this is beam which is scattered in these direction the action essentially is the beam is parallel beam and this parallel beam which is hitting on the lens this will all be focused to a point this will all be focused to an another point correct this what essentially it happens. So, all the parallel beams will be focused to the back focal plane, that is as far as the diffraction pattern is concerned so, but suppose I tilt the this sample a little bit here. You know that in the diffractions spots essentially we have a streaking which is perpendicular to in these this a direction it is there depending upon the thickness of the sample.

So, the Ewald's sphere if you consider it either it passing through the spots and through some of the spots it will be stilled cutting this streaking. Even if I tilt the sample by 10 degrees plus minus 5 degrees, still some portion of the streaks will be cut by the Ewald's sphere. So, we get the diffraction pattern. So, diffraction pattern remains stationery we see it whereas, the inelastic incoherent scattering the source is within the sample. So, if I tilt the sample the source is also shifting with the sample. So, because of that what happens is that kikuchi band will shift when we tilt the sample, but the diffraction pattern remains stationery. That is why the tilting of the kikuchi band is very sensitive to sample tilting we can utilize this to find out the deviation from Bragg angle and also we can use that to orient the sample correctly and the separation between them is very accurate because the Bragg angle is satisfied exactly at this particular point theta value. So, this could be used to find out the lattice parameter very accurately, these are all the 3 applications of kikuchi diffraction is this clear.

Student: I think he was asking whether the kikuchi band is also appear on the back focal plane only.

Yeah everything.

Student: Not on the Bragg angle.

See in an imaging what we do what we do it is that, if I use this back focal plane as the object for the next lens I will get the diffraction pattern on the screen. If I use the image plane of the sample then I will be getting the image this, this is the type of a ray diagram which you people are familiar with right.

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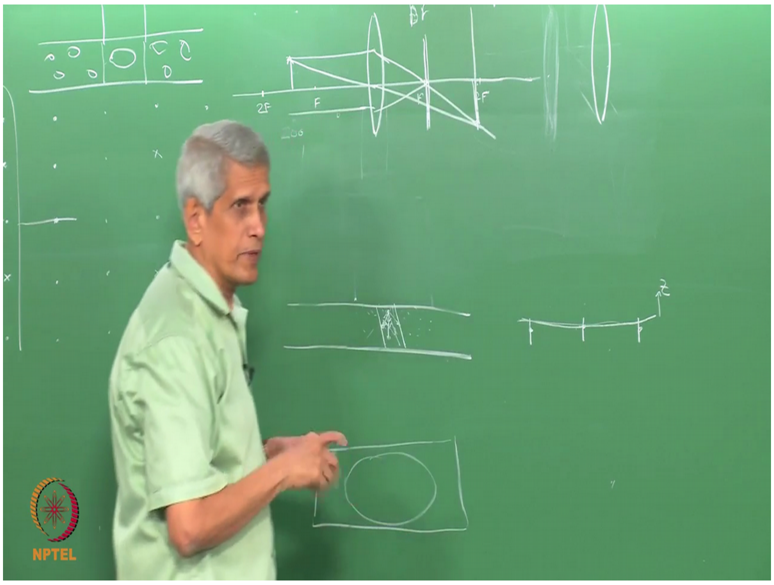

This is how it is drawn right and this is all paraxial ray consideration only I am drawing it, this ray which comes like this, this will through the focal point correct it will come and the ray which passes through the chief ray where these 2 meet we have the image correct and which is this plane, this plane is the back focal plane this is the image plane.

Suppose I keep a lens here, for this lens for the distance which is adjusted in such a way that this place becomes the object then what I will get it? The diffraction pattern on the final screen. Suppose this lens instead of keeping it here I can keep it somewhere else here. So, the image is the object then what it will get I will get a magnified view of the image. So, this lenses have to be moved in the case of an optical microscope; in an electron microscope what we do the lenses are nothing, but coils through which we pass the current if we change the current the focal length changes. So, we do not move the lenses, but we can change the focal length so that same thing can be affected. This in a microscope what you do you just press a button all these thing occur, but essentially all these changes are automated in the system is it clear.

So, so, far what we have considered is essentially the various types of diffractions these two. So, parallel bema we have considered in the parallel beam if incoherence scattering takes place what will be it is effect which is kikuchi diffraction; and another thing which is similar to kikuchi diffraction which has been seen that is what as essentially in the x-ray diffraction which is called a Kossel pattern we will come to it now.

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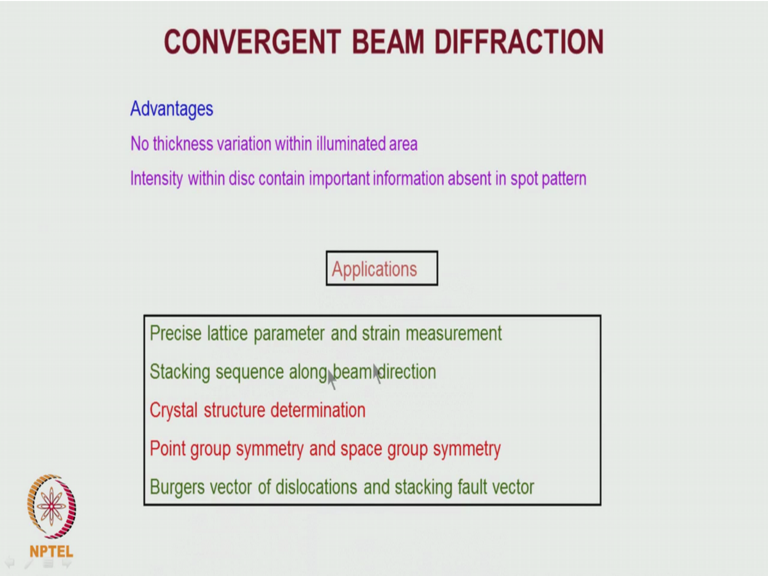

This we call this we will come back later I just mention what all applications applications are precise lattice parameter determination, crystal structure determination thickness of the file could be measured accurately point and space group could be determined. I will just give just a brief idea about some of these aspects especially the point groups symmetry on space group symmetry is a really a tough part of it which I will not go into detail, but I will mention, but the others I will just mention.

