Electron Diffraction and Imaging

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Lecture – 10
Diffraction – 01

I welcome you all to this course on diffraction and imaging, before going any further I would just like to ask you what have you understood in the last class, because let us have a recap of what has been done and then we will proceed from there. So, what did we study in the last class.

Student: (Refer Time: 00:35) a reciprocal lattice.

Reciprocal lattice what did you learn in this reciprocal lattice.

The relationship between the real space and the reciprocal space; what is the relationship between the real and the reciprocal space which you have learned?

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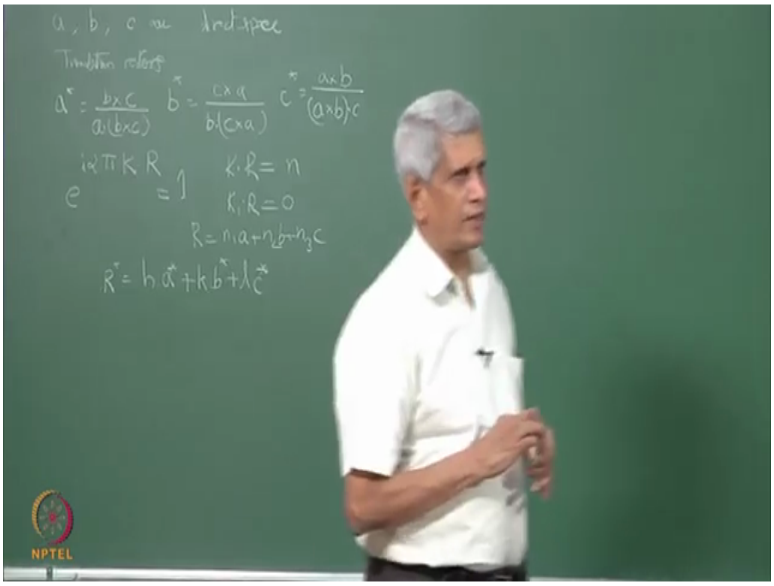

If a, b, c are translation vectors in I call it as a direct space, this is all constructed with respect to a primitive lattice correct the lattice is considered a primitive lattice, then the reciprocal space this is the relationship which c cross a, equals a cross b, dot c correct then what is the basis equation from which this was derived; what is the basic equation from which we derive this x relationship.

Student: (Refer Time: 02:18).

That is essentially e to the power of i 2 pi K dot R should be equal to 1 correct; or K dot R should be equal to an integer correct. This was the basic relationship from which this relationship between the real lattice and the reciprocal lattice has been derived.

So, from this relationship what one can make out is that for every vector K in reciprocal space, there are set of vectors in real lattice in different planes which satisfy this condition right. Like it could be that K 1 dot R could be equal to various value 0 1 2 3 like that any value which it can take right; similarly we can have K 2 is an another vector in reciprocal space, similarly for every vector in reciprocal space we have a corresponding lot of vectors which satisfy this condition; that means that all the vectors which satisfy this condition R equals b plus n 3 into c, this set of vectors R when they satisfy all these vectors are perpendicular to this vector K 1 correct that is what this indicates.

Then the other expression which we have derived is that the vector in a reciprocal space, if it R star that can be written us h into a star, plus K into b star right l into c star this way we can represent all these vectors, but both the vectors in real lattice as well as the reciprocal lattice are represented in terms of orthonormal coordinate system right that is the way we define this vector.

Let us just take an example with respect to a simple cubic lattice if we take it that is not simple cubic FCC lattice if you take it how are the lattice translation vectors of the real lattice of the primitive lattice is represented.

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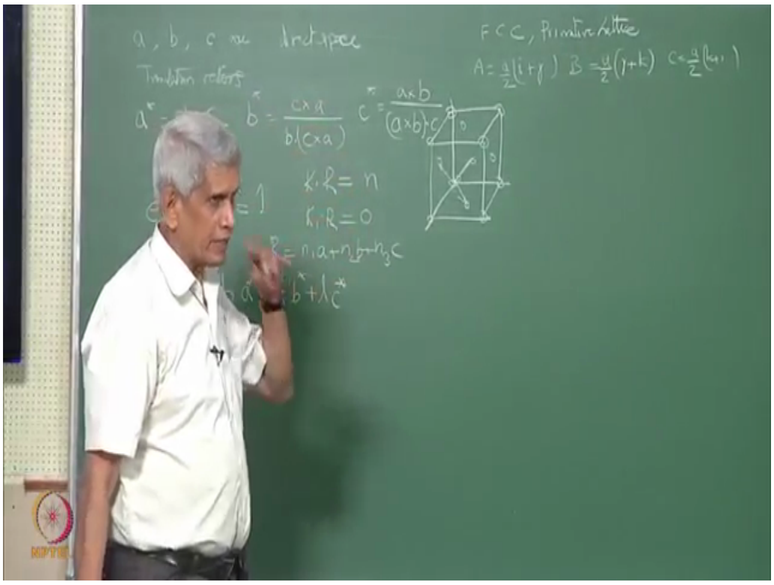

FCC, if we take it will be that is a vector A I will just write it as further primitive, that is for primitive lattice j plus k; c is equal to 2 into k plus i, this is how the vectors will come n a that is essentially if you take an FCC lattice, and this are all the position lattice points are there. So, this one this vector this vector these are all the 3 primitive translation vectors translation further primitive lattice of FCC.

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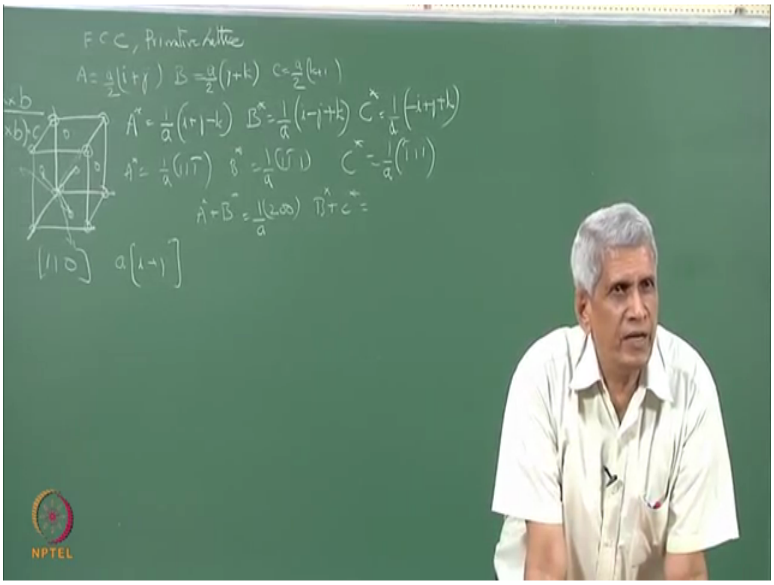

When you use this formula and try to find out these vectors this will turn out to be 1 I am just writing in, but you have to cross check it, it will turn out to be 1 by a, 1 is i plus j minus k, c star will be 1 by a into minus i plus j plus k, this is what the vectors will turn out to be.

Student: (Refer Time: 07:12) by j by 2.

Um no when you take it, it will just turn out to be this value; what this a star in the reciprocal lattice this means this vector.

Student: BCC.

No, BCC is a structure what essentially this because this represents the translation vectors of the reciprocal lattice which we are looking at it for the primitive lattice.

This will be nothing, but 1 by a, normally conventionally how do we represent a vector 1 0 0 right. So, if you write it like this this will be 1 1 bar correct this will be 1 1 bar 1, 1 by a, this is how it will turn out to be correct because when we write a vector are any direction in a lattices are 1 1 0, it actually means if a is the lattice parameter this should be a into i plus j this what it exactly means correct. So, essentially using that same logic this is what essentially turns out to be.

So, this defines translation vector of the unit cell of the reciprocal lattice, when this is defined how this will turn out to be we can mark this one n a all these one 1 will be going from here into the next cell in this direction, another will be going into this direction, another possibly will be going into down into the next one that is how this vectors will turned out to be and the magnitude is going to be 1 by a of a. So, once we know this basic vectors all other reciprocal lattice points, we can find out by taking a combination of this correct is it not? So, these are all the basic translation vectors if we take combination of it we can find out; if you do that what it will happen you take A star plus B star it will be.

