Chemical Crystallography

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Lecture – 60
Review of Reciprocal Lattice and Bragg's Law in Reciprocal Lattice

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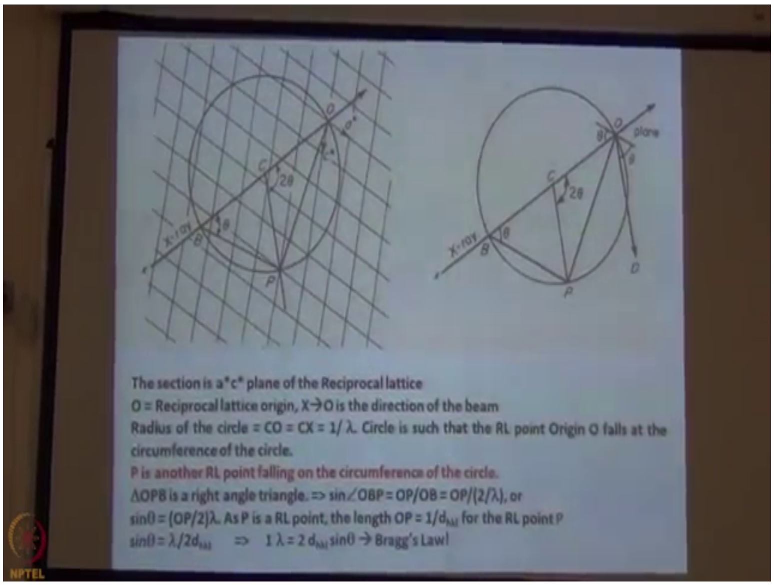

So, what we did yesterday is we try to represent the direct lattice using Reciprocal lattice constants. We define what is a reciprocal lattice and how the reciprocal lattice constants are related to direct lattice constants A B C. So now, we will try to see how Bragg's law is applicable to this reciprocal lattice and how that helps us in understanding the phenomena of refraction. See one is drawn here, I did not want to draw it and these two you have pictures or these two drawings are directly taken from (Refer Time: 01:02) textbook. So, I have a photocopy of that, I will give you that. So, today you do not need to draw these things, now better you try to understand.

So, what is represented here as that grid line represents the A star C star plane of reciprocal lattice. So, all the points point of intersections are reciprocal lattice points in A star C star instead of A and C plane I am saying it is A star C star. So, in that plane you have those points in a given added. Now, we use one such point which falls here as the reciprocal lattice origin and then I am trying to draw a circle like this in such a way that reciprocal lattice origin forms at the circumference and the radius of that circle is 1 by lambda which means this radius depends on the wavelength of radiation that is used, better we use copper or molybdenum, the size of this circle region.

So, now when I have drawn such a circle with reciprocal lattice origin here, we see that some points like this point P falls on the circumference of the circle, not all points fall on the circumference of the circle, some points exactly meet the circumference, some points are very close to the circumference say this one is meeting, this one is meeting, but not that or that or some other.

So, now, we assume that we exerting that I am using is in the plane of that A star C star lattice. So, beam is not perpendicular to that A star C star plane. It is in the plane of the lattice the A star C star plane. So, now, if I see that this direction is my the beam direction of the beam and I find that this particular point is at the circumference.

So, I am now drawing a triangle from B P O inside the circle. This same figure is drawn here without the grid now. You see there is a plane which is like that. This direction is giving you a particular plane and from this point to that point this is the distance between two sets of parallel planes. So, what is that distance in reciprocal space?

Student: 1 by.

1 by d h k; if the particular point P represents a plane h k l in the direct lattice, which means the reciprocal lattice point corresponding to a plane h k l. So, that distance from O to P is nothing but 1 by k. So, now, if we look at this diagram, X-ray beam falls on that planar angle theta and it should refract in the direction of O D. So, this would be the diffraction direction, which is then parallel to the direction C P. It was this angle when it is 2 theta this angle is also 2 theta.

So, this will be the direction of X-ray diffraction. So, now, if we look at the particular triangle O P B, that is O P B; this is right angle triangle. If this is theta that angle is also theta. Now if we try to see what is sin O B P; O B P sin O B P, so, what is sin O B P? O P by O B.

Student: (Refer Time: 05:43).

O P by O B, what is O P?

Student: 1 by d h k l.

1 by d h k l, what is O B?

Student: (Refer Time: 05:53).