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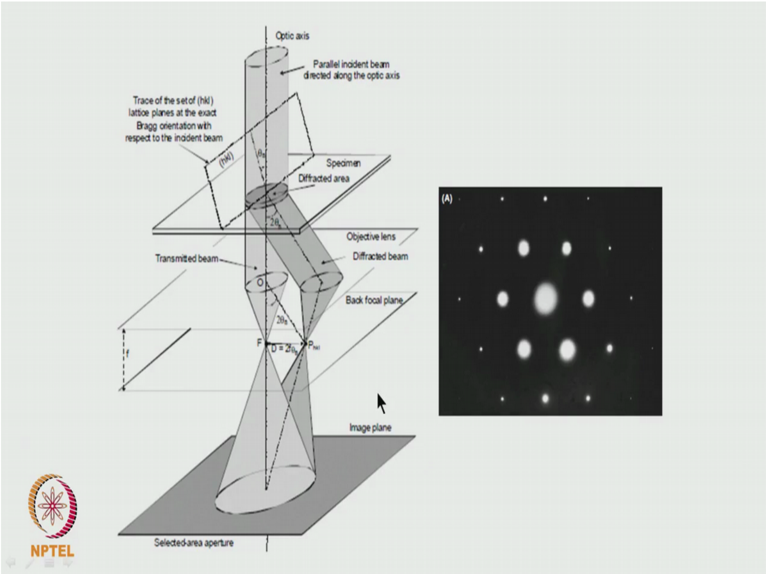

See this is just a ray diagram which shows parallel beam which falls like what we have shown here is that all the rays which are parallel to optic axis are brought to a focal plane right, but e if this is the sample from different points in the sample, there will be a variations in intensity could be there know. But still when they are all focused to the point you are not able to see any of those variations that is one drawback of it, but you will be getting just a spot pattern like this right this is how we get a diffraction pattern with a parallel beam.

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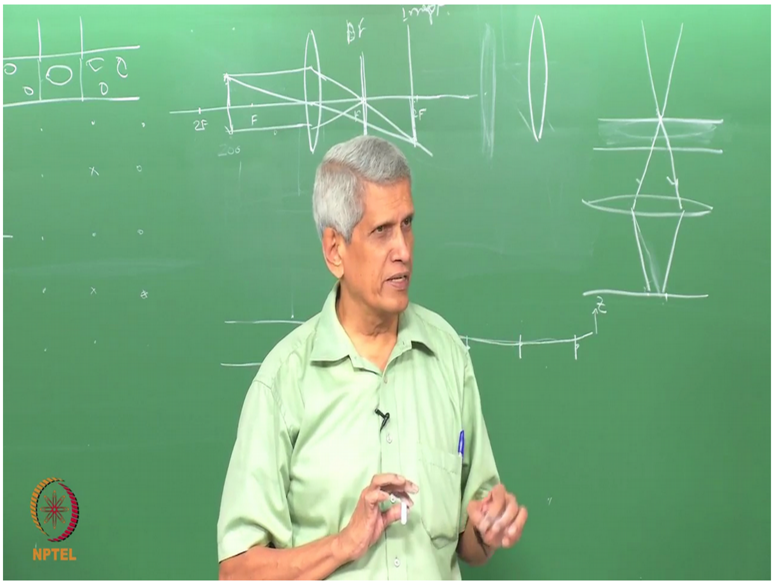

Suppose we make the beam convergent, instead of making the beam that is we have the lens I do converge the beam like this then what will happen no this is a sample I converge the beam onto the top of the sample, now what will happen this beam is going to enter into a sample like this know. So, this is the direction in which the beam will be coming and if the lens is going to be there, the lens will try to converge it this we converge it into this. So, what we will be seeing it here is since the beam is like convergent beam we are putting on the sample instead of getting very fine spot we will be getting a disc, that you can also understand that the beam which is coming like this in this direction.

Suppose as it enters it does not satisfies the Bragg condition this beam will be just coming like the full intensity this beam also will be coming like this with a full intensity. So, essentially you will be getting a disc of some uniform intensity we should get it correct if it is a suppose material is an amorphous material that is what it will happen. But if some diffractions takes place or some interactions takes place depending upon that some fluctuations in the intensity could occur. This fluctuations in intensity could be used to get information about point groups space groups symmetry then lattice parameter determination strain determination could be done, because in many gamma prime precipitates in material people have used the precise lattice parameter determination to find out how the strain varies from one region to another in the sample. Precipitate of one micron size they could map the strain distribution that is always possible.

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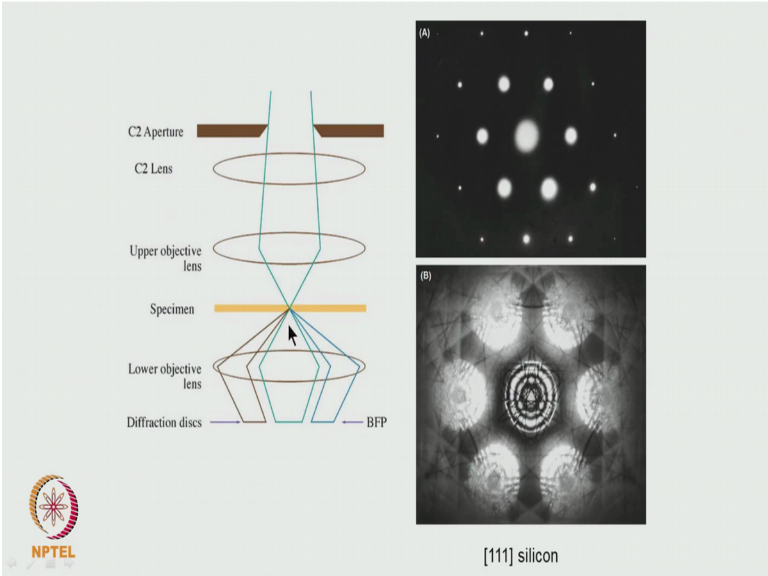

So, this is what essentially being shown, the beam is divergent now we can see that this forms and if something gets diffracted first order diffraction, this will also form a spot like this. So, now, you see that instead of getting a sharp points we are getting a disc and the disc has got some intensity distributions which are there. Some lines could be seen dark lines could be seen there are so many things which we are seeing this all this are carry information about crystal structures. The whole game here is that how to get useful information from this sort of pattern.