Student: 200

200 correct; similarly you can take b star plus c star like this if you do you find that the reciprocal lattice vectors which are there are 0 to 0, and the other 1 will turn out to be 0 0 2. Automatically if you look at it the structure factor consideration which you look into it is already taken care of.

So, you take whatever be the combination of all these vectors this and you can choose any value of h k and l you substitute this and (Refer Time: 10:50) finally, what you are going to get it is that various reciprocal lattice points. So, what I wanted to emphasize at this point is that the reciprocal lattice point which has been constructed using this relation automatically takes care of the extinction rules if we construct it with respect to the primitive lattice that is all which has to be done, that is one important point is it clear? 1 0 0 will not come in this because always we have to when you take that additional the addition is always taken with respect to integer values only because h k and l has to be an integer correct because I had explained earlier about how to construct and all the relationship in detail in the last class.

So, using these vectors we can construct a reciprocal lattice the same thing which we can do it is that what is the geometrical meaning of this vector algebra; what we have done is essentially if we take any lattice, we can construct the reciprocal lattice also in an another way that geometrical construction.

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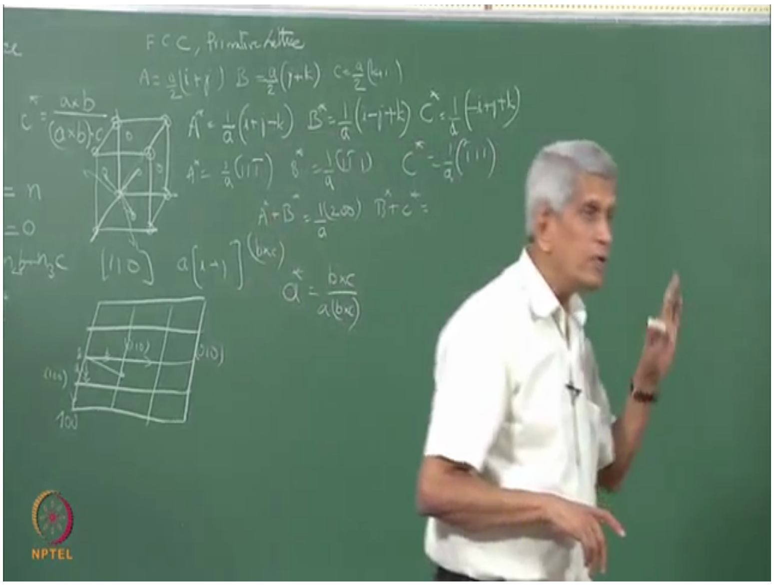

Suppose we take that the lattice itself is the 2 dimensional lattices, which we are considering it correct. You take this as the origin then this direction will be 1 0 0 this direction will be 0 1 0, the third direction is perpendicular to the board and assume that we are keeping the similar the same type of a lattice 1 on top of the each other to generate with a lattice parameter and here suppose this is a is the lattice translation vector here and you take this to be the b. So, what is this plane? This plane is nothing but a 1 0 0 plane right this plane will be 0 1 0 plane, correct, is it not ok.

What is the plane normal to this 1 0 0 planes it is essentially drawing a. So, this is the plane normal, what will be the magnitude of this value? This will be there is if this angle is theta it will be a cos theta that is what this value is going to be is it not. Similarly what will be the plane normal to this 0 0 1 it will be essentially in this direction it will be coming correct and this plane normal is nothing, but if this is b and this is the vector c, b cross c will be a vector like this correct that is the direction of the vector is the same as the plane normal.

Now what is going to be the magnitude? The magnitude is going to be essentially nothing, but inverse of the distance in magnitude whatever is the value it is the inverse of that that is what it will turn out to be correct. See this is this direction is b cross c, correct this is what this vector represents correct when we write a star a star is nothing, but b cross c by a dot b cross c right what is a dot b cross c.

Student: (Refer Time: 14:44).

It is nothing, but essentially volume of a unit cell good; what is b cross c is the area of the plane also; geometrically it means it is the area of the plane.

That is I can.

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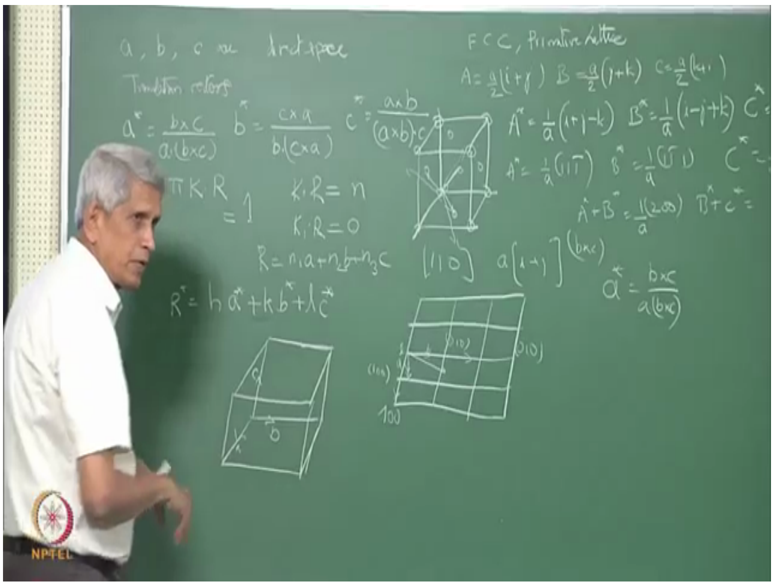

If this is a, b and if you take it c is it not. So, if that is the big area of the plane, a dot b cross c what it says it is essentially that divided by if you take the area of the plane that will be the perpendicular height. What is a cross the vector (Refer Time: 15:59) you are taking the inverse of that. So, essentially magnitude wise it is inverse of the interplanar distance correct; that is what essentially what we are taking it. So, on this direction if you mark the inverse of this interplanar distance at some point, then here also will be marking an inverse of this interplanar distance, the lattice which is generates that is the reciprocal lattice.

So, geometrically this is the way we can construct it; is this clear? Suppose we assume that there is a at this particular position at the middle of it there is some lattice point is there then what will happen? Then there is a plane which comes in between right. So, the interplanar distance is half of that. So, it is inverse is what we will be taking it, this plane will be nothing, but a 2 0 0 type of a plane, automatically this is equivalent to taking a primitive lattice. So, this way also geometrically we can construct a reciprocal lattice.

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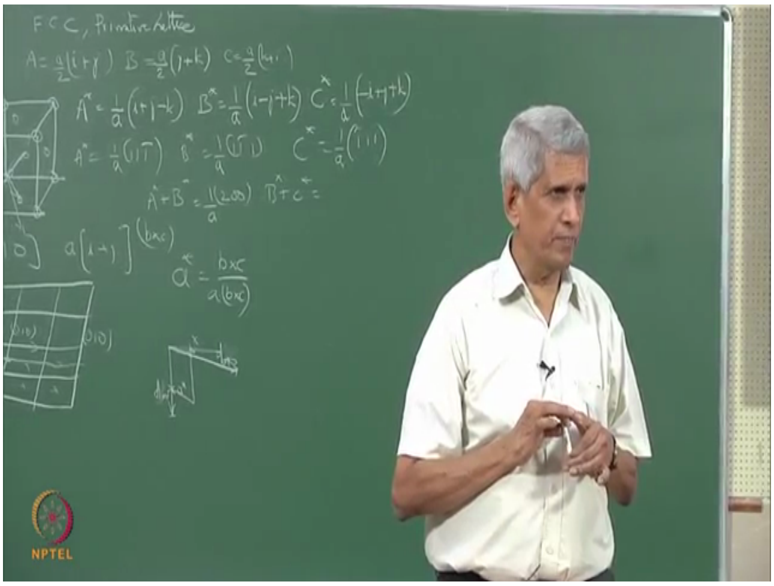

Essentially what we have to do it is that with respect to the same origin ok find out the vector suppose this distance is a and this distance is b, that is the not b I will write it as this as d 1 0 0; that is the 1 0 0 plane the distance between 1 0 0 plane, and here this we write it as d 0 1 0 plane.

