Nanostructure and Nano Materials: Characteristics and Properties
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Lecture - 36
Reciprocal Lattice

In this lecture we will learn about reciprocal lattice. We will see it is the reciprocal of the lattice. Now, how does it evolve and why is it essential we will learn about in this particular lecture.

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To learn about diffraction, it is highly essential that we learn in terms of reciprocal lattice and how does it evolve we will talk about that in this particular lecture. We might be already familiar with the Braggs equation and we know that Braggs equation is given by 2 d sine theta is equal to n lambda.

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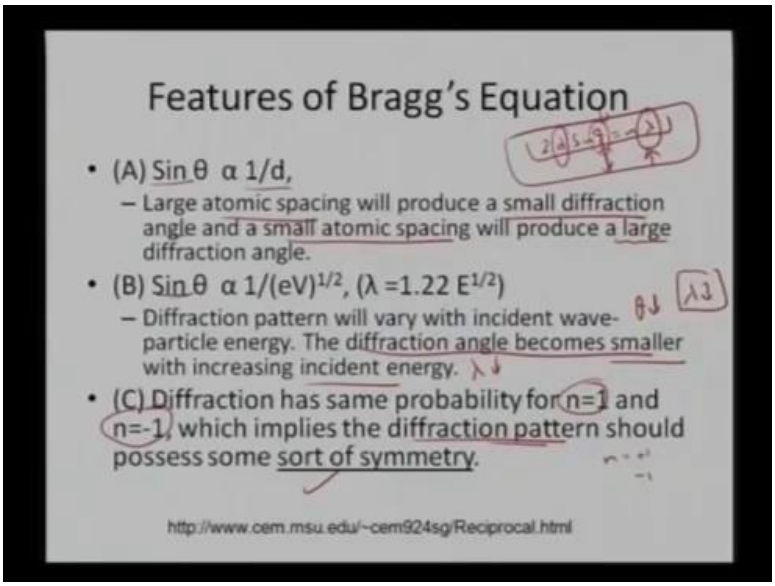

So, taking that particular equivalents we can directly see that, if we keep our lambda as constant, our sine theta is inversely proportional to the inter-planar spacing, which means that, if I have a large atomic spacing it will produce a smaller diffraction angle. So, that is what we can see that sine theta is inversely proportional to 1 by d. So, as my lattice spacing increases, I get diffraction which is at much smaller angles.

Also that is smaller atomic spacing will produce a larger diffraction angle. So, that is the inverse relationship of the inter-planar spacing with the diffraction angle. Secondly we can also see that, if we have for a particular lattice spacing for inter-planar spacing I can also see that my sine theta is inversely proportional to my energy or in other or words, if I start increasing my lambda I start decreasing my energy term.

Then obviously my theta will also start getting. If I start increasing my lambda then my theta will basically decrease. So, that is what the equivalence what we can see here because as my energy is higher my lambda is lower. So, eventually my theta has to decrease. So, for higher energy terms I can see diffraction at much closer points or theta as very very low, when I have very high energy wave length. So, I can see that with diffraction pattern will vary with the incident wave particle energy and the diffraction angle they become smaller when once I increase my incident energy or when once I reduce my lambda. So, my theta increases my theta decreases as I decrease my lambda.

So, that is the direct dependence I can see with see with theta with in terms of energy or the wave length. At the same time if I keep my n as either plus 1 or minus 1, I can see that this law will be again valid. It shows that there is some sort of symmetry which is basically which has to be incorporated for different values of n. So, automatically diffraction is, it will have the same value whether n is equal to plus 1 or n is equal to minus 1. So, my diffraction pattern automatically incorporates some symmetry into itself.

So, this summarizing it, if I keep my lambda as constant my sine theta in d have inverse proportionality or in other words if I have my d value as constant, I have direct proportionality of theta and lambda.

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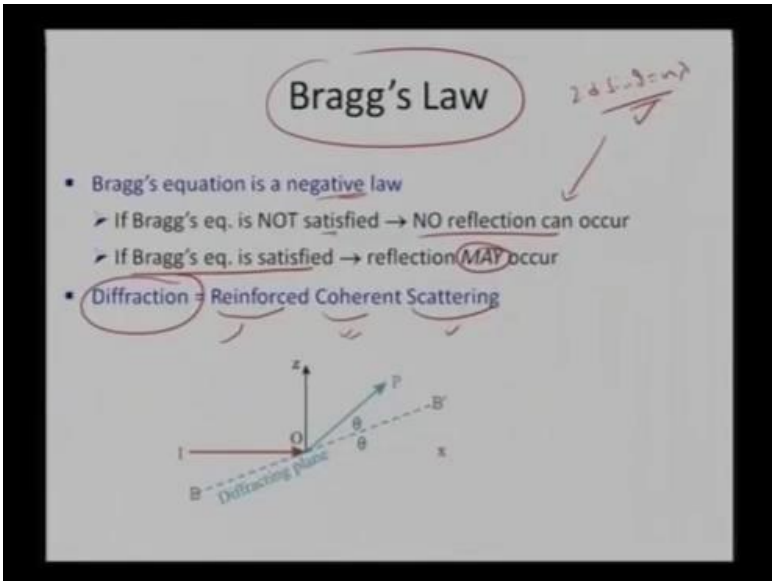

It means, if I reduce my lambda or increase my energy, my theta value will be very very low. So, that tells where my diffraction slots finally appear in terms of Bragg equation. Secondly the Bragg's law, it is not a positive law, it is a negative law. Which means that if I am not satisfying law no diffraction will occur, but once my Bragg's equation is satisfies, I am may see those diffraction. Diffraction is well defined as reinforced coherent scattering.

So, it is basically reinforcement of the coherent beams which are scattered. So, that defines my diffraction as such I will again Bragg's law or 2 d sine theta equal to n lambda this particular equation, is a negative law and that that tells me clearly. That if I

am not satisfying this particular equation my diffraction will not occur, but if this condition is it may occur.

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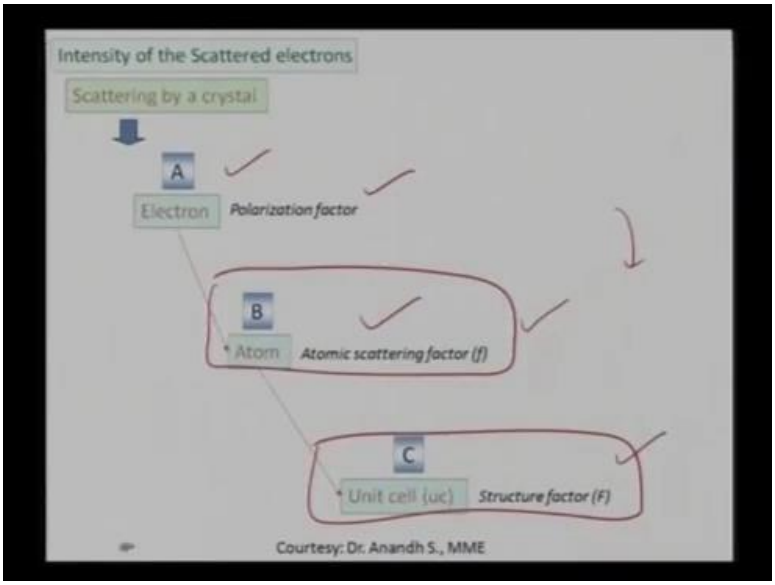

That is what is being defined by the Bragg's law. I will again there are certain factors of scattering by various electrons because initially we will have scattering by individual electron that brings out the polarization factor. I can have the whole atom because atom is consisting of so many electron, it will have something called atomic scattering factor. All those atoms will be arranged or organized in a particular unit cell in certain fashion. So, it will result on my unit cell structure factor. So, I have polarization factor which advances from the electron or I have whole atom which has many many electrons. So, this particular factor is dependent on my atomic number. Then I have the structure factor which is dependent on so many atoms which constitute or define a particular unit cell. So, this is how my intensity basically varies.

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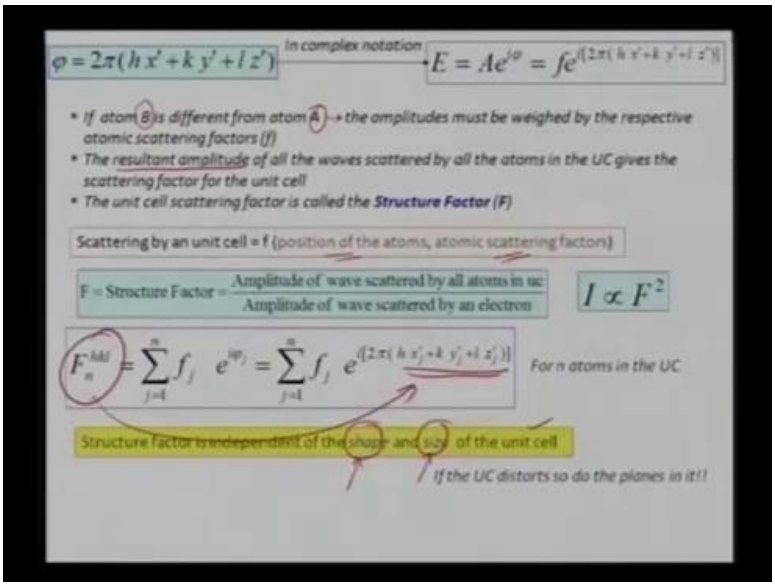

Then coming on to next part of it, I see that my overall structure factor is not dependent only on the positions of my atoms, which are there in the unit cell. So, I can see that structure factor is independent of the shape and size of the unit cell. It just depends on the location or the positions of the atoms and what their atomic scattering factor is. So, that part we can clearly see from this particular part.