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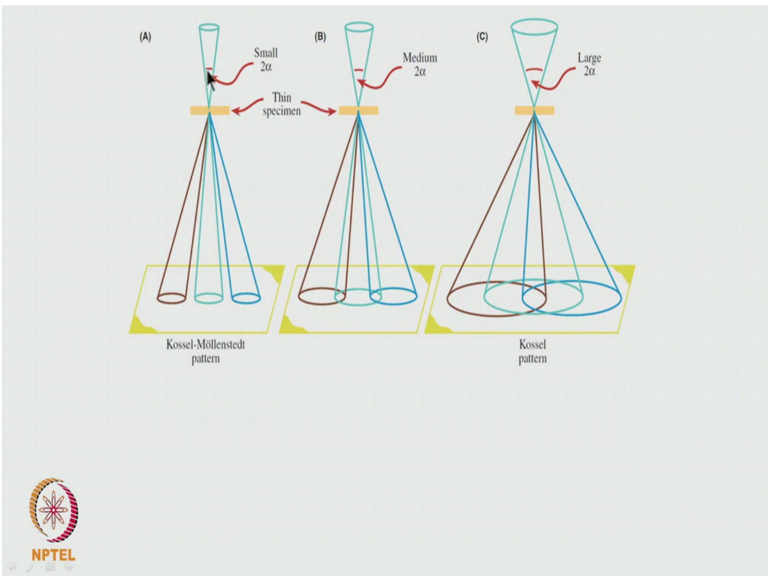

Suppose we make the beam size small we converge the beam, this is the case where the beam is converged in such a way that angle is very small. So, that the spots do not overlap and I can change the convergence to the large value, so that if I make the beam more and more convergent the width of this will increase. So, the diffracted spot and the transmitted spot can touch each other or if the angle is being made very large then what can they can overlap also, when they do overlap that sort of pattern is called as Kossel pattern. This is one technique this Kossel technique which is used in x-ray.

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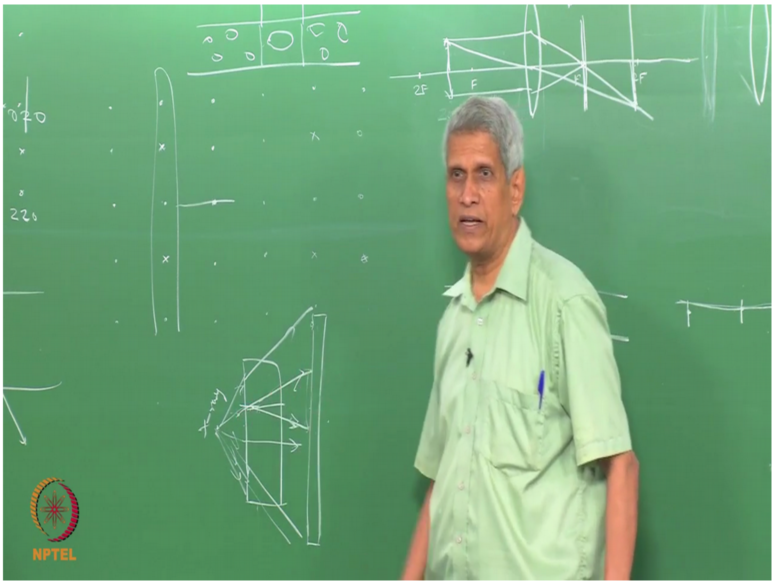

Suppose I have a sample here, I put a divergent beam of x-ray here keep it here, the beam is diverging like this as close as to a sample then what will happen? Will we get a diffraction there is this is x-ray source which is kept very close to the sample and the beam is divergent because normally you are used to seeing like parallel beam what will happen in this case.

Student: Diffraction occurs.

Lecturer: Diffraction will occur within the sample for planes which satisfies Bragg angle; others what it will happen the beam is coming and suppose I put a photographic film here or nowadays you do not use photographic film you use an image plate like for a taking chest x-ray. If you go to radiologist they have a film know such image plate I put it behind it then what it will happen is that all the rays as such it is an amorphous sample it should be coming and falling on this.

Suppose there is a plane which satisfy Bragg condition, then what it will happen is that in these planes since it satisfies one region where over the background excess intensity will come here there is a reduction reduction in intensity, and this separation is now very large because we are using a divergent beam. So, the distance which we can measure is very sharp lines you get it and the separation between them can be used to find out lattice parameter. You think this technique we can find out lattice parameter one into ten to the power of minus of 5, it is one of the most accurate technique to find lattice parameter using x-ray you could I do not think in a conventional diffraction diffract meter you can find up to a fourth fifth decimal place you can find out using this technique this one can done exactly that same thing is what is happening in this also the beam is being made it is a because it is a divergent beam. The beam though it is converged onto the sample what happens within the material from point it is a divergent.

Student: (Refer Time: 48:59).

Monochromatic beam which is coming correct.

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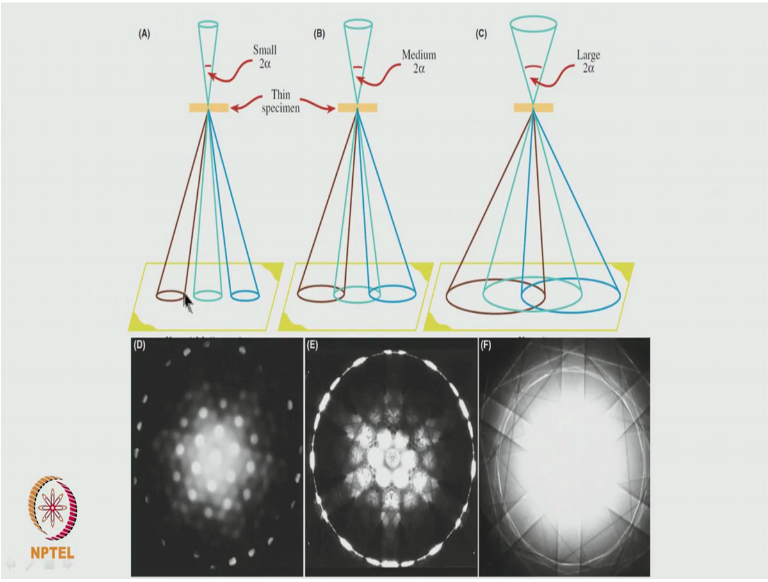

So, if you look at the spots which are corresponding to it, when the convergent angle is small we will be getting pattern like this and now you see some pattern which corresponds to the first order. Then if we increase the angle of convergence here they are almost touching each other this is the way the convergent diffraction pattern will look like if we make it all overlap this is the sort of pattern. All these type of patterns various types of patterns are used to find out point group and space group symmetry.