So, if we take the inverse of it that inverse this is going to be larger compared to this one right. So, when we mark any point they will be in this ratio n a. So, that will give raise to suppose this point we take it as here this is the vector corresponding to a star, the other one the vector maybe corresponding to it will come here as b star, and if you try to do vector addition we have the unit cell then we can by vector addition we can generate all other points and construct the reciprocal lattice. This is the geometrical way both are equivalent; but the geometrical way for simple lattices it can be done for visualization, but it can become quite complicated for many lattices whereas the using vector algebra it is much easier to do is this clear.

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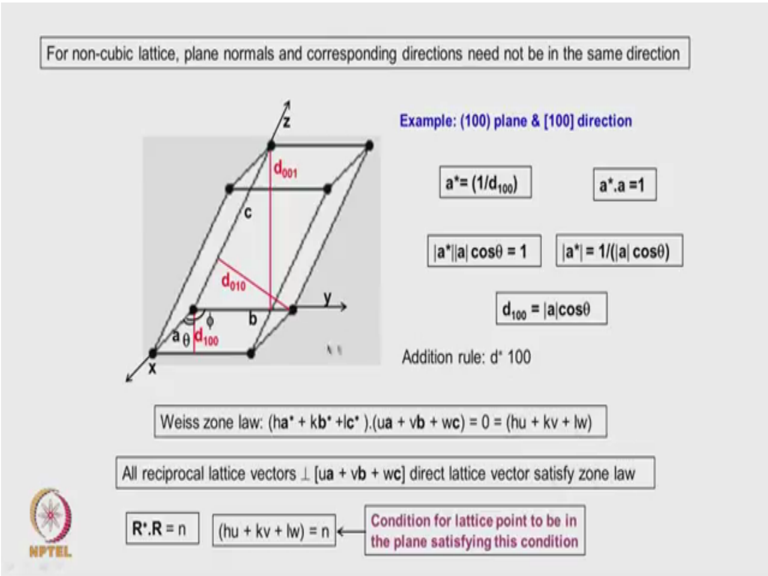

This is the same which I had shown here taking a triclinic lattice, and I have shown here what is this perpendicular distance these are all the distance between the planes, the inverse of it if it take it in these directions and draw that we will be able to; and the another information which comes if you take that R star dot R what will happen.

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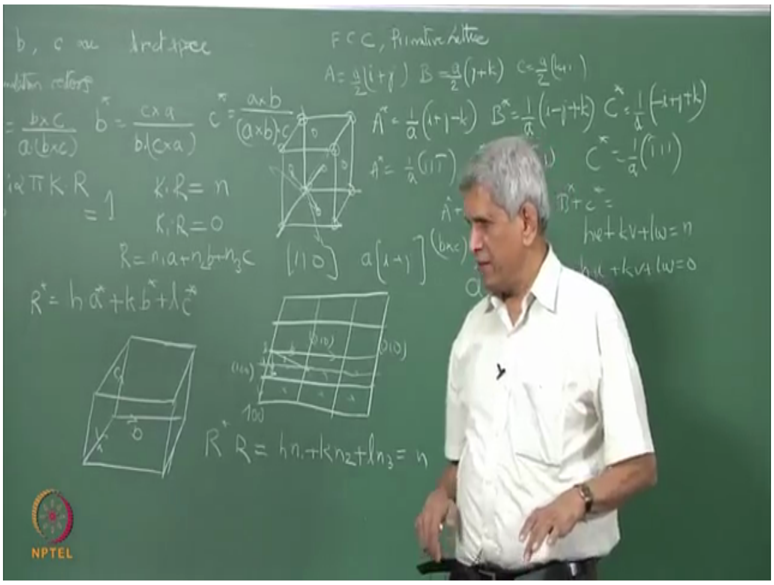

Plus K into n 3 right this should be equal to an integer, generally you find that in the books instead of n 1, n 2, n 3 for the vectors we write u v w right.

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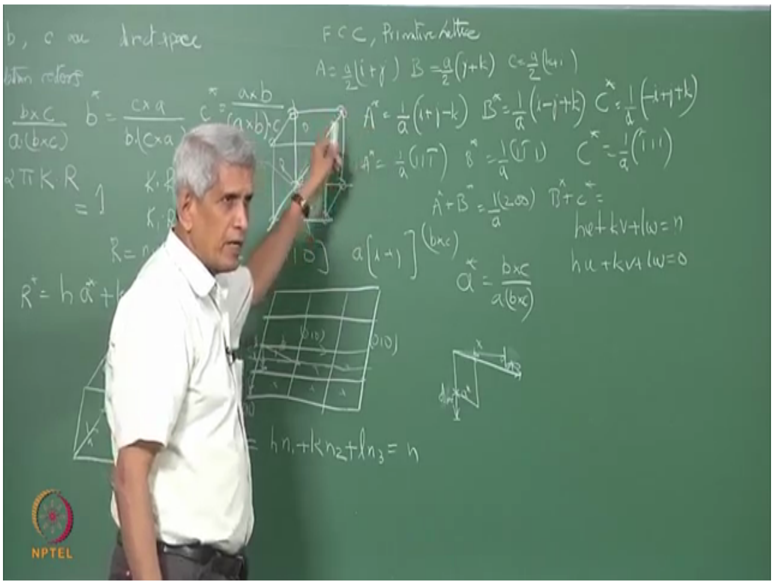

Then you write that formula h u plus k v plus l w equal to n when the n equals 0 this what is called as the Zone law right which you might have studied. And the 0 means that what we are looking at it is in the reciprocal space, the first plane is what we are looking at it. The zeroth plane when n equals 1 it gives information about the first place, then the second plane third plane like that it goes these are called as higher order weiss zones planes. Essentially by looking at these planes the information which we can get it is in the diffraction pattern, we can get information about the complete reciprocal lattice right.

So, when a reciprocal lattice is constructed for a this one the zeroth order plane is there respect to this one, the next plane is there, the next plane is there for a particular beam direction in which the beam is falling; when we get the diffraction pattern analyzing the pattern generally what we get it in the normal diffraction pattern is only zeroth order. But if you change the camera constant which I will come to later explain we can get information about the higher order Weiss zones also; that means, that in a single pattern we can get various reciprocal lattice sections information could be get in the we could get it in the diffraction pattern. If you analyze this pattern then we can construct the complete reciprocal lattice correct. So, in principle if you have the full reciprocal unit cell is available, from that we can get infinite construct back the real crystal structure that is the philosophy behind this.

So, this is essentially what we have looked at it is, is a geometrical construction. We have not talked about diffraction at all, but we said that there is a relationship between diffraction and reciprocal lattice phase correct this; what we will look at it now. What do we do in the diffraction experiment normally what is a diffraction.

Student: (Refer Time: 23:14).

What do you understand about diffraction?

Student: (Refer Time: 23:22) interference of waves.

Interference of.

Student: Waves.

Waves which have some phase relationship.

That you might have studied in optical radiation right how these waves interfere.

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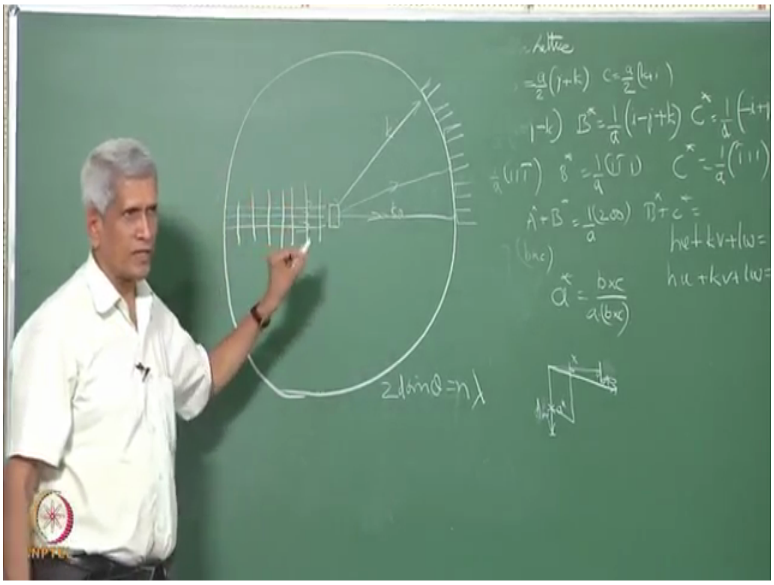

Suppose I we assume that a sample is kept here and another thing which is very important is that diffraction is essentially a like a group activity, are scattering from more than 1 point is necessary for this interference phenomena to occur correct. Suppose we keep a sample here and an electromagnetic radiation, because electromagnetic radiation can be considered as can be expressed as a wave, we assume that that is coming an (Refer Time: 24:32) and we assume that it is a coherent beam or we take that this is to be something like a plane wave which is coming, a monochromatic coherent beam is falling onto the sample surface. If it falls on the sample surface now what is it which will happen?