The overall structure factor is not dependent only on the ((Refer Time: 05:38)) and the location of my atoms which are located out there in a unit cell. So, it is independent of the shape and the size of unit cell. Again it can have various intensities, the overall atomic scattering factor can be different for different atoms. If I have 2 atoms a and b and what I will get finally, is kind of a resultant amplitude which is arising from the scattering of different kinds of atoms. So, overall I can see that my overall scattering factor is dependent only on the location of atom in a particular unit cell and is independent of the size of the unit cell or its shape.

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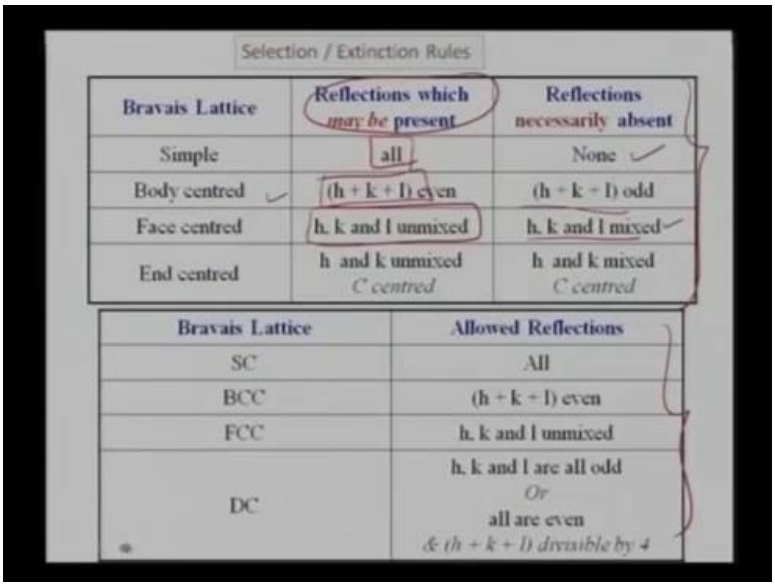

This thing also we might have learnt about a the diffraction, but all those reflection may be present simple cubic, have all the reflection to be present for a body-centered, I have only h plus k plus l ((Refer Time: 06:31)) indices which the combination when it is even I get my reflection. For face-centered I have, I should have h k and l which are unmixed, it means all h k have to be all odd or everything has to be even.

Then for end-centered I need to have h and k unmixed for a c centered 1. For necessary absence reflections are totally absent for simple cubic, I should have everything like everything is present. So, I do not have any reflection which are absent and absent might have h plus k plus l is equal to odd or for BCC and for FCC I have h plus k plus l they are all mixed. So, then I would not get any reflection. So, these are all the criteria for diamond for a SC BCC FCC DC or SC cell.

Now, coming back to which forms the basis of my, of the reciprocal lattice is. Like if I see I start seeing a particular crystal and I start defining each and every plane by their normal. So, I can see the points begin at fractional coordinate of one.

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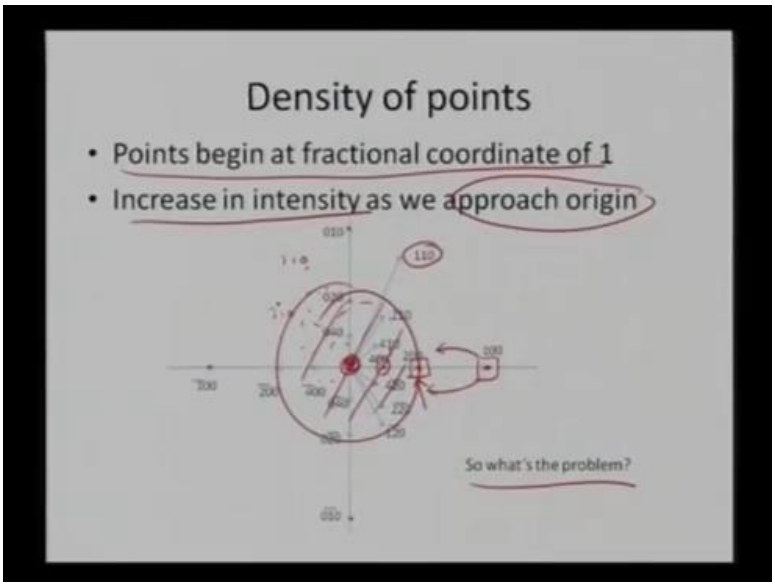

So, this is what is defining my particular unit cell. So, this is the end limits of that particular unit cell. It will have a dimensions of 1 on each side, but as soon as start coming into the particular crystal, I see that I have the different planes plane 2 0 0 0, plane 4 0 0. They all start falling from the outside to the inside. Similarly, I will have all of points available here as well I have 1 1 0. So, I will have my 1 bar 1 0 somewhere here.

Along with same side I will have my 2 2 bar 1 0 somewhere here 2 bar 1 0. Similarly, I will have more intensity of points along this side which is near the origin point. So, I will have more intensity of points which will start crowding my central location. So, this problem is that we have increase of intensity as we start approaching the origin. So, this is my origin as soon as I start now creating all the planes or labeling all the planes. I will have more intensity in the central part because my 1 0 0 is at this particular part this particular point and 2 0 0 is at the half the distance. So, I will have more agglomeration of points in this particular region. So, to basically come out from this problem.

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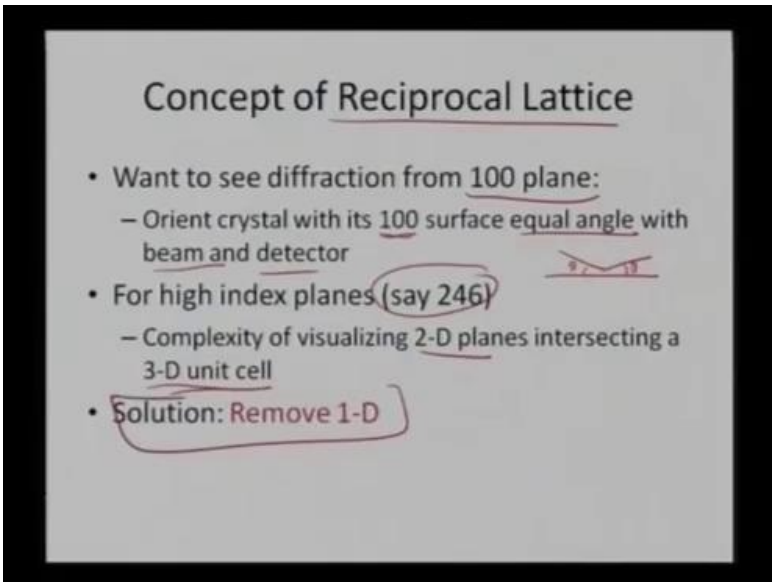

We define something called a reciprocal lattice. The problem arises say if you want to see a particular 1 0 0 points. I orient my crystal in a approximately with 1 0 0 and which has a equal angle with the beam as well as the detector. So, I can define that my theta is basically obeyed and I can basically obey the Bragg's law for a particular alignment. So, this becomes very easy for 1 0 0 or lower index planes, but what happens if I want to go for a higher or complicated higher index planes as 2 4 6.

So, basically this creates some problem or complexity. Once I want to visualize all those things in 2 dimensions so, actually what I have is 2 d planes which have intersection of a free unit cell. So, this creates much more complexity. So, if you want to visualize this 2 4 6 plane, what I can do I can just remove the one dimension of it. So, once I remove 1 dimension I can see looking 2 dimension and that for I am more comfortable.

So, I can remove those 1 dimension from my unit cell and what I see everything in the reciprocal lattice spacing, I can see I can form the same crystal in a reciprocal lattice I remove 1 dimension, now I have much more simpler view for analyzing. So, I have everything a representation of crystal itself in a reciprocal lattice and I am removing my 1 dimension no I have the same plane with much more simplicity.

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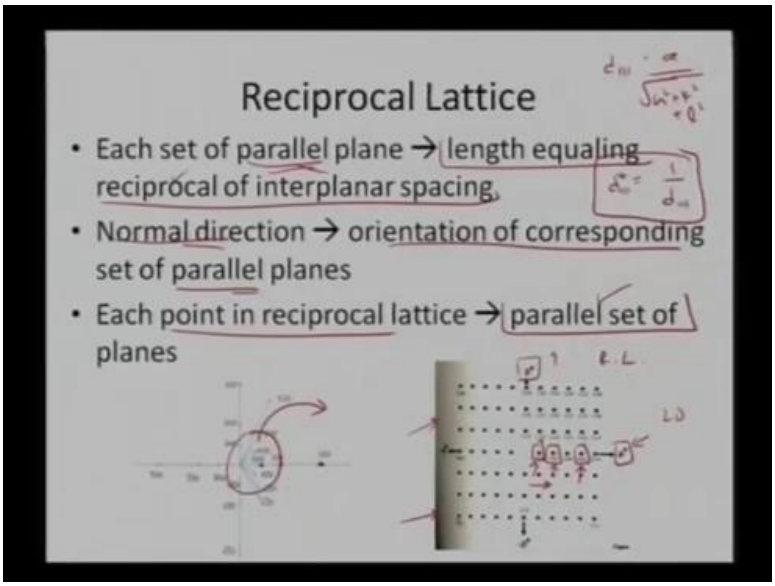

How do we go about that, it is more like this. That we have more set of parallel plane and that have length which is equal to the reciprocal lattice. So, let us say I had reciprocal lattice for a unit cubic cell say for d 1 1 1 is equal to under root of h square for k square plus l square for a cubic a for a cubic cell. So, what I can do in my reciprocal space my new spacing will become 1 by d 1 1 my d 1 1 1 star will come 1 by d 1 1 1.