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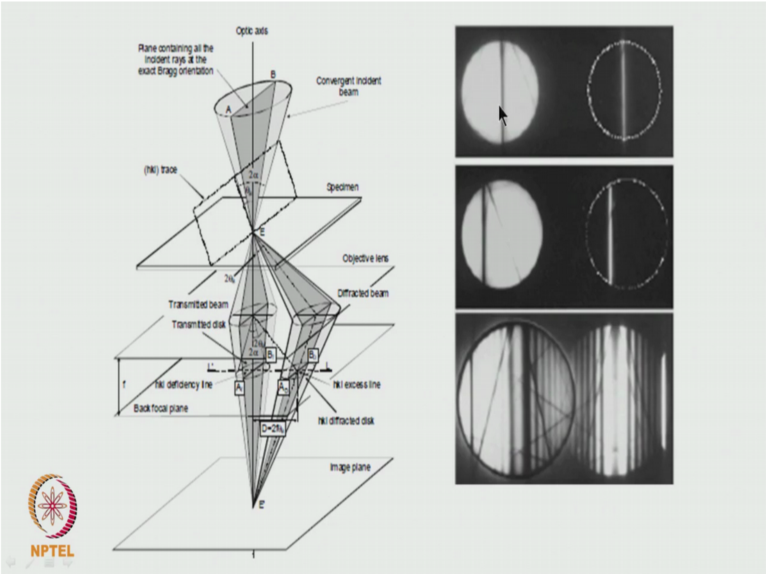

See here I have taken a case the same ray diagram which is being shown, it is a beam which is convergent onto a sample. It is a cone and the angle of the cone is such that it is larger than the Bragg angle for a some planes which are parallel to it. If it is larger than the Bragg angle what will happen is you will be getting a intensity of the spots then in addition to it the when it satisfies Bragg angle from that lot of scattering has taken place. So, what will happen to the intensity in the diffracted spot you will be getting a line in the transmitted spot.

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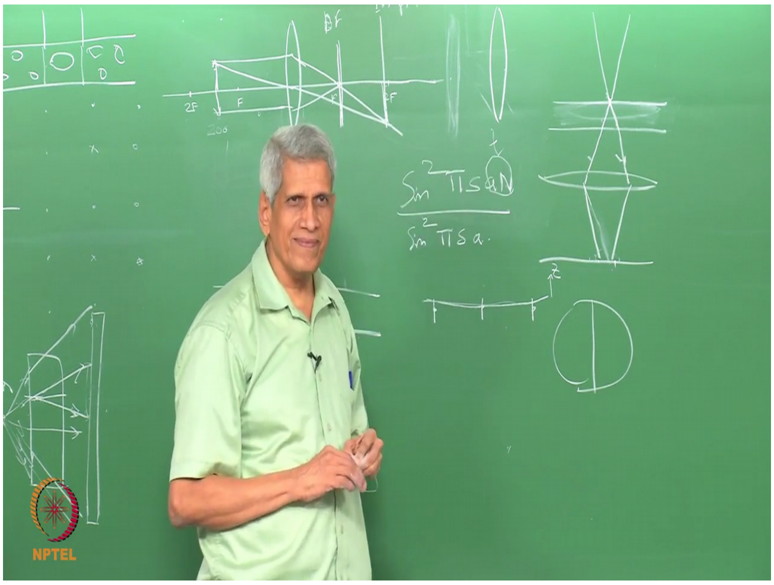

Now, in this ring you will find that the there is a reduction in intensity which will happen. This is exactly like a kikuchi diffraction kikuchi diffraction also this what you concern know divergent beam which falls only a planes satisfies the Bragg conditions ok.

You see this you look at this one, it is a two beam condition because there is only one plane which is giving rise to

Student: Because this transmitted.

This is the transmitted beam almost uniform intensity, at the center you have a dark line and corresponding to it in the diffracted one the intensity is maximum which correspond to x axis. So, if you measure this separation this will tell you exactly what is going to be the lattice parameter, but from the spot when you see spots have always some finite thickness; however, fine they are focus. So, measurement error will be high and when I tilt the sample then what happens is that, this diffraction plane is getting tilted. So, this spot will also shift that is exactly what is happening. But in many of that samples this is only with respect to one beam which is considered; quiet often not only this we get sort of a French pattern which we get it within the sample.

Why this French pattern arises? The reason is I had given an assignment to find out the intensity of the different shape pattern correct that effect how does the shape pattern what is the formula for the intensity yes still we sin squared pi s into a into N, pi s into a comes correct a is nothing, but the number of unit cells which are there in the is a direction which you take it. So, this should become t right that can be considered thickness of the sample, what is s into t.

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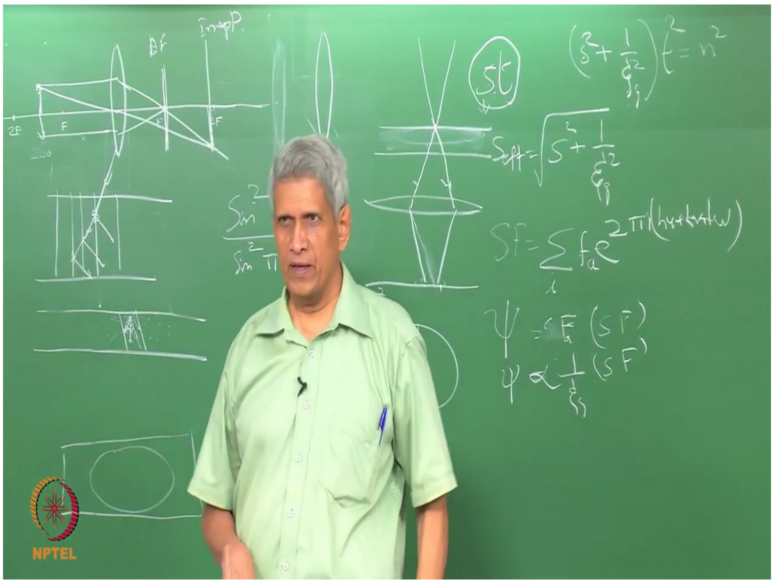

So, suppose s is the deviation from the Bragg angle, suppose this s into t s becomes 0 then what will happen this term one because (Refer Time: 53:23) you have to use it and this term can be made 0 right 2 different ways, this product also could be equal to some integer s into t is it not? This s which we considered was a deviation from the Bragg angle that is if a finite size of the sample is there delta k in the reciprocal space there is some extension in which the broadening of the peak occurs, and where is the first minimum takes place that is what it corresponds to the that has corresponds to that value.