The diameter of the circle, or is the radius of the circle? 1 by lambda. So, diameter of circle is 2 by lambda. So, I have put O P by 2 by lambda and then I am changing that sin O B P as sin theta and rearranging it as O P by 2 into lambda. So, now, P being the Reciprocal lattice point with I am replace O P by 1 by d h k l. So, if you put O P equal to 1 by d h k l it simply becomes lambda by 2 d h k l. So, on rearrangement it is nothing, but Bragg's law. What we get to know from this? We get to know from this that if we draw a circle of radius 1 by lambda taking the crystal as the center and the corresponding Reciprocal lattice is drawn with respect to the crystal position then any point which falls on the circumference of that circle meets that condition and gives you diffraction. No other point gives you diffraction.

So, if I place my crystal at point C static. I have a star c star like this maybe a star b star like that and b star c star like this; so, three different sets of orientations. So, now, instead of thinking that this is the circle if we assume that it is a sphere of 1 by lambda radius. So, all the points around C crystal which falls in the circumference of a sphere of radius 1 by lambda, we satisfy that one and will cause diffraction.

So, by expanding this circle into a sphere we can think of that if I correct crystal here. There is an imaginary circle around it or sphere around it rather the imaginary sphere corresponds to a set of Reciprocal lattice point which is not the circumference. Of course, there are Reciprocal lattice points everywhere in the sphere, but those will not cause deflection, until and unless one Reciprocal lattice point falls on the circumference of the sphere it does not cause diffraction.

So, now we can easily understand if I have a mechanism to rotate the crystal. If I am able to rotate the crystal above this axis, suppose, I mounted the crystal in such a way that b star is that direction and this plane is my A star C star plane. If I rotate it what I am going to rotate? Is this grid? If I rotate this grid, at some point this Reciprocal lattice point which is inside will cross somewhere here because diffraction. If something is here at some point we cross this region will cross diffraction in different direction. So, all the points which are there in this diagram all the point of intersections by rotation of the crystal can be make to pass through the circumference of the of the sphere that we are constructing assuming the wavelength is lambda.

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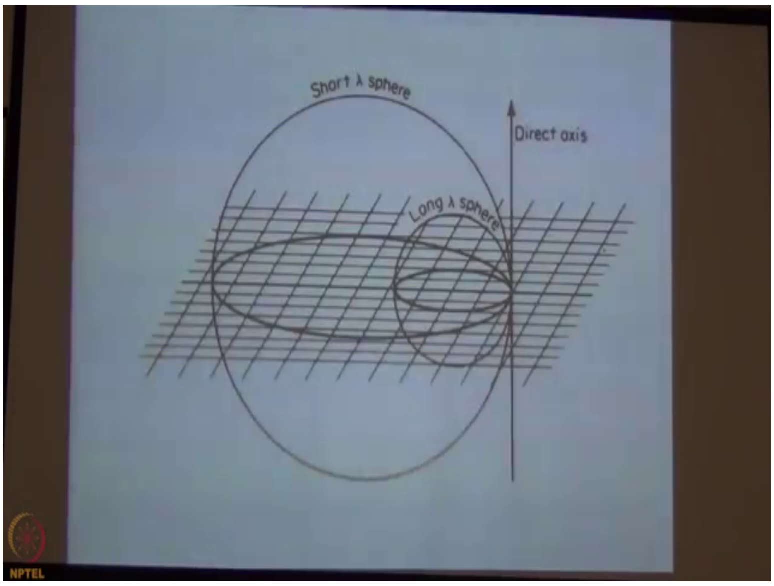

So, now we can have different wavelengths. If lambda is large for suppose for copper 1 by lambda is small. So, the radius of the sphere is small. So, if I use a large wavelength I have only a strain small sphere. So, only is much smaller number of Reciprocal lattice points can be made to pass through this small sphere. Whereas, if I use silver molybdenum radiation or silver radiation, which are much smaller in wavelength. What is wavelength of copper? Approximately 1.50, molybdenum is 0.71, silver is 0.68. Just let me know and I think it is 5 unit, 0.5 unit.

So, it is so small that this sphere becomes much larger. When the sphere becomes much larger immediately your conclusion is I can access larger number of Reciprocal lattice points. How the position or reciprocal lattice point is related to revolution? Smaller the d value larger is 1 by d further is that reciprocal lattice point provide (Refer Time: 11:32).

Student: (Refer Time: 11:35).

That means, for a particular lattice if you skip on chopping thinner, thinner, thinner, thinner slice with smaller wavelength you can go to much thinner slice much thinner d values because 1 by d is large and that large d value can be accessed by the larger sphere that we have considered here that is the short lambda sphere, short lambda means smaller wavelength sphere, smaller wavelength sphere is larger. So, it can access more number of reflections, more d values which are smaller and smaller and smaller.