So, I have this set of parallel planes of 1 1 1 which have their length equal to the reciprocal of the inter-planar spacing. The normal direction normal direction to this particular plane is the orientation of the corresponding set of parallel planes. So, I can also define its orientation, I can also define its magnitude. How, what is the overall spacing between all the particular planes.

So, each point which being observed in the reciprocal lattice that is nothing but a parallel set of planes. So, all the planes 1 0 0, all set of the parallel planes which are shifted by a particular unit cell distance all those I can represent by a single point. Now, I know it is direction because I will have the normal direction which is orientation of a corresponding set of parallel planes. I know the magnitude that is nothing but the 1 by inverse the inverse of the inter-planar spacing between those particular set of parallel plains. So, I can define each point in the reciprocal space as a parallel set of planes.

So, what I was seeing here 1 0 0 in the normal nomenclature 2 0 0 out here 2 0 0 out here, but in terms of reciprocal lattice my 1 0 0 is out here, my 2 0 0 is double the

spacing aa 4 0 0 is 2 times the spacing of 1 0 0. Now, I can see all these parts. I am basically opening it to go on the other side and to see my lattice more clearly. So, my 1 0 0 is here 2 0 0 is out here 4 0 0 out is here, what I can see. I can see uniform or periodic distribution of all this points which I can define by either by the vector quantity.

Now, I have a star which nothing but a reciprocal lattice and on this star I have a b star. Now, I could see everything now is in 2 di have removed 1 dimension to it which is nothing but the 0 0 1 part of it. I have already removed it that becomes its own axis and I can present all my points all my planes so nicely by a single point. Now, I know my direction as well.

I know my direction this thing is my 1 0 0 direction that is what I am going here with this this of my direction is 0 1 0. So, that is where I am going, it is perpendicular to the 0 0 1 1 plane. So, that is what I can see here that becomes a zone axis. So, now it becomes much more simpler for me to represent all the planes. I know their magnitude what is the inter-planar spacing. That becomes 1 by d of the inter-planar spacing in a reciprocal lattice spacing. I know its direction, so I can represent now a set of parallel planes by a single point in a reciprocal lattice. The concept of reciprocal lattice becomes more like this that I have incoming x-ray b.

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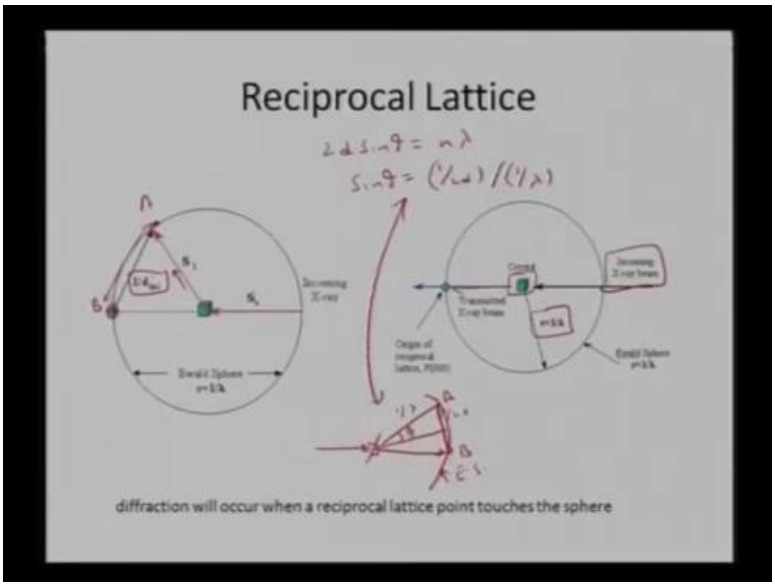

It can again be electron b depending on kind of diffraction which is occurring. Then I have the Ewald sphere, this is nothing but the Ewald sphere which is a radius of 1 by

lambda. Upon interaction with the crystal from the beam get transmitted, but those which are following, which are obeying the Bragg's law, they get diffracted out here. What I get the diffraction chord on the evolved sphere.

So, this is my first chord that will come out here this is my transmitted beam. This particular distance nothing but 1 by d or the inverse of the inter-planar spacing. So, I have 2 d sin theta is equal to n lambda I can define this sin theta is equal to 1 by 2 times d divided 1 by lambda. I can see that if I take a particular thing like this. I can define that my incident b interacts with the multi crystal goes away.

Then everything is falling on the Ewald sphere these 2 particular points I take a and b. I can take them a and b n half of it is my theta. What I am saying is 1 by 2 d, this is my 1 by lambda that is what is being shown in this particular equation. So, I have particular crystal plane which are oriented in certain direction. They give out my theta and 1 by lambda and I can now see that everything is now falling on Ewald sphere, this particular part. I can see this is my Ewald sphere.

Then what I get is a spacing of 1 by d out here that is what is presented by reciprocal lattice. So, it means that all the points which are falling on the Ewald sphere all this points on the reciprocal lattice which are falling on the Ewald sphere only they are producing my diffraction chord because they are the ones which are obeying the Bragg's law. We can see sin theta is equal to 1 by 2 d, whole divided 1 by lambda. So, I have my Ewald sphere which is the radius of 1 by lambda and also I am getting theta value of 1 by 2 d. Our 2 theta becomes 1 by d that is what I am seeing out here in the Ewald sphere construction. That I have my 1 by d I have my 2 theta out here.

That is what is giving my diffraction chord. Again this is what is being stated that diffraction will occur, only when a reciprocal lattice point touches the sphere. That is what is obeying and that will create a diffraction chord. Let this be the construction of a reciprocal space. I have my reciprocal lattice out here r l.

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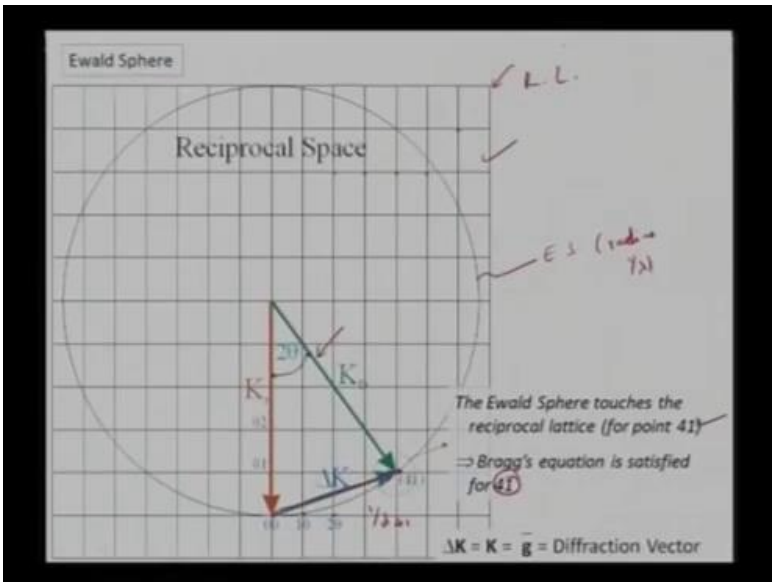

This can be individual plane which can be represented by all this intersection of all those points. So, I have all my points it is a 2 d reciprocal lattice. So, it is 2 d 001.0 2.0 and 3.0 and so on. This is my Ewald sphere and this has a radius of 1 by lambda radius of 1 by lambda. So, what I can see this particular distance. It is touching the Ewald this particular point is touching the Ewald sphere. I have 1 by d of 4 1, this is again 2 d only 2 dimension. I am seeing that my Ewald sphere it has a radius of 1 by lambda and I am getting 1 by d which is of a of particular plane, which is being satisfied by 4 1 plane.

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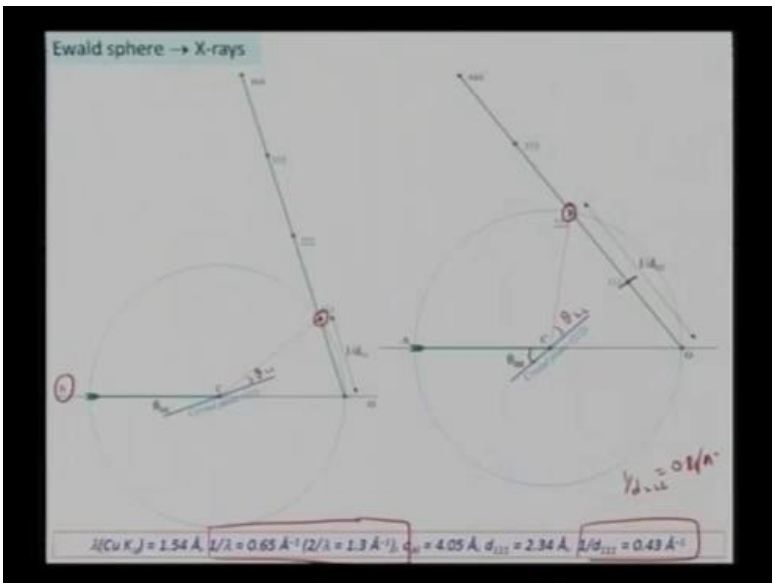

So, when the point is touching 41 I am getting a diffraction chord. So, my reciprocal lattice, once it coincides with the Ewald construction I get a diffraction chord. So, it is more like this. I am sending a beam out crystal plane is oriented at certain theta value. I must obese the theta value I have theta 1 1 1. In this particular case I have theta 2 2 2. So, once it is touching the Ewald sphere say my plane is exactly oriented.

So, I will get a diffraction chord out here for plane d 2 2 2 I will get diffraction chord at some other point because now my d 2 2 is different than theta 1 1 1. For a particular material once I recognize a proper key alpha I fix my lambda value or my inverse of lambda that comes out to be 0.65 per angstrom. In this case I have units of 1 by length because it is an inverse construction of a particular length scale.