Just I will jump a little bit which I will talk about it later is that this s is in the kinematical condition which consider. In the dynamical theory this s is written as the factor called as s effective s effective is nothing, but root of s squared plus 1 by written as psi g square what is psi g psi g is nothing but which is called as an extension distinction. I do not know if you have thought about it you would have got a feeling for what psi g is because I said as the sample is very thick as the beam enters into the sample the intensity the beam gets scattered in the diffracted beam.

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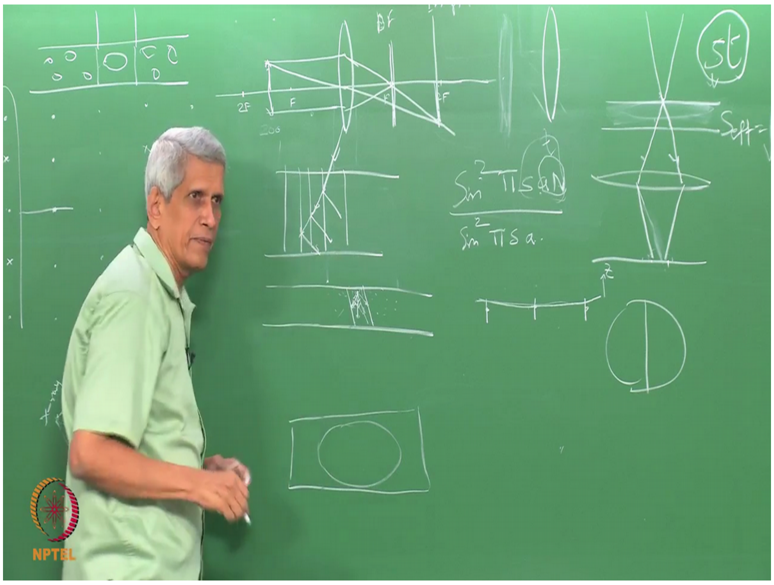

Similarly, the primary beam also like if suppose this is the sample, that they the beam enters like this it gets scattered these are all the planes are there know as it comes here again it gets scattered in this direction, again it gets scattered in this direction right when it gets scattered at some distance into the sample the intensity of the beam will become 0 that distance in the crudous way if you define that is called as the extension distance. That extension distance depends upon what sort of atom which is going to sit here, suppose it is aluminum for the same beam the scattering intense the scattering of the beam will be poor because the atomic scattering factor is small.

Suppose instead suppose I have uranium here, the scattered intensity will be more; that means, that as the atomic number is that increases the extension distance size g will be getting smaller is that clear? Now let us talk about scattering this one structure factor what is structure factor? Structure factor equals 2 pi I h u plus k v plus l w you write it know if f A become large what happens.

Student: (Refer Time: 57:01).

The scattering for structure factor scattering factor will increase what does the scattering factor say? It says that how much is going to be the intensity or the amplitude of the scattered wave. So, amplitude of the scattered wave increases if f A increases; that means, that f A the atomic that is the structure factor and extension distance are inversely related you understand that. What exactly relation we will come later, but now we have got some idea of that if the structure factor is going to be high then the more scattering will take place as the beam enters. So, psi g will be small. So, they are inverse relationship this much is clear.

In fact I can write it in a very simple form that this psi equals structure factor into I put it as a f A into shape factor right this structure factor I can write as equivalent to 1 by psi g some other constant terms will come proportional to structure factor this way also we can write it that is what essentially will happen this. You will see it later you understand this what this psi g is; that means, that if I use the dynamical theory consideration and instead of s write as s effective this term will become s square plus 1 by psi g square into t square should be equal to some integer and square know for which the intensities will become reduced.

That means that either if the thick if the thickness varies or if the no not the extension distance, if the deviation from the Bragg condition varies both the effect will be to give raise to some fringe the black and white fringe has to come. So, these fringe which it comes is because here when the beam enters this satisfies when in when this plane satisfies the Bragg condition there s equals 0 correct, because perfect Bragg condition is being satisfied and all other ones though the beam is all falling on to the same region, but it is with different s. So, that will give rise to a fringe pattern this is a fringe pattern which you get it. In fact, this equation if we know the material which is there if you know psi g, this expression could be used to find out the thickness of the file this is what it is being done.

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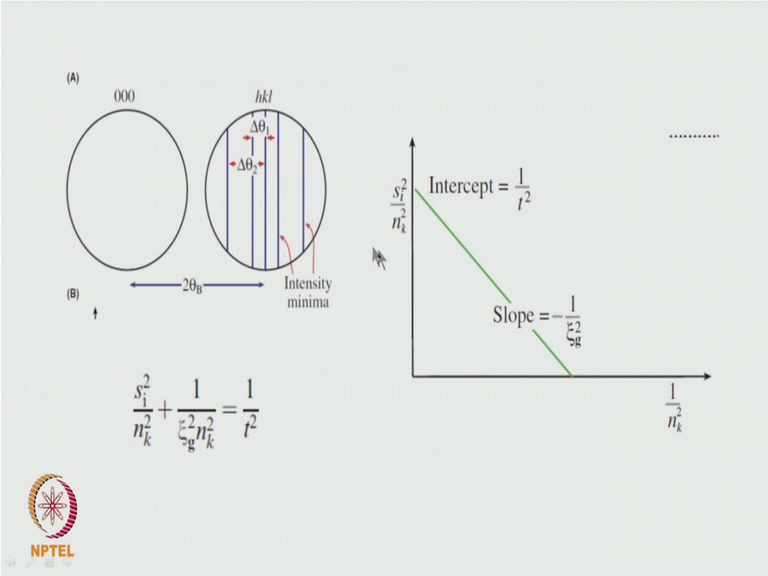

There is looking at a fringe pattern like this finding out what is the if we know the lattice parameter and this distance, I am only just this is the formula which is used and there are ways to do it I am not going into a detail which you can see it from this you can study it later. Essentially if we try to plot S i squared by n k squared because this is only the mathematical jugular which we are trying to do it versus 1 by t square the slope of it will be 1 by t square from which the thickness of the file could be determined because for many applications.