Student: It will either absorb (Refer Time: 24:55).

Student: It get either absorbed or.

What is absorption, what do you mean by absorption?

Student: (Refer Time: 25:09) energy electromagnetic wave which whatever the wave carries is transferred to the atoms in the (Refer Time: 25:17).

Suppose it does not get scattered essentially what happens is that if the intensity of the radiation which comes out on the other side is less than that we say that the beam has been removed, it could be due to a physical absorption or it could be due to scattering. There are many processes which can happen finally, there is a reduction when the reduction in intensity takes place we say that absorption is taking place, but processes could be different; let us not bother about it.

So, if we take we assume that this is the direction in which it is travelling. So, direction you take it be k 0 coming. Around the sample you take a sphere of radius some radius; suppose I keep a detector I can move the detector like this everywhere I am just only showing a cross section of it, if I move the detector what will happen? At some particular positions at each position if I look at it the intensity which the detector is seeing it will be different some regions it will reach a maxima, some regions it may be 0, some regions will have some intermediate value that is what essentially is going to happen. Provided the sample (Refer Time: 26:54) material when such a phenomena occurs, we say that interference of the beam has taken place. Any direction which we can take it in this direction suppose this I can take it to be k wave vector because we are choosing a reciprocal space to represent it, because we are using a wave the incident wave this is the direction in which it is coming this is the scattered wave correct, is it not ok?

Do you expect this to happen in a sample if you do diffraction? There is you allow the beam to fall on the sample surface the sample in around 4 pi at different positions on the surface of the sphere, there will be intense be maxima or minima. So, essentially 2 d sin theta equals n lambda. So, if this condition is being satisfied and there are many methods in which this experiment is being carried out; normally in the deflectometer you move the detector and also the source that is why we collect peaks at one particular point, but it is always possible that when the beam is coming in one direction and falling on to the sample, there are many directions in which you will be observing diffractions parts it is not that one position.

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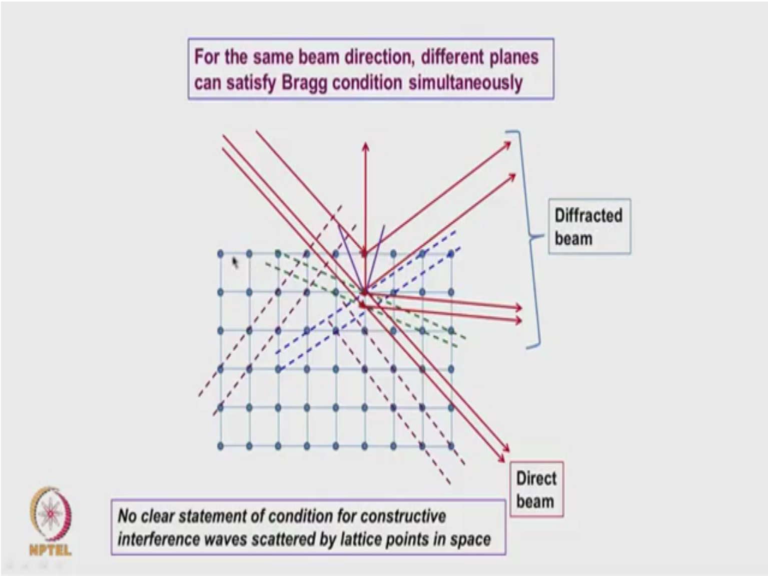

That is what essential is being shown in this particular slide; that is this is the direction in which the beam is coming in this lattice you can have planes like this you can consider; you can consider planes in this way, you can consider planes various directions you can have in the planes n a. So, whichever planes with respect to the beam direction it is satisfy the Bragg condition, we are able to get some intensity maxima will be taking place. What is a major problem about this Braggla? The lies very fine, but this equation does not talk anything about discreetness of the atomic lattice.

It is a lattice which is it is telling that between these 2 planes if the spacing between the planes is a particular value this is the angle theta which you should correspond to correct at which the diffraction will take place. But scattering is done by individual atoms correct; where are the atoms, that information does income from this expression, correct? It only tells that between these 2 planes, that is what it is talking but not about at what positions the atoms are sitting on the plane at what point atoms are sitting on the plane that information is missing from this law.

The basic derivation if we try to look at it is that each lattice point is a scattering centre, the coherent beam when it falls on to the sample surface it is scattering from each of the point, from each lattice point it is scattering in all the directions and these scattered radiation is what we are trying to collect it. Like if I put a detector here what I am trying to do essentially in this direction all the electromagnetic waves which has been scattered from every point on the atom, I am trying to measure it correct that is the intensity which is being measured. So, like here if I consider in this particular direction, all the rays which are scattered because this sample is very small is large.

So, essentially all the rays which has scattered from the various points on the sample, in this direction it is being collected. So, the intensity which we measure is essentially the intensity of the atoms scattered in a particular direction from by all the atoms in the sample correct that is the information which we are trying to look at it; will just try to find out what this value will be in terms of the incident beam radiation.

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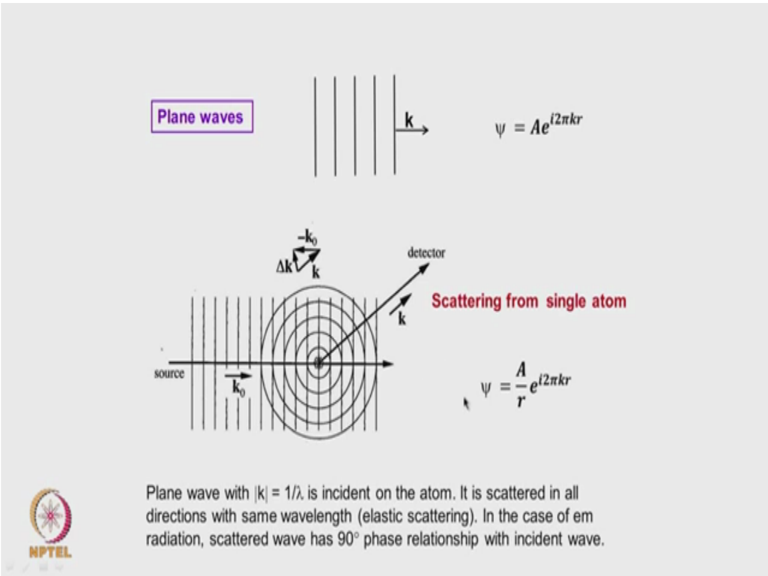

That is essentially if we consider the incident beam as a plane wave, this is essentially where the crust which we are showing it; that means, that the separation between them will be there corresponding to wavelength of the radiation correct. K represents the wave vector like the incident waves in reciprocal space and so, psi will be A into e to the power of i 2 pi k r. Here what we have talking about is with respect to this A e we have not defined it, we will not define it what it is this a can have different values depending upon whether it is an x ray or whether it is an electron beam, whether it is a neutron (Refer Time: 32:43) types there will be that part of it we will not talk about now, but essentially what is important is that wave nature is described by this phase term only correct that is what we will concentrate on.

If this wave encounters an atom when it encounters an atom this plane wave is from this point it is scattered in all the directions correct? This is the incident wave vector K 0 this is the if you put a detector we are trying to measure the intensity here then at any particular point on this circle because this circle is essentially cross section of a sphere any point what will be the intensity of that radiation? It is wave function and the intensity will be if the intensity here is i 0 it will be i 0 by 4 pi r square correct that is what the intensity at a distance R from the centre.

So, amplitude will be because generally intensity we write as psi, psi star correct. So, the amplitude will be (Refer Time: 34:00) root. So, that is what essentially is being written that is why 1 by R (Refer Time: 34:05) comes into what will be the phase factor here? It has travel from here to here if it has travel e to the power of i 2 pi k into r should be the phase factor correct at any point on the surface. So, this describes the wave which is scatter from by an atom at any point is this clear.