That eventually brings out the 1 by d value around 0.43 per angstrom. If you realize if I calculate 1 by d 2 2 2, it comes out to be approximately 0.86 per angstrom. We will see that it much product in nature and this length is exactly half of my d 2 2 2 and that is what brings the curiosity in this particular construction.

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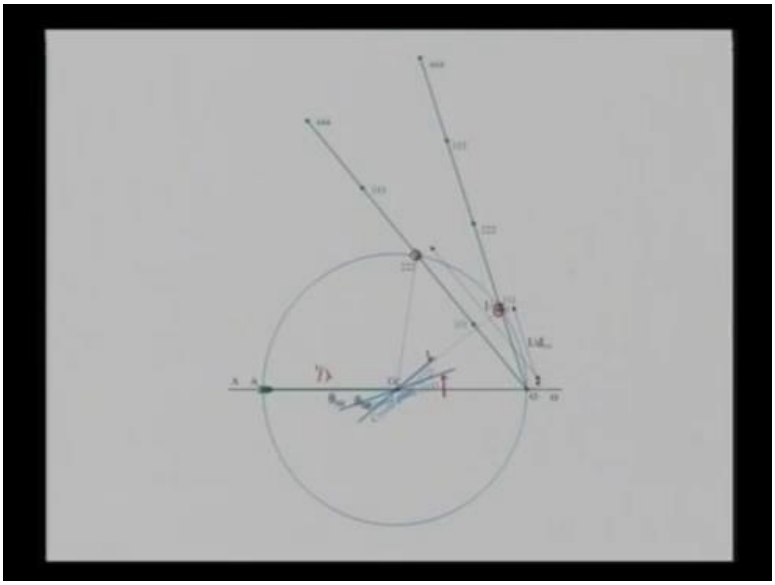

So, if you want to see again as the merger of this 2, I can see that I have plane 1 1 1 and I have plane 2 2 2 and how do they can fall on the same Ewald sphere because my 1 by lambda term is constant. For a particular radiation and now I can see that plane 1 1 1 has to be aligned differently as compared to the plane d 2 2 2, to give me a diffraction chord. So, I need to have a kind of poly crystal material with a proper orientation with my plane

1 1 1 and plane 2 2 2 to produce a diffraction spot, at particular location in the Ewald sphere.

So, my reciprocal lattice has to be such that it basically comes out or fetches the Ewald sphere. So, that I need to have poly-crystalline material. So, my reciprocal lattice will be accordingly to particular plane and my Ewald sphere is constant because my lambda value is fixed for that. So, I can get the diffraction chord at some location, so coming back to it.

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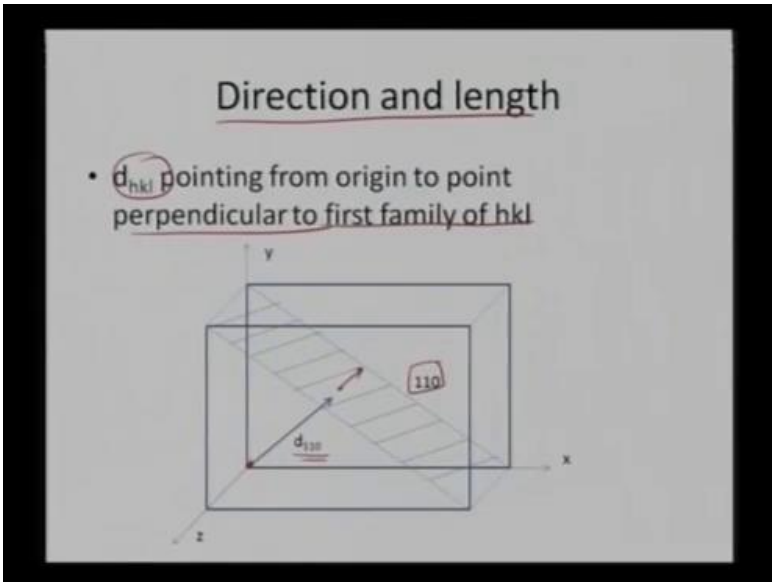

The direction and length of the reciprocal spaces will more like this. That my d h k l plane is pointing from origin to the point if this is origin and it is to a point. So, this is the plane 1 1 0. Now, this particular point is now perpendicular to the first family of h k l. Now, I have plane 1 1 0, the overall point towards it or the d h k l pointing from origin to this particular point will be my particular plane in the reciprocal lattice, with the direction of d 1 1 0. To construct a reciprocal lattice my directions is this be the normal a lattice construction.

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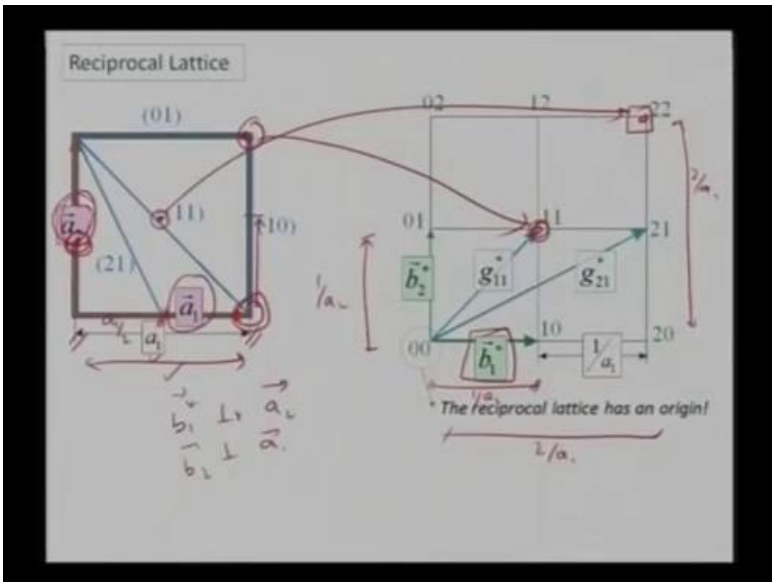

So, I have a 1 factor and a 2 factor which are in the real space gives length along a 1 direction is a 1. So, reciprocal space I have this particular length which is a 1 that becomes now 1 by a 1, 1 by a 1 in my reciprocal lattice. I had a length of unit 1 which becomes 1 by a 1, I had a length of a 1 which becomes 1 by a 1 in my reciprocal space. So, this particular point which was a 1 by 2, now that becomes 2 by a 1.

I had this particular length this becomes from 2 by a 1 and so on. Similarly, a 2 that becomes 1 by a 2 something like this become 1 by a 2. Any point out here in the center part, this particular length now becomes 2 by a 2. So, that is how the reciprocal lattice gets constructed. So, I had this 1 1, this particular point this now becomes this particular point. If I had some true comma true that becomes basically out. So, any point 2 comma 2 out here will now be at this particular location.

This particular point now has converted to this particular point. This point has now gone to this. That is how I construct my reciprocal lattice like this. One more condition to be to be noticed is, that my new b 1 vector is perpendicular to my a 2 vector. My reciprocal lattice vector of b 1 is perpendicular to my a 2 vector and my b 2 vector is perpendicular to a 1 vector. So, my reciprocal lattice it is a unit vector which are perpendicular to my real lattice real space lattice vectors. So, seeing it properly, again we can have again this a 1 and a 2, which are the real space coordinates real space vectors.

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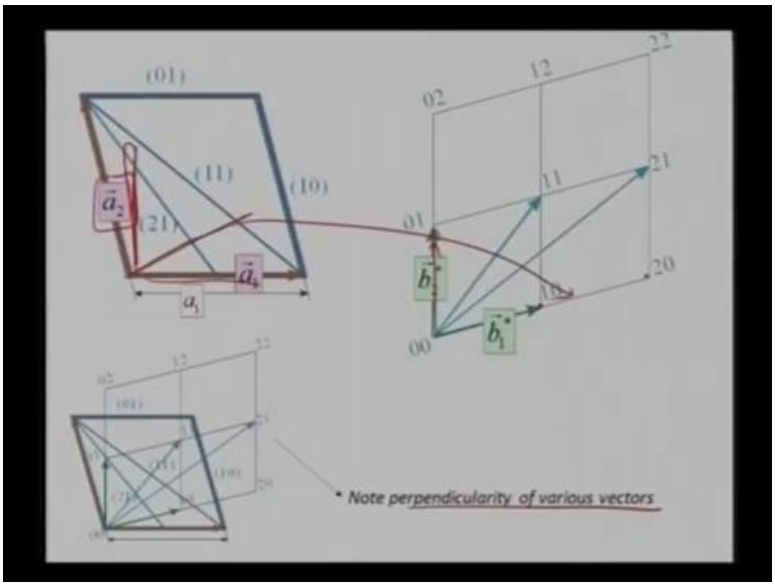

Now, my b 1 will be now perpendicular to a 2. So, my b 1 or the reciprocal lattice will be perpendicular to a 2. So, my perpendicular to will come out approximately like this and that is nothing but this particular plane. So, that is what I am seeing, that 1 0 plane is falling here 2 0 is falling out here. For a 1 it was, it has become b 1 and now b 1 is perpendicular to a 2 and now 1 b 2 will be now like this in the reciprocal space.

That is what I am seeing out here now b 2 is perpendicular to a 1. So, that shows the perpendicularity of the various vectors in the reciprocal lattice. So, it is very essential that, it is not only it is diminishing the dimension 1 by, it is also becoming perpendicular to the original other axis. So, I had a 1. So, it is now helping the b 2 form which is perpendicular to a 1 and my b 1 is perpendicular to a. So, that is how it becomes in the reciprocal lattice spacing.