Suppose I wanted to find out the dislocation density in a sample what I should do to find out the dislocation density if I have to do it I can see the dislocation how they are distributed, but if I do not know thickness of the sample how will I find out because we should know the volume of the sample know look at the area where the beam has fallen that defines the area, but unless we know the thickness. So, many applications we require the thickness of the sample accurately these technique could be used to find out the thickness of the sample is this clear. So, the basic philosophy is just how the s when it changes because these expression when you are familiar with this is what the intensity it gives the, but depending upon the variation of s r t.

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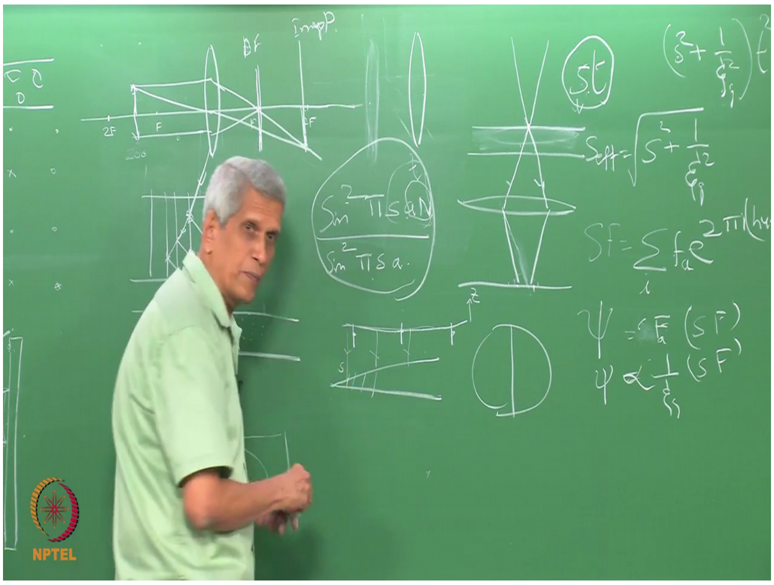

Similarly, suppose s remains that same if the thickness of the sample changes like suppose we have a wedge shaped sample the beam is falling at some particular angle, but with respect to the diffraction plane it is satisfying some value of s. But the thickness of the sample is changing know as the thickness of the sample changes what it will happens is that, we will be again getting a fringe contrast this I will come to later and show you some examples where you can see fringes near the edge of the sample all samples invariably you will be seeing it, that is because of this effect that is all coming from this expression of the intensity. In fact a similar form expression only will come after dynamical theory also, but some of the terms like I just have told you that instead of s this is the way will come these are all some modification which will come in those expressions.

Now, an another effect which it can happen is that, whenever beam enters onto the sample the Ewald’s sphere whichever that spots which it cuts those are all the only spots which will which will see as a diffraction pattern correct know.

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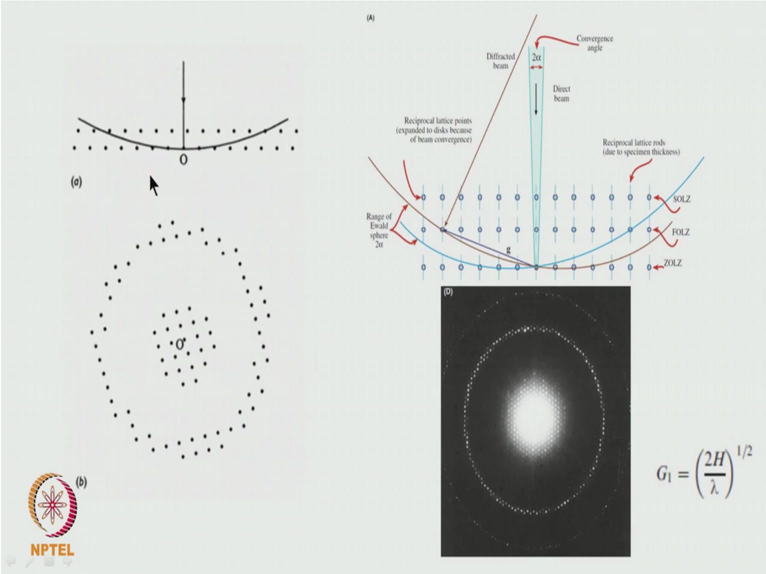

suppose I make the camera length very small that is distance from sample to the screen very small, then what is going to happen is that in the same area instead of only the central spots which are enlarged now because you can see that some of this spots are also being cut by the Ewald's sphere they will also appear. So, this is the 0 th.

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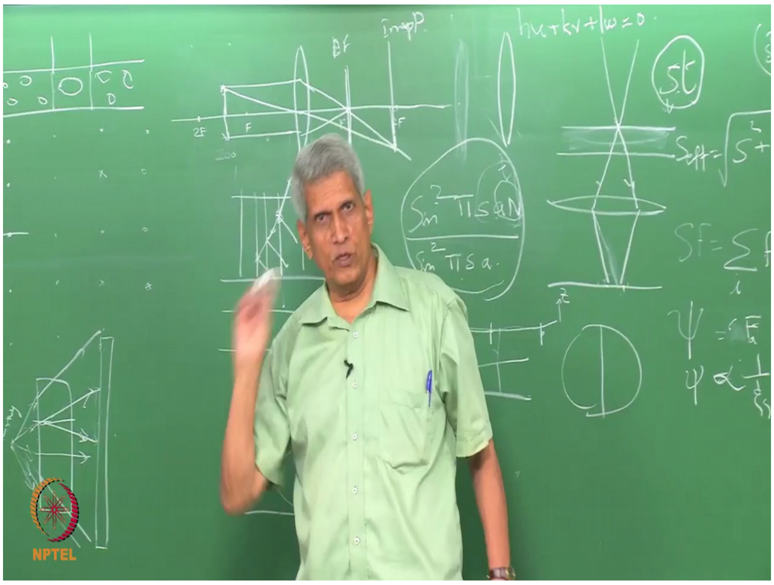

So, the one which corresponds to this spots to the zeroth order lavezone or for which we write h u plus k v plus l w equals 0 ok.