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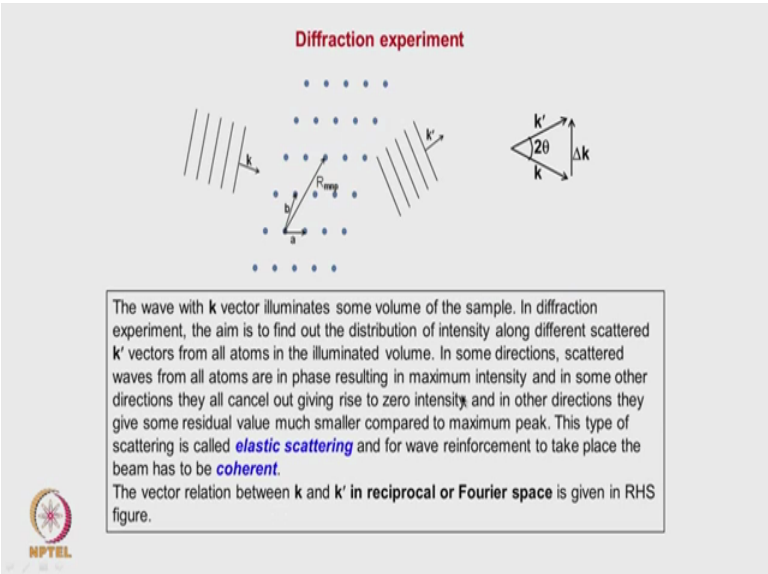

Now what we have done it is the sample contains lot of atom pole atoms are there at a periodic interval they are kept. So, if this is the plane wave which is coming and if this is the origin, we assume that at that origin suppose R equals 0 it have got the maximum amplitude. So, we try to write it to be psi is equal to some a if it ignore you can write (Refer Time: 35:14) a equals 1 if you put it, psi will be equal to 1 and then it is been scattered from here it is by scattered from here in this direction. So, in this direction by all the atoms what is going to be the phase with which scattered wave is coming, that is what he have to look at it and at any point R distance where we have kept the detector. So, we will be getting above which is scattered from this point away which is scattered from this point from this point all of them will be joining to the let us consider just 2 point this as well as this point.

So, this scattering we call it as elastic scattering because there is no loss of energy, that is the incident wave and the scattered wave was got the wavelength is not change no energy is loss and his coherent.

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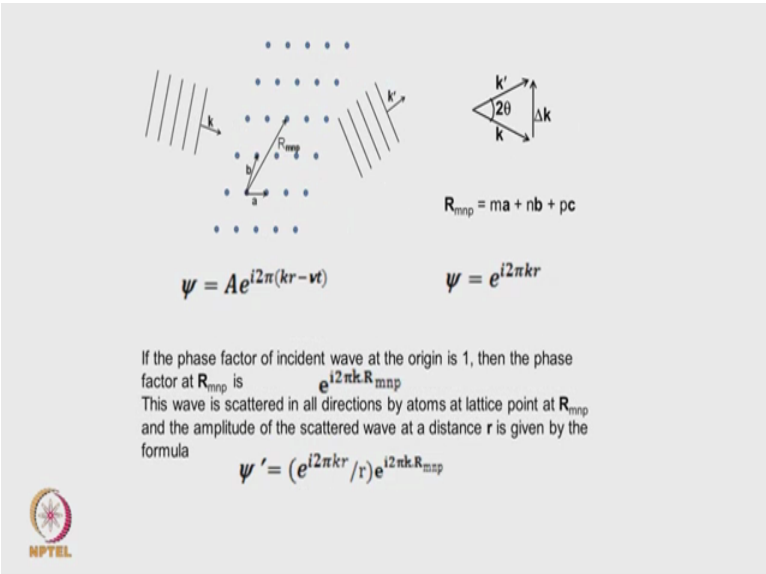

So, let us consider this particular case that is what essentially is being done. So, if it is being scattered from here at a distance R, what will be it is the amplitude in the function that will be equal to psi into because though we have to represent it as k r minus omega t this factor we are ignoring it for the present because that does not at any instant of time if you consider the time factory can ignore only this spatial this one factor we are taking into account then psi will be e to the power i 2 pi k r divided by that r will be there correct that is what essentially it is going to be (Refer Time: 37:05).

But the incident wave itself when it reaches here if it has a psi equals 1 when it reaches here, what it will happen the incident wave because some distance it has to travel na what is the distance which it has to travel that incident wave that is given by k dot R m n p. So, that that means, that the phase will have this much phase also will be added to the incident wave right and then this is what it is going to be essentially is the amplitude which it will have finally, of a wave which is scattered from here at a particular point wave which is scattered from here at a particular point we have, if the scattering if the we consider the beam to be a coherent beam all the amplitudes will add together right the wave functions will add together, if it is and incoherent one it is only the intensities will add not the amplitude, that I will come to later, but now you can take it that it is essentially all the amplitude add together.

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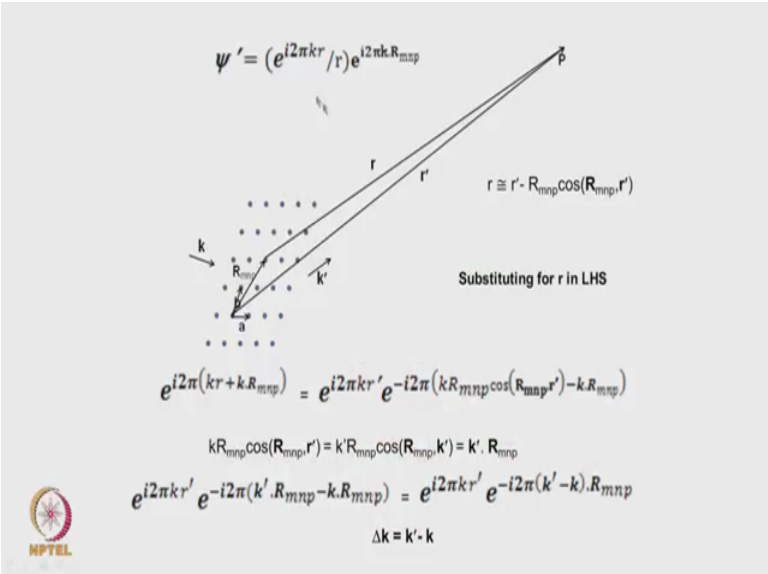

That is essentially what is being done this is the amplitude of the wave sider is set, this particular point. From this particular point if you consider it this will be with respect to R dash, from here this is the amplitude, just if we considered scattering from 2 points in the same direction please little bit of mathematical jugular if you do it. Finally, an expression will turn out to be of this type e to the power of i 2 pi k r dash into e to the power of k dash minus k will come what is k dash minus k? This is incident beam direction this is K dash right and the difference is what is a vector which is going to be that is represented as delta k is this clear see.

What are we trying to do? From this point at this particular direction we try to find out if I put a detector here which is very far away compared to the atomic distances, correct.

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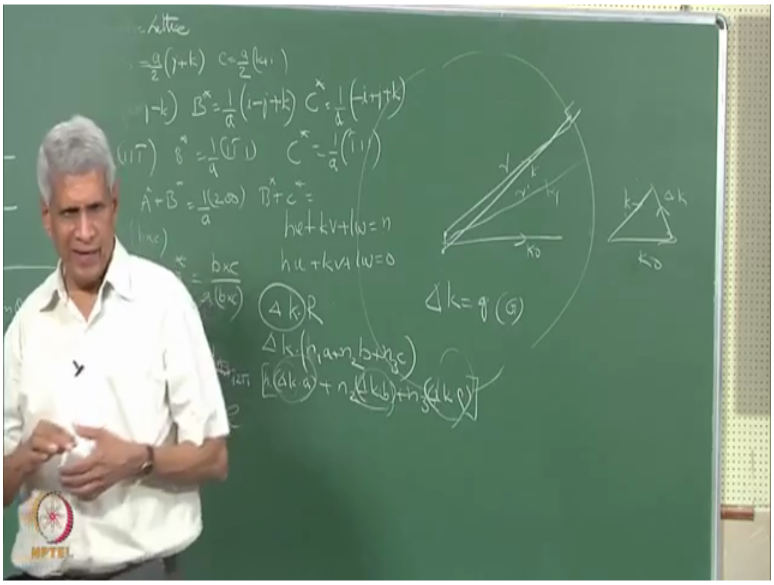

What is the distance between atoms in a lattice it is essentially 2 or 3 0.2 or 0.3 nanometers, where do we keep the detector and measured it most of the time? It is at 20 centimeters, 30 centimeters right. So, the distance if you compare it compared to the intern atomic distances it is a very huge distance. So, from here to here if I take a small another atom position essentially the beam which comes from here; here also the direction we can take it to be a essentially in the same direction.