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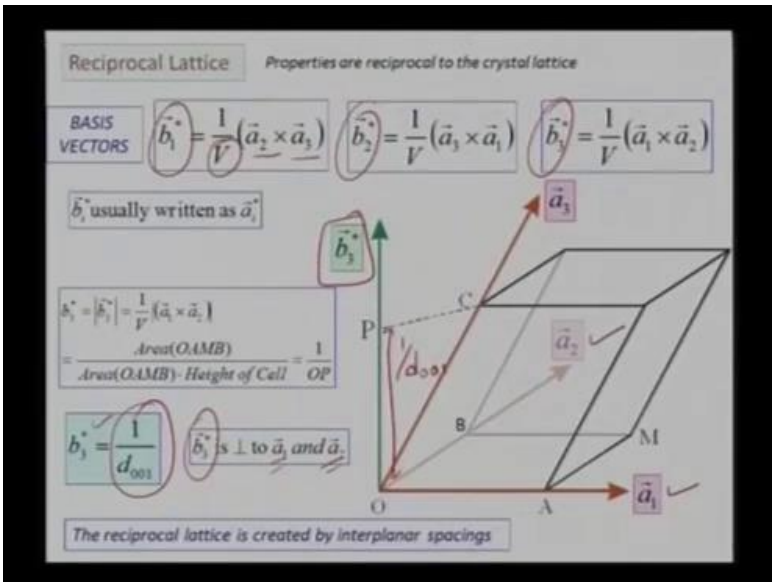

All the basis vectors in 3 dimension can also be defined as their cross product of the other two. So, my b 1 star becomes the a 2 cross a 3 divided by v, where v is the volume or b 2 becomes the a 3 cross a 1 by v and b 3 becomes a 1 cross a 2 by v. Again particular thing is that b 3 is again the reciprocal inter-planar spacing and again b 3 will be perpendicular to both a 1 and a 2.

That is how I can see how the overall lattice, reciprocal lattice spacing is being constructed. So, I can see my b 3, it will remain perpendicular to my a 1 as well as a 2 and this planar distance is nothing but 1 by the inter-planar spacing of particular plane, which can be 0 1 1 or it can be something else as well 0 0 1 approximately here. So, that is what is being shown out here how one could construct my reciprocal lattice.

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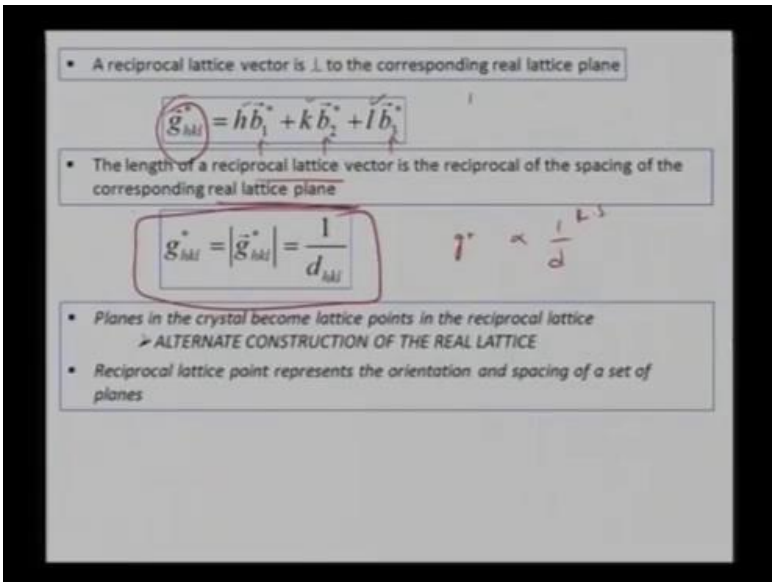

So, what I can get finally, as my inter–planar spacing is nothing but my miller indices plus the reciprocal lattice vectors. So, that is how we will define my 1 by d 1 by d of h k l it is given by the lattice, reciprocal lattice vector which is again nothing but the corresponding to the real lattice plane. So, I have this g vector corresponding to the 1 by d vector in the real space. Again this reciprocal lattice construction becomes an alternate way of representing my lattice space real lattice.

So, what is so good about reciprocal lattice I am eliminating 1 dimension at the same time I am able to mimic my real lattice. So, that is how it assess me visualizing things much more clearly, again coming back to the relations of the reciprocal lattices.

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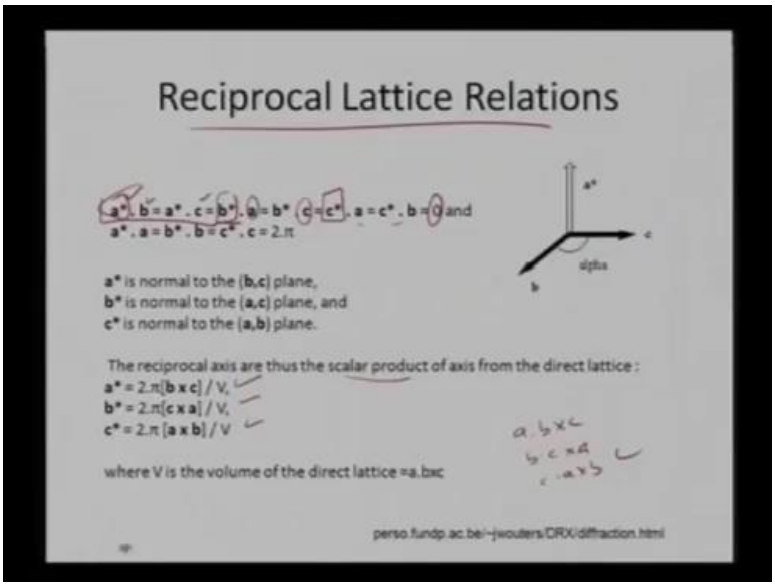

I can see that my a start b, a star c or my reciprocal lattice spacing with the original b c it becomes 0 or it is perpendicular to the original axis. Similarly, my b star, the dot product of my b star with a and c it again brings 0 and again my c star with a and b it brings out 0. It means that everything is all these things are perpendicular to the 2 axes which have it form. Again the reciprocal axis are the scalar products of the axis from the direct lattice. That is how it basically forms the reciprocal lattice.

This is nothing the v volume is nothing but the a dot b cross b dot c cross c or c dot a cross b. That is how I get the volume of the correct lattice and for a simple cubic lattice I can see that if I take the dimensions to form a cube.

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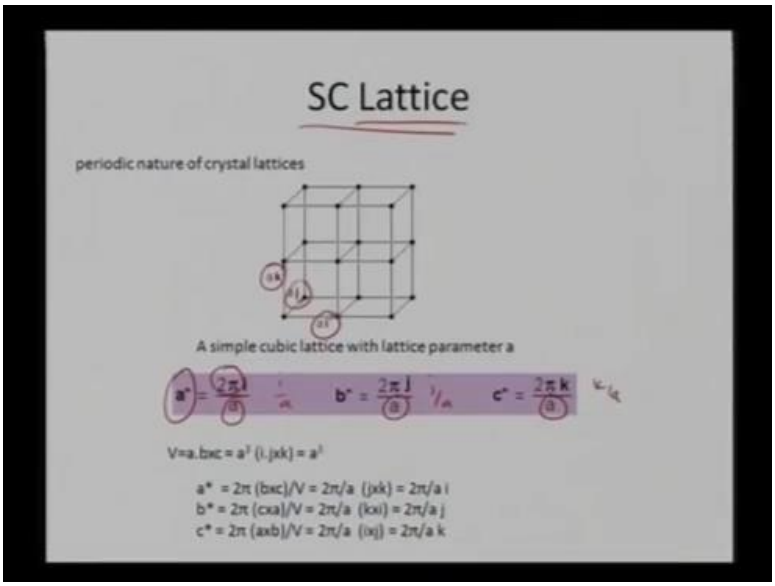

Again I will have to go again 1 in direction 1 in j direction and 1 k direction. That is how I get my reciprocal lattice parameters of a b and of a star b star c star all the 3 axis to form a unit cell. This particular thins is nothing but my lattice parameter. So, I get i by a j by a and k by a. Ideally 2 pi comes this factor particular comes to maintain the periodicity of a certain particular structure.

So, it is converting it into more into radians part. So, that is how it maintains as well the periodicity of the particular crystal in terms of taking it to the reciprocal lattice. So, finally, get a star is equal to 2 pi a multiplied by a b star is 2 pi j by a and c star is equal to 2 pi k by a and now coming to the BCC lattice. This a is again my lattice constant for a cubic for a cubic lattice.

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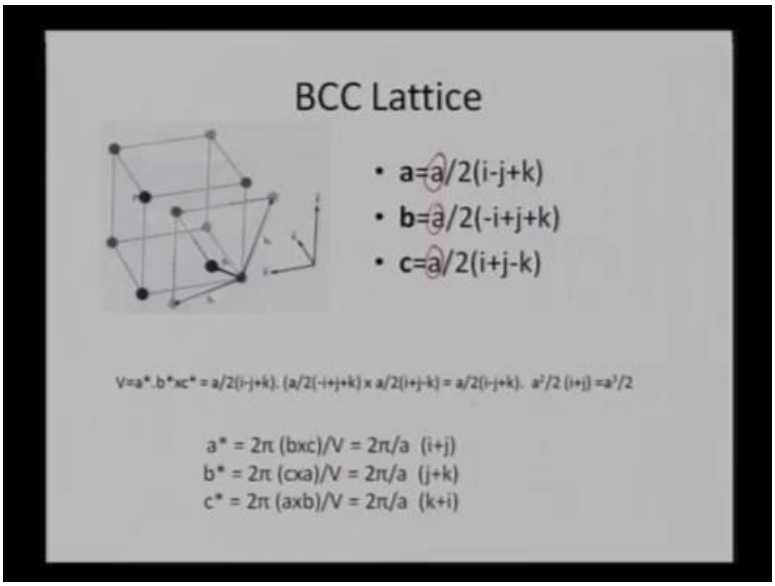

Again a b c are the new axis which will relate from the new crystal. So, to define a particular volume, I can take a dot b, b cross c.