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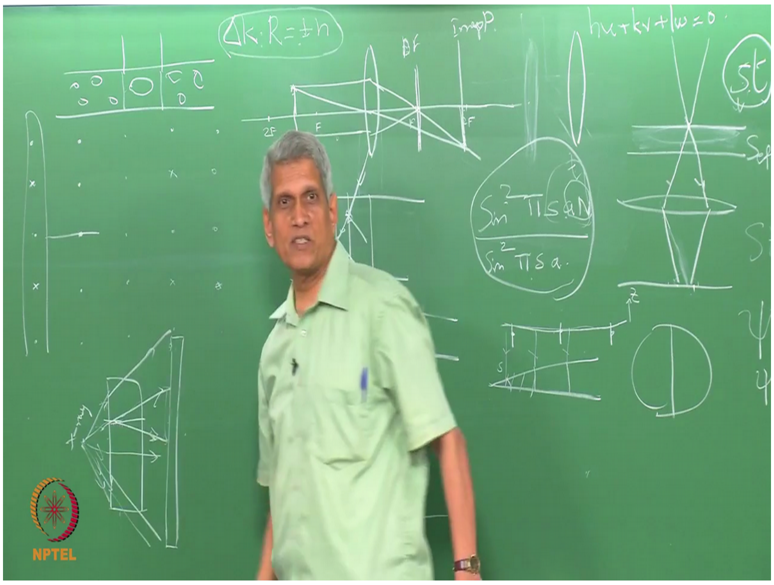

This is also nothing, but what we have written the when we start at the class itself equals plus minus n. This all the various interpretation of this expressions only when n becomes one then this is the first order n becomes 2 it is the second order that is nothing, but the reciprocal lattice which you have constructed for a simple cubic structure itself or an FCC if the beam is falling along 0 0 1 direction if you see it, see the plane which corresponds to the passing through the origin that is the where it will be satisfying the zeroth order lavezone condition.

The one which is the next plane like this plane it will corresponds to the first order the next one will be the second order like that it will happen. So, when we reduce the camera constant, we can get first order planes also and if we index this and try to superimpose onto it, then looking at that structure we can find out what is the type of Bravais Lattice all this information we can get it; that means, that essentially in one diffraction pattern we have got the full reciprocal lattice spots corresponding to full reciprocal lattice spot is risk already come is this clear.

Student: Super imposing means super imposing means what.

Super imposing means that because since only these touch we have got these spots know suppose we know this is the separation between them, now I can extrapolate it by putting this spots at regular intervals this distance it has to come which they are not appearing it because their own satisfy the Bragg condition. If I do it right at the center I will be getting the spot which is corresponding to it. Suppose this central one corresponds to with respect to a reciprocal lattice which we are constructed the unit cell the first plane the on which comes above that will be corresponding to the next plane that way you will be able to do that know that is how you do the analysis is it clear ok.

So, that is what I am showing it here. So, that is what I am showing it here how and in a kikuchi diffraction pattern happens we are making the beam little bit convergent; that means, that it is not a one of Ewald's sphere corresponding to each direction you can have a series of this one. So, over a range of value in which it curve so, first zeroth order first order second order all the spots we could get it, but generally what happens is that to get all these spots it is not that easy. Because as we go to higher diffraction which are taking place, the vibrations of the sample will come into play atomic thermal vibrations will come into play in such cases what is normally done is that when you wanted get second order third order and all you cool the sample to liquid nitrogen temperature then this vibration thermal vibrations will get reduced then we will be able to get a sharp pattern.

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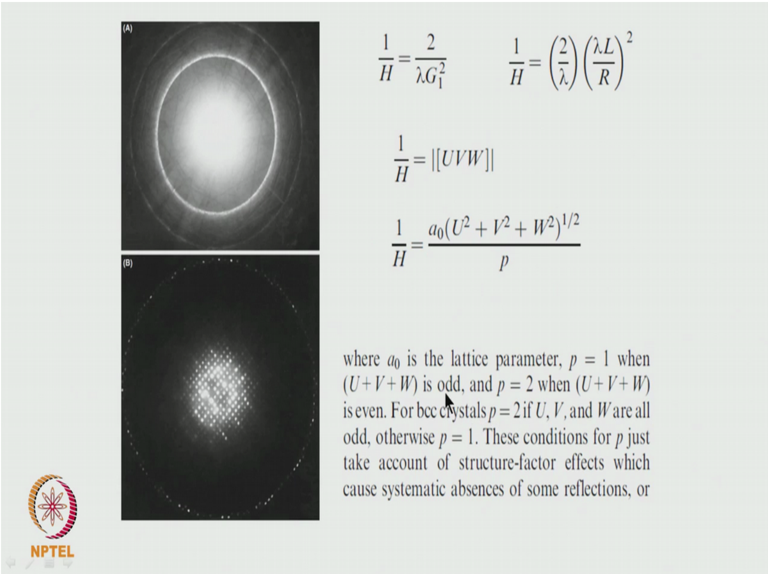

Here if you see this is zeroth order this is the first order and this is the second order, and another thing which you can see it is, if you see here this is a we know the Ewald's sphere is radius right if we can measure this distance because from this spot the center if I measure I get this distance [FL]. So, where this the ring cuts that distance I can get it, and this is nothing, but a what is it is a cart. So, for the cart the length of the cart we can find out from the geometry this all things you have studied so; that means, that if the length of the card you can find out then you can find out from here to here what is distance is; that means, that from this one to this one at what height it is going to occur you are got that information.