So, what we are trying to do is that the wave which is scattered from here what is going to be there because you can take a sphere find out what it is going to be. From here the wave when it reaches here between this and this there is a phase shift has been introduced, you get supply in wave when it reaches there then from this it is at a distance if that is at r dash this is at a distance r, then again we can find out what will be the amplitude of this these 2 amplitude we add together. When you add together you get a term which comes like this, this is essentially what this turns out to be this a dash by r what I have taken it is that is an amplitude factor which we have not talked about what that it is to do with the scattering atom as well as with respect to the incident radiation that part of it we will talk about it later.

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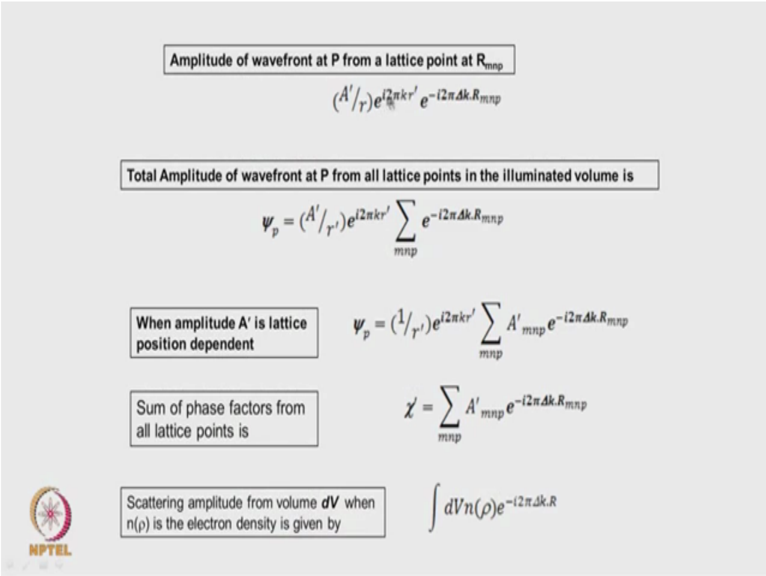

So, essentially what is interesting here is that this factor e to the power of i 2 pi delta k dot R m n p this is for with respect to origin 1 atom we have considered. In this sample there are in each direction in 1 direction m (Refer Time: 41:36) atomic point lattice points are there, another n and another p then it will be we have to submit over all these factors correct that is what essentially is written and in this term if it depends upon each particular site this factor turns, it has to be within the bracket sigma. If it is independent of the atomic position then you can be taken out as a common factor, but what is important is there this is what essentially is important. Supposed what is R m n p it represents a position of each atom or each lattice point. So, for each lattice point this term if it turns out to be 1, then all these will add together right, is it not.

So, this amplitude of the wave scattered in this particular direction will turn out to be maximum, then we say that a constructive interference is taking place. In between points where it is not k some value k 1 if you take it here for this value k 1. Suppose all of them do not add together some of them subtract intensities will come to and at some point they could completely vanish then we say that the sum is 0.

So, this; what it is? So, the condition for constructive interference essentially is nothing, but this delta k dot R m n p should be equal to 1 for each point correct is it not? And this is essentially what we have written is the amplitude part of it correct of the wave which is coming the detector at a particular direction and this can be considered in (Refer Time:

43:48) we can write it in an integral form also right. If you write it as an integral form then what happens is that this is over a particular volume we have to consider it; here what we have done it is every atom position we have taken and added it correct. Instead we can integrate it over the full volume also instead of taking each lattice point then this will be integral d v, this factor is a factor which depends upon the sample and the primary beam correct (Refer Time: 44:22).

So, this turns out to be if it is x ray diffraction, this factor will turn out to be the density of electrons; otherwise in the case of electron diffraction should be a electrostatic potential how it varies. So, this is characteristic of the sample .

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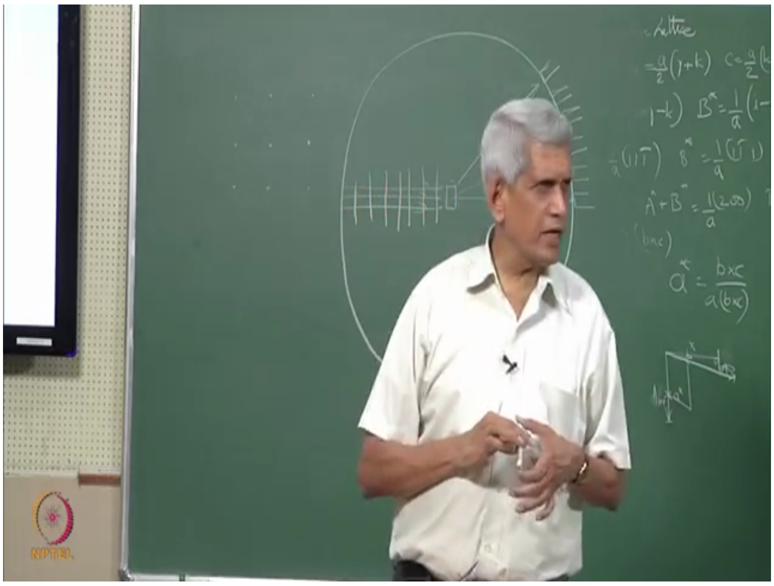

Because in the sample which we have considered has consign of if we represent it like this each of the point atoms are there, what is it exactly which is happening here? Around each point there is a nuclei surrounding it which there are a electrons are there, that turns out to be some ions and then in a periodic lattice in between regions also there are electrons are there which are distributed correct. So, maximum passing charge will come here like this here. So, this density of electron will be varying from the core of the nuclei to here if is the density is (Refer Time: 45:30). So, density is going to fluctuate electron density is going to fluctuate is it not in the sample. So, that itself is essentially another periodic function. So, this is what the dendroid represent nothing, but the density and e to the power of this term which turns out to be this way also we can write it.

So, important thing essentially is that delta k dot R should be an integer and this we can write it as the same delta k in the last class what did we represented that is in an another form as a capital K.

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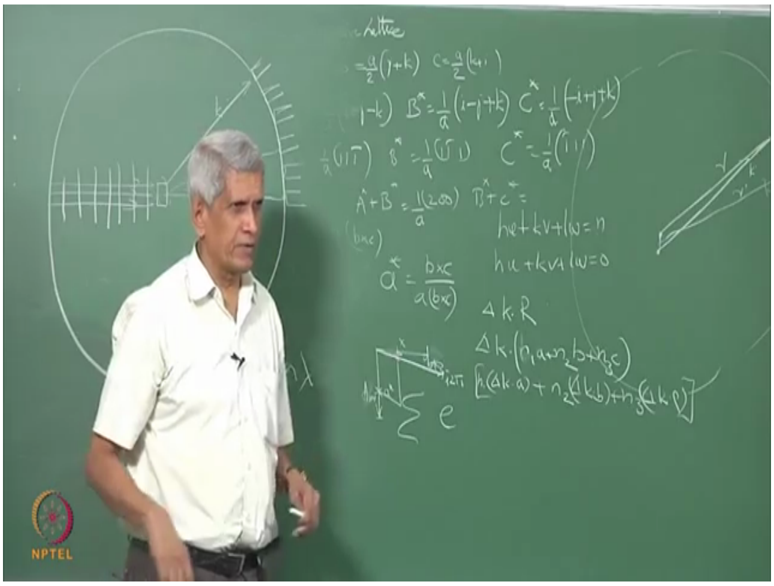

That will come to it this k dot R we write it R can be written as n 1 into a, plus n 2 into b plus n 3 into c right. So, this will turn out to be n 1 into delta k dot a plus n 2 into delta k dot b, plus n 3 into delta k dot c this is what it will turn out to be all this things we have looked at it the last class.

What is interesting about it is that this into i into 2 pi into exponential, that is what sigma of it we write it correct this how we can write it e to the power of i 2 pi i, h 1 into this one correct into e to the power of i 2 pi i n 2 into delta k dot b. So, when each of this exponential term becomes 1 then only it will become; that means, that n 1 is an integer then delta k dot a should be an integer this should be an integer, this should also be an integer independently is it clear.