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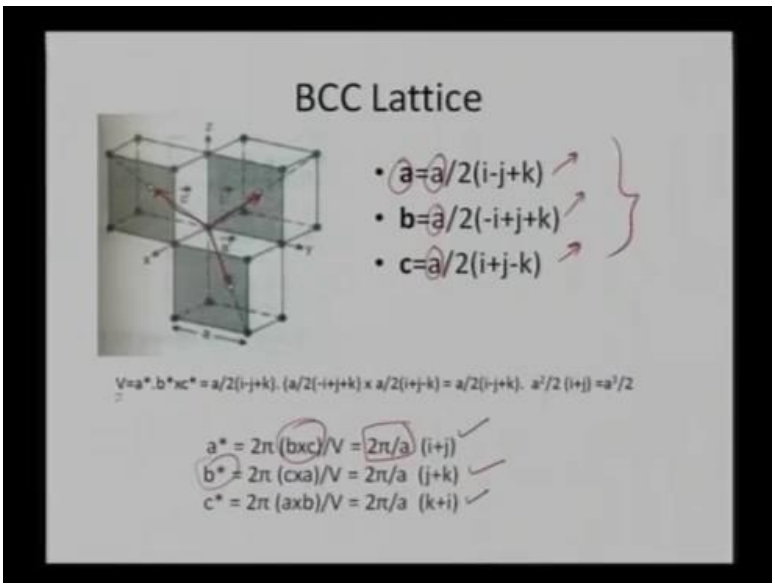

It eventually comes out that my a square is equal to 2 pi by a, I plus j b star becomes 2 pi a j plus k c star becomes 2 pi by a k plus I. This ideal construction comes from the equality form points which will from a particular unit cell. So, I can see that from origin, I had to go certain distances out here like this, 3 different to be able to form 3 axis of the new crystal or the new lattice which will form.

So, I can see if for consulting particular x, for a particular axis my a direction I have to go i minus j plus k whole by 2 or second thing for b, I have to go minus u plus j plus k or for c I have to go i plus j minus k. So, eventually taking doing all those vector algebra all the cross product I can see that it eventually comes out i plus j, j plus k and k plus i to form my final crystal final lattice.

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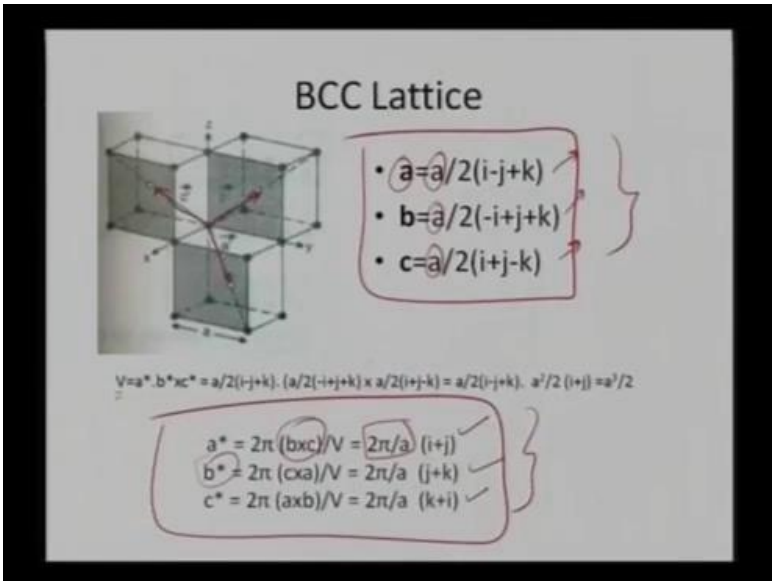

Similarly, for FCC lattice, my 3 equivalent point basically are these particular points which are sitting on the 3 different places. So, those correspond to i plus j, j plus k and k plus i. So, I can say I have traverse 1 1 and each direction because this my bottom face this is my front face and this is my side face the center of that. So, I can say that I had to travel i plus j by 2 j plus k by 2 and k plus i by 2.

Taking the periodicity of 2 pi I take my again the cross product of b cross c and I divided the volume. So, I can get some parameters which are more like this. Eventually turns out that the reciprocal lattice of BCC is equal to FCC. So, I can see that this particular part is similar to what I had started with in a BCC. So, I can see that this particular part and this particular part is now similar to my i minus j plus k. So, it is basically i minus j plus k, it is similar to this particular part. So, I can see that reciprocal lattice of FCC is equal to BCC and reciprocal lattice is equal to FCC.

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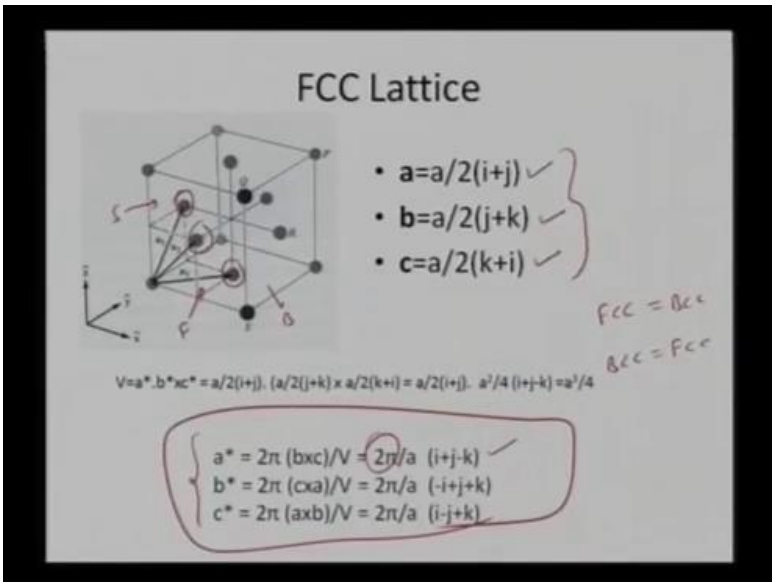

That shows the correspondence or correlation from the BCC to FCC lattice. It simple cubic remains a simple cubic, but my FCC becomes BCC and reciprocal lattice spacing and then my FCC becomes BCC. So, what I can see out here is the reciprocal lattice is the reciprocal of the primitive lattice.

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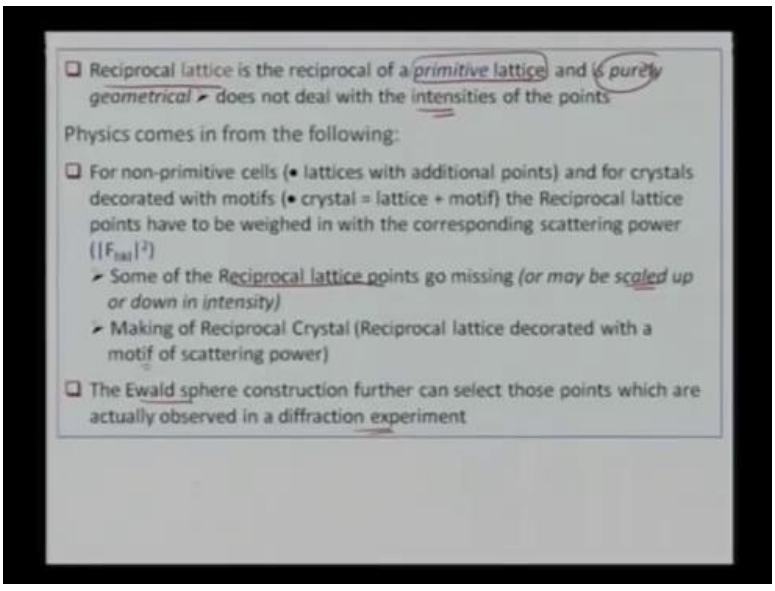

It is purely geometrical. Since, it is only geometrical, it is not dealing anyhow with the intensity point. What I am getting particular point, it is just showing me that it is just reciprocal lattice or it is forming the reciprocal of the primitive lattice without taking

care of the intensity of any particular point. So, I can have some primitive cells, something with the non-primitive cells, but then again how do I decorate them, it fully depends on the location of my particular points.

It might also happen that some reciprocal lattice points may go missing or they can be scaled up or they can be scaled down in the terms of intensity. Or it can have a decoration of some motive because depending on the scattering power. Again the Ewald sphere construction can select those particular points which are actually demonstrated in a diffraction experiment.

It is again a problem that, whether it will come or it not, totally depends on the scattering power a particular plane or a particular element or a particular atom which is being present there. For location and the scattering power the combination of that decides whether a particular diffraction part will be present or not. So, the construction of Ewald sphere plus the construction that is coming here, they jointly say that a particular spot will be present or absent.