And then this spots if you have indexed it the unit cell in this and suppose we take a high symmetry zone axis if you get it take the diffraction pattern. So, then we have got a and b parameter here and measuring these distance we can find out the c parameter. So, the unit cell parameter could be obtained from this pattern itself is it clear. So, from this one diffraction pattern, the full unit cell parameter we can get it is it clear this is all the expressions which are given that you can read it.

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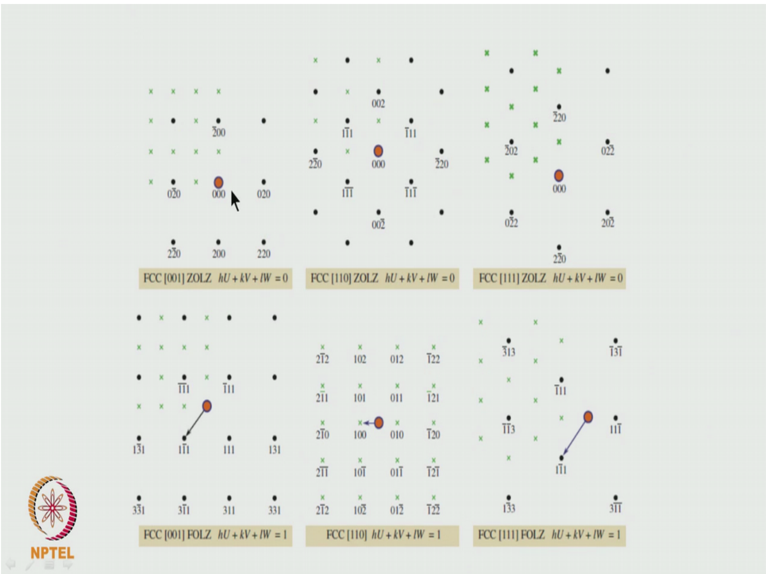

So, here what I have shown is a simple thing like for an FCC for the zeroth order diffraction pattern this is what the how the diffraction pattern looks like for a 0 0 1 zone 0 0 2, 0 2 0, 2 0 0. The reciprocal lattice section corresponding the first order lavezone if I take it, no no this is corresponding to for the 0 0 1 zone, this is for a 1 1 0, this is 1 11 type and this one corresponds to the first order lavezone how the spots will come. If I superimpose these 2, I will be getting how with the first and this one how they should appear correct.

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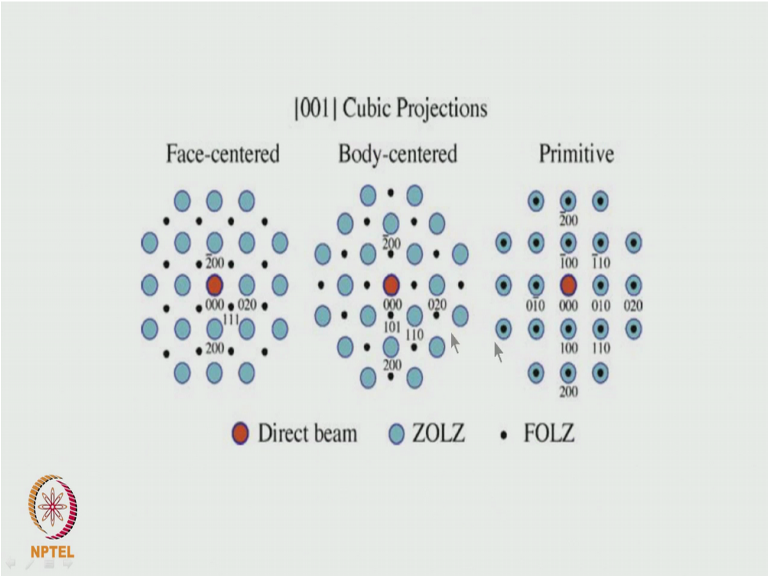

That is exactly what is being shown here. So, this is how this for a face centered in primitive what it will happen is that it will coincide here this is the where the pattern will appear then the zeroth order and the first order or overlapping. All these thing you look carefully then you will these are all very simple things 2 patterns which are being superimposed one on top of the other and once this pattern is analyzed we have the full information about the reciprocal lattice, if you have the information about the reciprocal lattice about the corresponding Bravais Lattice you can get that information.

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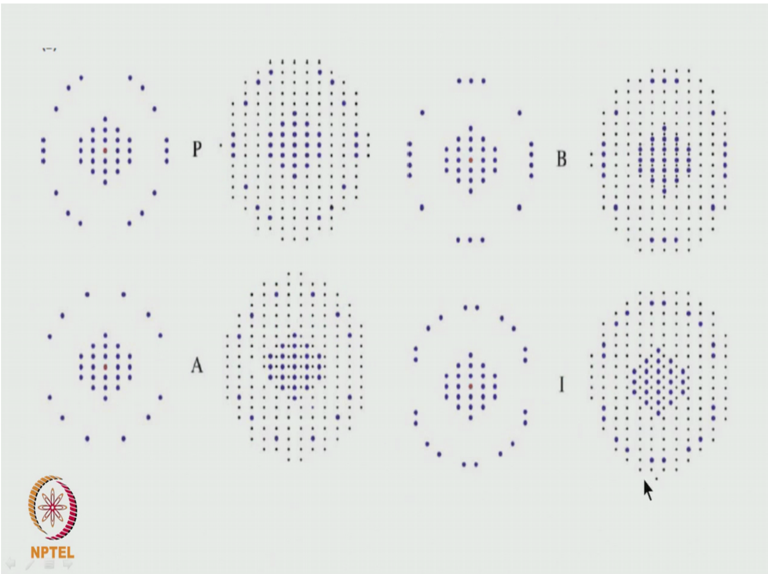

And this what exactly it is being shown this is what how the diffraction pattern looks like what you get it and then when you know this distance you create a lattice of this type and just overall expand it and superimpose it then you can make out that this is for a primitive lattice. So, when you superimpose it this is how the pattern should appear. If it is face centered cubic lattice this is how it will appear in the diffraction pattern which we get it when we do a super imposition this is how it appears.

Body centered lattice this is how a pattern will appear for a 0 0 1 zone, when you superimpose it happens this is for no this is b centered this is the body centered like this these are all generated a patterns, then you can compare it with it and match and measure it that way you can do the analysis this way we can identify the crystal structure you understand that.

What I will do it is I will stop here, in the next class we will take it and complete this.