Student: yeah, yeah.

That is what has to happen; when that happens then the scattering from all the atoms are adding together there in phase correct and then will get a maximum intensity.

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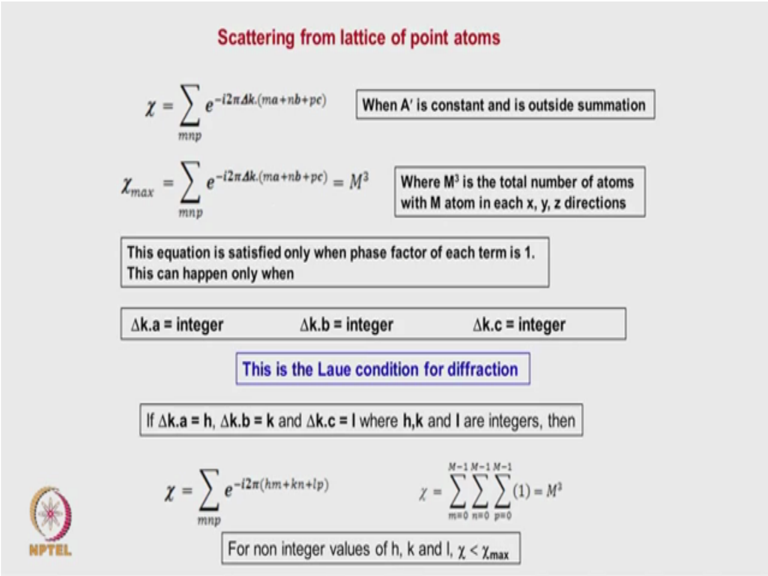

So, if the total number of atoms are in any one particular row is m in each direction maximum value of n m n and p equals m, then this maximum value what it can have this phase factor should be equal to m cubed it can happen correct. This if you remember last time we have derive the explained the delta k dot a should be equal to h all these things which we have derived it, instead of delta K we wrote it as K right capital K (Refer Time: 48:50).

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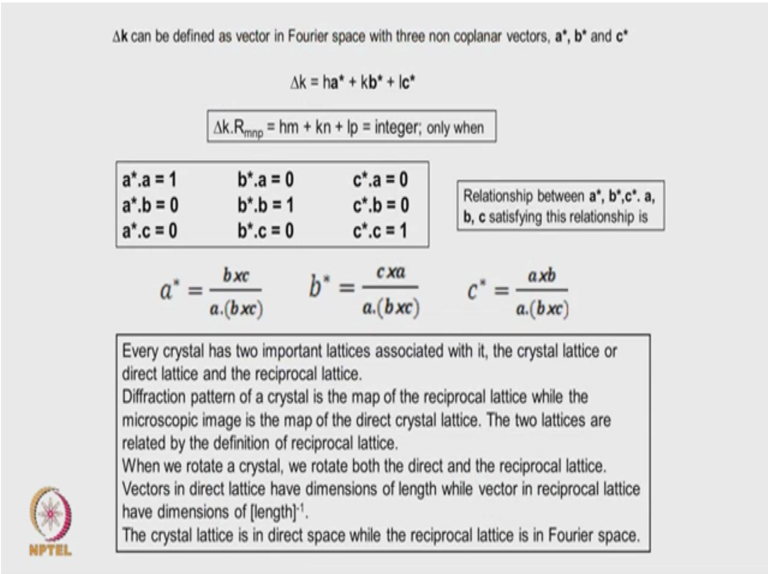

And we derived that expression that delta K should be h into a star plus all this expressions come, the same derivations follow which I had mentioned just sometime back in the class.

So, what is important from this derivation is that, every crystal has 2 important lattices associated with it the crystal lattice and the reciprocal lattice right direct lattice and reciprocal lattice. The diffraction pattern from this what we can make out is that the diffraction pattern is related to the reciprocal lattice right that is one; what is the relationship which happens is that when because this delta K which we have considered here is between if this is K 0.

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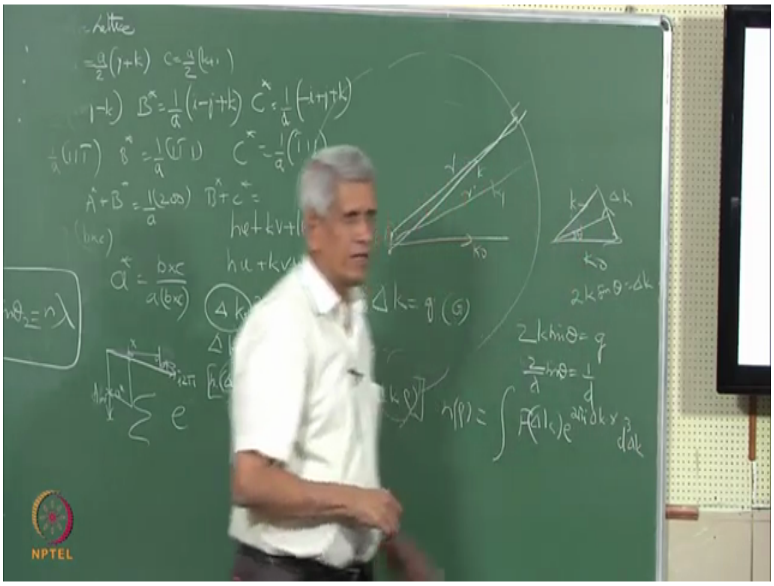

And if this; the direction which you are scattering k, this is what the vector will be which is delta K correct is it not.

But if this vector turns out to be a reciprocal lattice vector, then constructive interference will take place because this could be this could have because this value of k could be any value n a in this sphere what we have consider we are putting a detector here measuring it putting a detector here and trying to measure it. Only at some points that value turns out to be maximum for that delta K will have also some special value, that value is that the delta K equals at that time equal to g the reciprocal lattice vector, and another important factor which you should understand is that the crystal lattice which we have drawn earlier and the reciprocal lattice the origin for both of them remains the same. If I rotate the crystal what will happen.

Student: different phases will (Refer Time: 51:03).

By the same angle the reciprocal lattice also will rotate they are tied together real lattice and the reciprocal lattice, the relationship is fixed. So, it is as if I take a real lattice and represent it in terms of an orthonormal coordinate system, with the same orthonormal coordinate system reciprocal lattice is also defined. So, if I rotator l lattice the reciprocal lattice also has to rotate along with it, it cannot remain separately right that is what it is this factor is very important. Tilt a sample in the holder what we are essentially doing it is that we are tilting the reciprocal lattice also along with it. So, what will be the consequence of it? The reciprocal lattice has cut a direct relationship with the diffraction. So, the diffraction pattern also will rotate there is if you put a sample the beam is coming like this and falling on to it if I tilt the sample what it happens the diffraction part which has come, when a tilted that will also rotate; that means, the reciprocal lattice is also rotating along with it.

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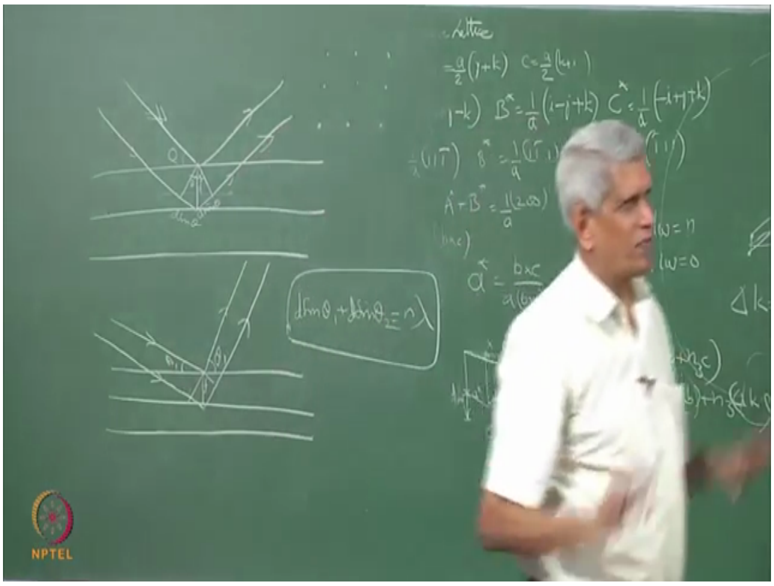

I have planes like this conventionally you draw like this is what it is, right this is d then you are try to find out if this angle is theta this angle is also theta, then you are trying to find out this is d sin theta correct this is also d sin theta, this is how the derivation is done.