Now, the question is which Reciprocal lattice points can be pass through these sphere? Are those only the ones which are very close to that, is there any restriction on that or those would be only inside the points, but inside this sphere?

Student: (Refer Time: 12:46).

What is your answer?

Student: (Refer Time: 12:50).

Which are the reciprocal lattice points that can be made to pass through the circumference of the circle is it only those which comes inside during rotation or we the ones which are at some distance from here or anything ?

Student: (Refer Time: 13:16).

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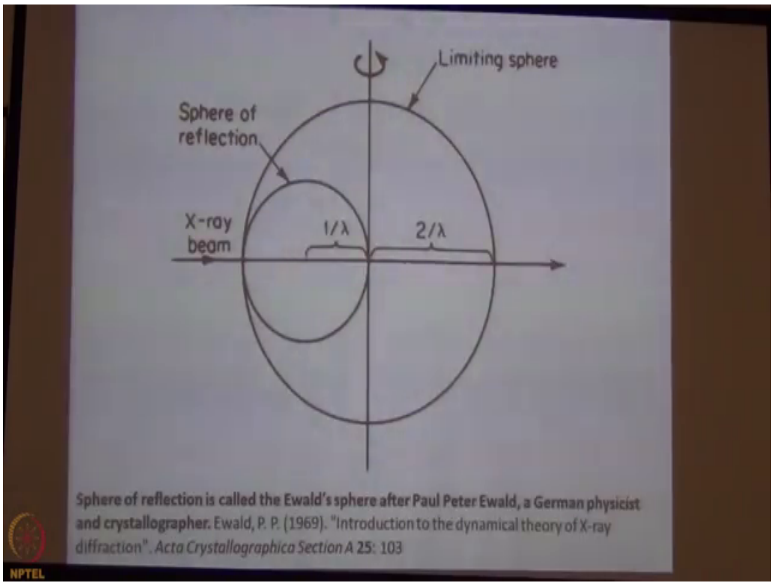

The answer is here.

Student: (Refer Time: 13:24).

The sphere that we are talking about is this one of radius 1 by lambda, diameter 2 by lambda.

So, when a spot when a Reciprocal lattice point is passing through that sphere in progress diffraction. Now, taking that as a circumference and this as the center if I draw another sphere of radius 2 by lambda I get something called a limiting sphere. Geometrically all the Reciprocal lattice points which fall within that sphere of radius 2 by lambda by rotation of the crystal which is placed here can be made to pass through that sphere? The ones which are outside this sphere cannot be made to pass through that sphere right. If I rotate the crystal in this plane whatever planes are there, whatever directions of Reciprocal lattice are there in that particular plane which is inside the sphere can pass through that sphere outside, no.

So, this particular smaller sphere is called the sphere of reflection and that one is called the limiting sphere of reflection. So, limiting sphere is a larger sphere which can be accessed. The reflections falling in the limiting sphere can be accessed and can be recorded provided when they pass through this sphere of radius 1 by lambda right. So, this concept was introduced by Peter Ewald and the sphere of reflection is called Ewald's sphere after the name of Peter Ewald.

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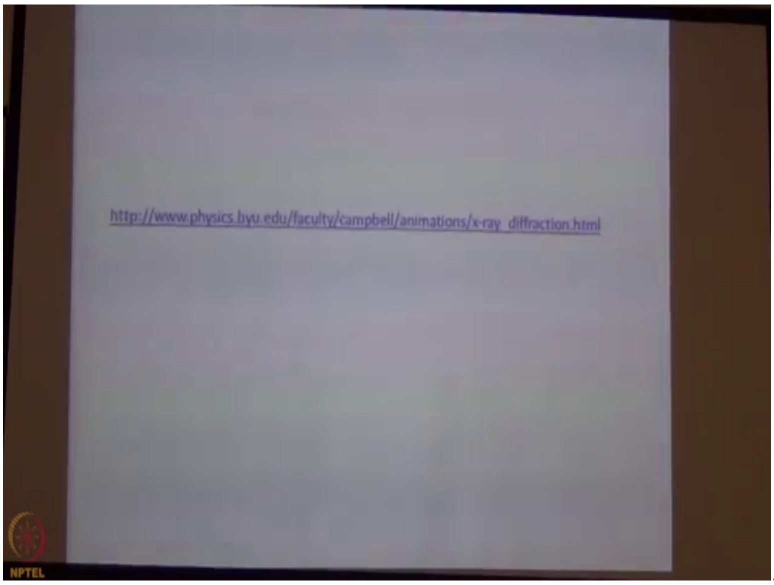

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So, let us see one video hopefully the internet Ewald's sphere at internet Ewald's right.