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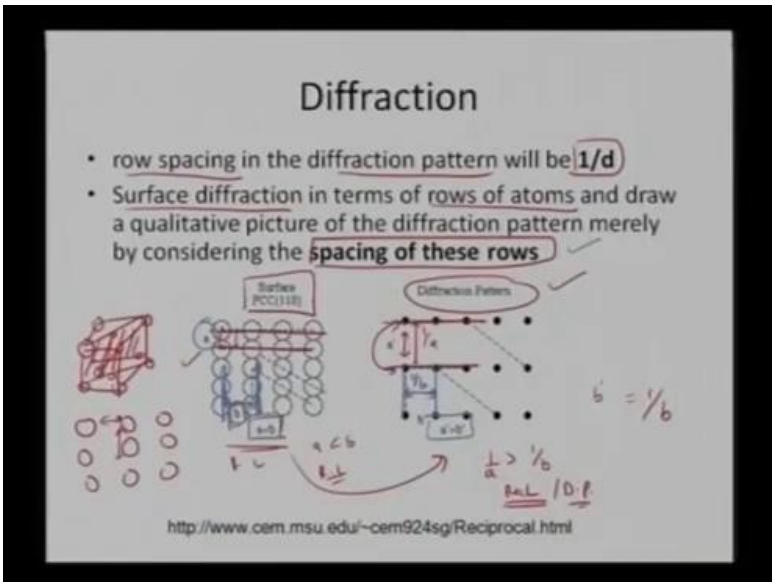

So, seeing it in a different manner. So, I can see that in my diffraction, once the diffraction is recurring my row spacing in the diffraction pattern has become 1 by d. So, initially when I had inter-planar spacing of d, it becomes 1 by d in my reciprocal spacing. Again I can see this surface diffraction is either in terms of rows of items or ((Refer Time: 32:41)) quality to picture of the diffraction pattern just by considering what kinds

of names are present. So, just by considering the spacing between those rows, I can construct my reciprocal lattice.

So, from that I can eventually bring out my diffraction pattern. So, if I had a real space like this where I have say for surface of FCC 1 1 0 plane, then I can see that in my FCC 1 0 0 plane, it becomes more like this. I have atoms which are associated at this particular location as well on the face center. So, I have something on the faces as well. So, I can get something more like this and seeing their 1 0 0 particular plane, this particular plane, I can see that I have planes which are more like this.

I will get some sort of a construction where these atoms are much more closer as compared to these particular atoms. So, that is what we are seeing here that in this particular case we have a is less than b. It means I can even have, the atoms touching one another or they can have spacing much smaller than that of b. So, my spacing along plane b inter-planar spacing along bids much more scarce or spread quite far apart in comparison to my lattice spacing along this particular a direction.

What once I bring it to the reciprocal spacing, I can see if I keep my b constant if I keep my b and represent it as some b star it becomes 1 by my b. So, I have this particular thing is 1 by b. Now, I can see that in this particular case, in the real lattice I had a closer to one another, but in diffraction once I am getting a diffraction pattern.

This a has gone to a has gone much far apart. So, this particular 1 by a, has become much more sparse or much spread apart. So, here I had a less than b, now what I will get in reciprocal lattice spacing is 1 by a is much greater than my 1 by b. So, that is what happens in my reciprocal lattice. This happens in the real lattice this happens in the diffraction pattern I get 1 by a is much greater than 1 by b.

So, that is being retained in the diffraction pattern. This part I can also see is that the spacing of the rows, this was the spacing of rows in a. This has now become much further apart. My spacing of b was this much. So, let use a different color pen. So, I can show it more clearly that I had something b around this part. Now, it has decrease as compared to the a. So, in the real space I had a, I had b, in this case I had a less than b, but in this case in the reciprocal or the diffraction pattern my a dash has increased in comparison to the b dashed.

So, that is what we are able to see from the diffraction of those particular things. Once I consider only about the rows. Alternately seeing are following up only with this particular spacing or the spacing between the rows, it becomes much more difficult. Sometimes it is necessary that instead of following my rows I can go back to the particular item and take their diffraction pattern. So, I can also follow the position of atoms or planes and then come back to my diffraction pattern.

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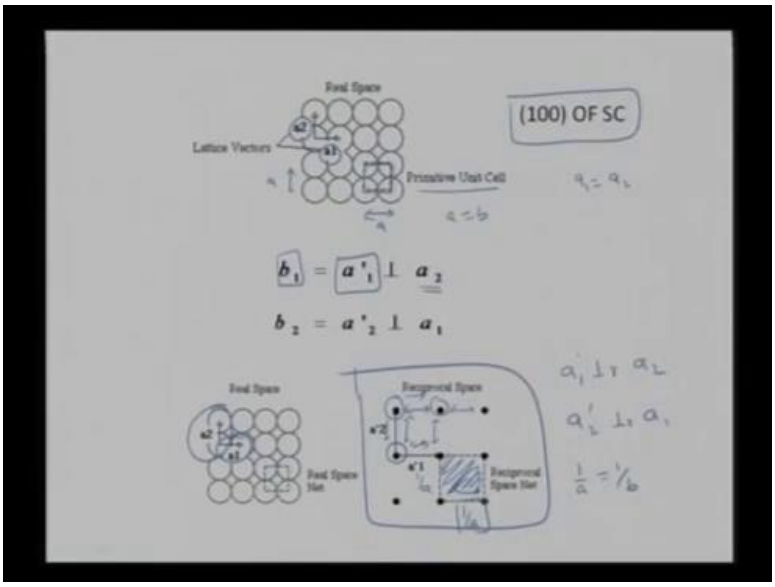

So, just tracking the rows or the spacing the rows it is sometimes not convenient. So, what I will try to go I will try to go with individual atom. So, let me come back to 1 0 0 plane of a simple cubic. If I take the real space as the vector a 1 as a vector a 2 and this is the lattice factor and they will a primitive unit cell. If I take a particular point it will form my primitive unit cell. Now, if I come back to my reciprocal lattice what I can see is my b 1 is perpendicular to the a 2 or I can also give it by a 1 dash. Now, my a 1 dash is perpendicular to a 2 and my a 1 was out here and my a 2, a 2 dash or my a 2 dash is now perpendicular to a 1.

So, I can see that, my a 2 dash is now perpendicular to a 1. That part I am seeing out here and again my a 2 is now creating a lattice vector in the reciprocal space, which is perpendicular to a 2. So, now my a 1 dash is perpendicular to a 2 and I have my a 2 dash which is perpendicular to my a 1. At the same time I had a 1, the distance a 1 which is equal to distance a 2.

So, I have this particular unit length this one was a, this one is also a. Once I come to the reciprocal lattice I can see that the distances are now similar. So, this was forming a square in the real space, it remains that 1 by a is similar out here 1 by a also similar in the along the a 2 axis. So, my a 1 dash axis is similar to the a 2 dash axis in terms of magnitude.

So, I have that it is still forming a particular square. So, this particular part I can see. So, I have my because in this case I had a is equal to b. So, 1 by are mains equal to 1 by b that is what I am seeing in the reciprocal plane 1 0 0 of simple cubic. So, in 1 0 0 plane of simple cubic, I have then it cell which has length constant similar in two direction. So, I have my lattice vector along the a side or the x axis equal to a along y axis is also again equal to band a equal to b. So, once I take it to the reciprocal lattice spacing I get vectors.

Which have magnitude of 1 by a and 1 by b. Since a is equal to b I get a similar reciprocal space which has again 1 by a equal to 1 by b. So, it forms a diffraction spot which are basically much more periodic, much more similar and which have similar spacing between the diffraction. Along this side my distance is same as along this side in the particular case of simple cubic of 1 0 0.

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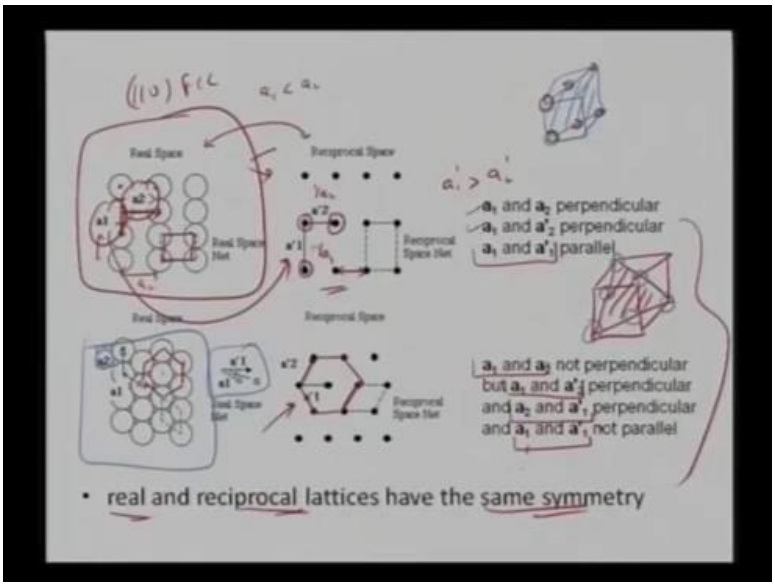

Now, let me go back to a different a different way in which we had considered the FCC lattice. So, in this particular case I take a particular FCC cell. I take 1 1 0 particular plane 1 1 0 and I can see I have particular items which are sitting along the sides. It will come

back to the different color. So, I can see that my atoms are located along these particular points. So, what I can see is, it is similar to the real space lattice or like here. So, this is a 1 1 0 plane of FCC and then what I can see along a 2 I have much more larger distances compared to the a 1. This will be the real space unit cell for this particular case, but once I come to reciprocal space, I can track each and every atom like this or a particular row of items for a particular plane.

What I can see is now my a 1 it has become 1 by a 1 and now my a 2 as become a 2 dash has become 1 by a 2. Now, I can see that initially I had this particular magnitude in a 2, which is now decreased and I had now a 1 which has now increased. So, in this particular case I had a 1 which was lesser than a 2. In this case I can see my a 1 dash is not greater than a 2 dash. That is how it is forming my reciprocal lattice and the distances are being defined by the original magnitude of the lattice vectors.

Again a directionality is also being retained. You can see the symmetric part is also being retained in the reciprocal space as well. That thing is again being given in the 1 1 plane of the FCC. So, if take the 1 1 1 plane of the FCC that becomes more like this. If I take 1 1 1 plane it becomes the 1 1 1 plane of the FCC. In there I can see that I have atoms which are located along the sides. So, those are basically located out here, out here, out here.