Suppose you considered a case it is not. So, how do you measure this angle theta is with respect to a beam this is the angle theta.

Student: (Refer Time: 53:09).

Student: (Refer Time: 53:12).

Is this how we measure angle theta? Suppose the beam comes like this if gets scattered in this direction will diffraction take place away from this.

Student: (Refer Time: 52:43) apart from n d lambda (Refer Time: 53:44) n d equals (Refer Time: 53:44) n lambda is 2 d sin theta we should also have periodic scatterer and (Refer Time: 53:45).

No, no that is not there is diffraction only, we are talking about no periodic scattering we are not talking about atoms we are talking about diffraction from plane bragla.

So, what it is that if I take it here if this angle is theta 1 this will (Refer Time: 54:08) theta 2 this is d correct d sin theta 1 plus d sin theta 2 should be equal to n lambda. If this condition is satisfied that is Bragla actually a special case is when theta 1 equals theta 2 is a symmetrical condition that is what you always see in books this also is given in books, but nobody looks at this pages, this is the most general formula does not mean that angle has to be equal for a brag diffraction to occur.

What is essentially important is that the total path difference has to be a multiple of n lambda that is what the diffraction conditions says, you understand that. That is precisely is the reason when we consider a sample here at the centre when the beam comes in this direction, there are various directions in which where the theta is not the same as the incident beam direction, we are still able to get maximum of intensity. So, this is what you should remember as a Bragla, now you can find out what will be second order first order all those things we can find out only from this. Then in this condition when delta K equals g that g can be written as small g and some places you will find that the g is written as a capital G that does not matter, this is actually is the condition for diffraction. What does this g correspond to? This g is nothing, but 1 by d correct what is delta K delta K is this vector correct this is this angle is nothing, but 2 theta right and if you take this one this delta K will turn out to be if this angle is theta, 2 K sin theta will be equal to delta K right is it not.

So, 2 K sin theta equals g this is 2 by lambda sin theta equals 1 by d and this is what the bragla is. So, this is the condition for a Bragg condition is. So, in vector space this is way only in which it has to be written when the between the incident beam direction and the scattered beam direction, the difference between them when it is equal to the reciprocal lattice vector, the Bragg condition is satisfied what diffraction. So, in those in that in those directions that the angle which correspond to it you will be getting maximum in intensity will be coming is this clear.

So, here this R m n p what we have considered as essentially like there are different lattice points are there right; it is each lattice point we are representing it, if it is a primitive lattice how do we represent the lattice or a primitive lattice. Primitive lattice how do we represent with only one point n a, the primitive lattice only the origin we giving because the total number of lattice points per unit cell is 1 n a. So, we can represent it by the 1 by the origin if we represent it so that means, that if this is a primitive lattice this will represent 1 lattice, and this will represent the another lattice this will represent the third lattice.

So, each point represents 1 of the unit cells correct (Refer Time: 58:56). So, when you take the sum of it what we are essentially taking it is what is going to be the intensity from all the atoms put together right or the amplitude which is going to be scattered from all the atoms here in this particular direction right; that we add together that is nothing, but that condition delta k dot R equals to n is also the same n a, there what it means is that delta k for a specific value of delta k, K 0 is initial direction which is fixed. So, the k is fix for a particular value of k, what is going to be the amplitude which is scattered from each of the atom positions there which adds together that gives that intensity.

That will have all the information about the shape also. In this what we have to consider it is that suppose it is going to be from a very few atoms if you consider it if the length of the sample is very small the peak will be broad. If the length of the sample is very large the peak will be sharp this if you relate it in a space if you look at it between a furious space real space and the diffraction space, also the furious space also this is exactly what happens. If the length is large in real space furious space will have a shorter distance if the length is small in furious space, length is large in furious space in real space it will be short.

Student: (Refer Time: 60:01) distance from the (Refer Time: 60:02).

No total lattice size itself the crystallite size if the crystal is crystal size is very large the peak become very sharp if the crystal size is very small the peak becomes very broad.

This intensity what we are trying to calculate psi dash equals this factor this is one which is a function of the real space information, and here this is we have written with respect to d v correct and what is this factor this factory is essential in a particular direction K we have calculated psi dash right adding intensity. So, this is something like a function of delta K you can take it and inverse Fourier transform will be that enough row should be equal to integral of F of delta K to exponential r into d cube delta K right this is how delta known to be.

Student: (Refer Time: 60:02).

Which one?

Student: from that how we can say (Refer Time: 60:02).

No, no, wait a minute, these 2 are related these 1 is a Fourier transform of the other this can be derived, that part I think I will not discuss in may be in tutorial like we can discuss these aspects.

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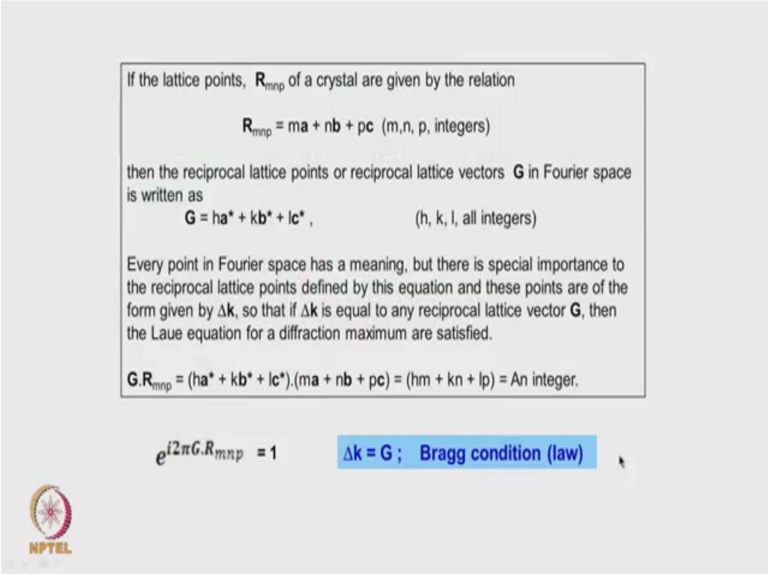

So, from this what you can understand or is that, there is a direct link between the diffraction phenomenon and the reciprocal lattice right and whenever delta K the difference between the incident vector wave vector and the diffracted wave vector that equals reciprocal lattice vector the Bragg condition is satisfied.

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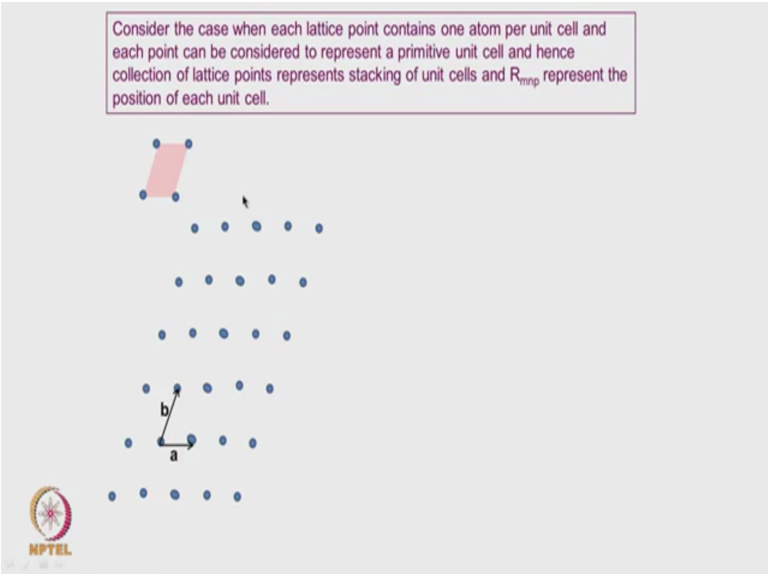

So, essentially what we have done today is a find out a relationship between reciprocal lattice and the diffraction phenomena we have looked at, it now what will do in the next class is what is a relationship that how the what are factors which control the intensity of the diffract us part we will look at it. We will stop here now.