Then again on the center of the edges and if I if I keep expanding it, I get something which is more like this. Here in I can see that a 1 and a 2 they are not perpendicular to one another and they have some lattice vectors that are given along certain directions certain angles. So, I have certain some value of alpha which is associated now with the real lattice spacing. So, but my a 1 dash will remain perpendicular to a 2. That is what I can see this is my a 2 and now my a 1 will now be perpendicular to my a 2 direction.

So, this is my a 2 and the a 1 dash is now perpendicular to a 2. I had my a 1 now my a 2 dashed will be perpendicular to a 1. So, I can see that my a dash is perpendicular to a 1 and my a 1 dash is perpendicular to a 2. That is what the requirement of a reciprocal lattice. Again the spacing part, the spacing is basically same between this particular point to this particular point. So, from here to here and from here to here my lattice spacing is the same.

So, I can see that the space which has been traversed from this particular point to here or from here or from this point to here remains the same. That part is being shown out here, at the same time I can see that this particular symmetry is now being retained in the reciprocal lattice as well. So, this particular part I can see I have my this particular point it is being retained as such. So, I can see that the symmetry part is now being retained in the reciprocal lattice. Though it has changed by particular angle, but the symmetry part now, it is also 6 fold this also remains the 6 fold symmetry in the reciprocal lattice.

So, I see that my real and the reciprocal lattices they have the same symmetry. So, that part is also retained in the reciprocal lattice out here. So, all these the kind of similarities I can again show them that a 1 and a 2 are perpendicular a 1 and a 2 dash are perpendicular. At the same time a 1 and a 1 dash are parallel in my 1 1 0 FCC, but that is not true. In the second case where I have a 1 and a 2 they are not perpendicular, but a 1 and a 2 dash are perpendicular. Other way also a 2 and a 1 dash are perpendicular, but a 1 and a 1 dash are not parallel.

So, there can be certain complexities which can generate, but how it retains the symmetry of a particular crystal that is being given in the reciprocal lattice, that it retains the symmetry of the real lattice. In certain cases once we have some surface adsorption. So, I can have some matrix which has some adsorption of some particular other entity which is again ordered in certain manner.

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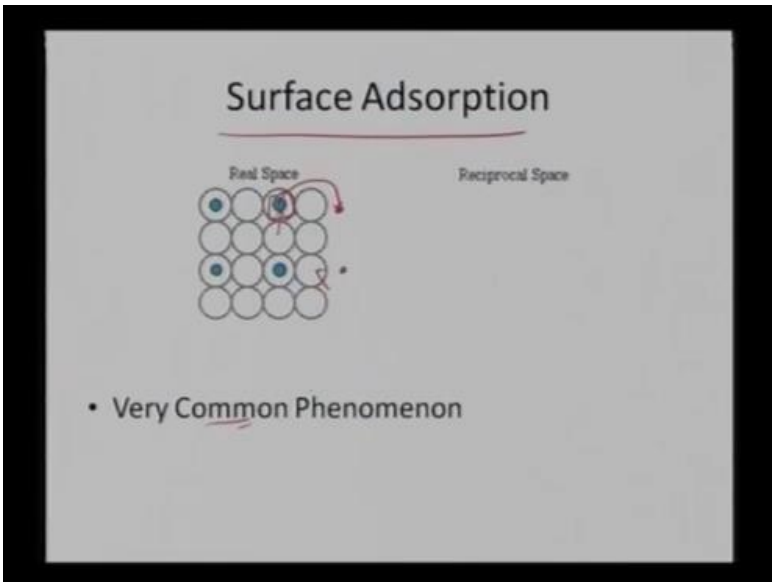

So, I can have this adsorbate which has a kind of symmetry in the, symmetry of couple monolates on the top of a particular matrix. This is very common phenomena because we can, we do see there is some specific adsorption of couple monolates on a particular material. So, how do they give out a particular diffraction pattern is more like this.

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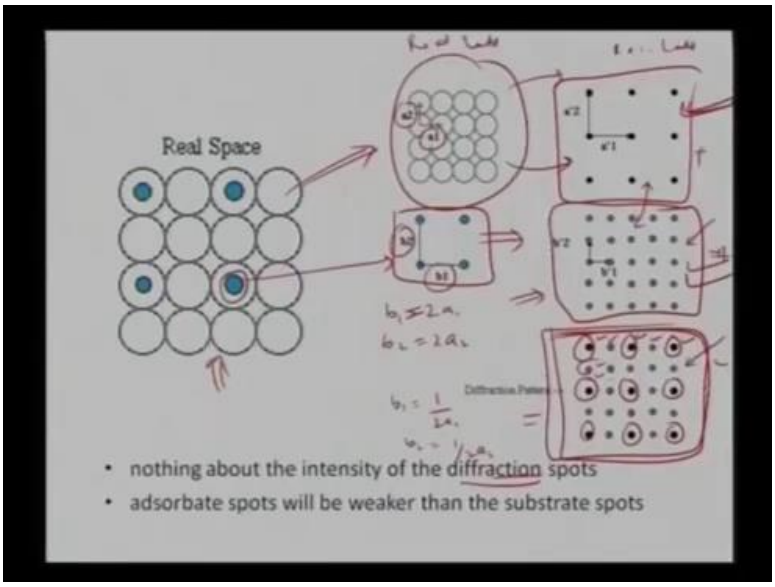

The matrix it the overall such can be divided into the matrix and the adsorbate which is being adsorbed on the surface. So, for a particular matrix I can see my length is a 1 a 2. I can take it back a dash 1 and a 1 a dash 2 in the reciprocal lattice, this is the real lattice. So, I can take it to the reciprocal lattice, reciprocal lattice. I can see that this particular part gives me certain diffraction pattern.

In the second case I have my b 1 and b 2 which are much greater than which are twice the a 1 and my b 2 is also twice the a 2. So, from the construction I can see from here. So, I can see that my b 1 is equal to 2 times a 1 b 2 is equal to 2 times a 2. So, what happens in the reciprocal lattice is my b 1 becomes half of that and my b 2 becomes half of that. So, what I get, for this I get much more diffraction spots as compared to my first case. I will see that my diffractions spots are much more in number.

Once I have a adsorbate which has spread much more scarcely, as compared to my overall matrix, but the problem is I have so less number of adsorbate on the surface of a matrix. That it is intensity might not be that great, but they will be overlapped over one another. So, if I combine this and this I get something which is this. So, what I am seeing

here is I am combining this part, the diffraction pattern which is coming out from the matrix, I am combining it with the diffraction pattern which is coming out from the adsorbate.

Then what I get finally, is the combined diffraction pattern and I can see I have a dark spots which is coming basically from the matrix out here. Then I have also some overlapping of these particular points, which are coming from the adsorbate. This is from the adsorbate, there is some overlapping of these points even at this particular points. So, I can see those things those particular things that I have combination between the matrix.

That diffraction spot which are coming from the matrix, the diffraction spot which are coming only from the adsorbate, but at the same time it is not telling anything about the intensity of the diffraction spot. So, I do not know what their intensity will be, but I can predict that this adsorbate spots will be weaker because they are few in number, the diffraction spot the intensity with which they will come out will be much more feeble.

So, I can see that I can overlap all this particular intensity point in 1 because I have combination of these 2. So, I can combine it and find out whatever initially the diffraction will look like. So, in summary we can say that to eliminate the complexity some complexity of representing a particular real crystal, the diffraction occurs. When the Ewald sphere stretches my reciprocal lattice plane and reciprocal lattice can be given by a set of parallel planes with all those planes can be represented by single point.

If I know their magnitude is equal to 1 by the inverse of the reciprocal, the reciprocal of the inter-planar spacing. So, reciprocal lattice what I am getting is a point, which represents a plane and the magnitude of that particular point from the origin is equal to the 1 by the inter-planar spacing between the planes which we have to represent. So, that is how I can spread it around and I can open it up because if I take a real crystal all the points all the planes tend to agglomerate at the origin.

So, there is much more segregation of all the points, if I start representing each and every plane. So, reciprocal lattice I am more or less I am like opening it up. So, I can see a much more periodic way of representing all the planes, all the set of parallel planes. I can define the direction, I can define the magnitude. The magnitude is equal to 1 by d, where d is the inter-planar spacing. So, I can in reciprocal space it will become 1 by d and I can also find their zone axis. I can also find the overall magnitudes and directions of all those

planes. So, that eventually tells the how the diffraction spots will appear once it is, once the particular material is getting diffracted.

So, it is the construction or the nature of the Ewald sphere and how it basically coincides with the lattice point, the reciprocal lattice point to give me, to obey the Bragg's law and give me a diffraction point. Again Bragg's law is a negative law. So, once so even when the Bragg's law is being satisfied it may not give a diffraction spot depending on what is the overall scattering factor and how it is basically merged into or what is the intensity of that particular point I may not even get a diffraction spot.

Also we learnt about how different planes can have, how different planes can provided kind of reciprocal lattice and how we can either go about following the row or the spacing between the rows or we can go with individual atoms which can get constricted back into the reciprocal lattice. We also saw how we can combine if more than one particular matric and how can we combine it to form a set of reciprocal lattice and it also maintained the symmetry of the real crystal.

So, that is the advantage with the reciprocal lattice. It can have it can accommodate wide variety whether we have access a 1 or a 2, whether they are parallel or not, whether they are, whether they are perpendicular or not, we can always grab it back into the reciprocal lattice. The axis are perpendicular to the other 2 or other 1 axis which basically defines the particular unit cell. So, that is what we learnt about the reciprocal lattice. I end my lecture here, thanks a lot.