Chemical Crystallography

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Lecture – 58
Review of Reciprocal Lattice

Today, I will start a new part of Crystallography, which is very important. I will introduce into Reciprocal Lattice, because this is the most important part that one should understand in the theory of diffraction. What is reciprocal lattice, and how is it important?

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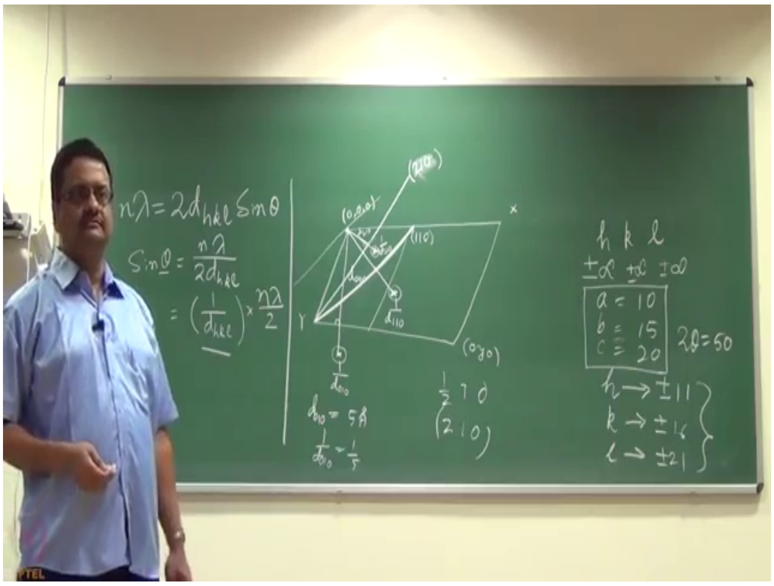

See we have gone through Bragg's law right. What is Bragg's law? n lambda equal to 2 d sin theta. So, the relationship is sort of inverse, when you calculate what is the work of sin theta, which is n lambda by 2 d h k l, which actually means the d h t l involves with respect to theta. And larger the d value smaller is d value of sin theta. And it is also difficult to understand, when we lattice is considered, and you try to draw the planes inside the ring itself with different d values.

What happens is in the lattice, suppose it is this is my unit cell. Some planes, which are parallel to the faces are easy to see. Some planes, which are like that are not so difficult to see. But, then with the planes are intersecting all the three axis in all possible directions, it becomes difficult to imagine. And then what are we saying in Bragg's law is the constructive interference of X-rays upon diffraction occurs, when? The phase difference.

Student: Path.

Path difference is.

Student: (Refer Time: 02:43).

Integral multiple of wavelength. So, now what we are trying to see is let us try to see the diffraction across the set of parallel planes. What we want to do, we want to measure all the reflections from all different planes. So, what we need is all the crystallography planes that one can consider inside the plane itself has to be placed in front of the beam in such a way that it meets diffraction condition, otherwise you will not get a full data set.

Because, as I said a full sphere data corresponds to h k l values ranging from plus minus infinity to plus minus infinity with this gives you the complete data set. And when you have suppose a, b, c values like 10, 15, 20, then h is about plus minus 11, k is about plus minus 16, and l is about plus minus 21 gives a full sphere data up to 50 degree 2 theta. (Refer Time: 04:18) see at give requirement for a full data set for an beam structure solution.

So, if you want to collect data up to 2 theta equal to 50 degree on such element itself, this is set will represent the full sphere data. So, you can imagine, how many large number of combinations are possible, and how many reflections are to be corrected that means you have to orient the crystal in that many ways. Then only, the beam will meet the reflection condition, because here the beam is fixed, you have to only rotate the crystal in different directions.

So, you have understand or to make a procedure or a strategy for data collection it is not very easy, if we just consider the planes. So, instead what is considered is points every plane in the direct lattice is converted to a point by a particular method. And then we will see that those points, which are the imaginary points originated from the real planes in the lattice. We will correspond another matrix, we form a new lattice. And then it will be easier for anybody to understand how, when you place a crystal those lattice points or reciprocal lattice points are around the in itself around the crystal.

So, what we try to do is to suppose, I have a two dimensional lattice. I have drawn two unit cells. And this is my origin 0, 0, 0. So, now what I am trying to do is I have one set of parallel planes going like that. So, the perpendicular distance between them is what see these plates suppose, if I say that this is direction X, this is directional Y, and Z is for view, this plane which is like this is parallel to X axis, and parallel to Z axis.

So, a corresponding mirror index for this plane will be parallel case means 0 y 0. So, this distance is d 0 y 0. What is y, it is nothing y at 1 unit. So, this distance is 0 1 0. Now, if set up parallel planes, which are 0 1 0 set up planes, I am extending this line or cutting this line at a point start, which is at a distance 1 by d 0 1 0. So, this particular start mark point represents, this set of parallel planes in the lattice.

So, this is the reciprocal lattice point corresponding to d 1 0 d 0 1 0 corresponding to 0 1 0 plane. So, for this plane this is the point, it can be outside, it can be inside depending on what is the value of d. If the d suppose, if d 1 0 1 0 is 5 inch, so this is 5, so 1 by d 0 1 0 is 1 by 5, so it should be somewhere there like that. Now, you can have a plane like this, what is this plane?

Student: (Refer Time: 09:30)

It is parallel to Z.

Student: (Refer Time: 09:35).

One sorry 1 1 0. So, this is 1 1 0 plane. So, if I drop a perpendicular from here to there is my d 1 1 0, but then I am stopping that at a point here at a distance 1 by d 1 1 0. So, 0 1 0 plane makes a reciprocal lattice point here, 1 1 0 plane makes a reciprocal lattice point there. What about this plane?

Student: (Refer Time: 10:37).

This cuts X at half.

Student: (Refer Time: 10:39).

Y at 1 parallel to Z.

Student: (Refer Time: 10:44).

So, it is 2 1 0 now 1 2 0 right 1 2 0, because it does x intercept is half, y intercept is 1, and 0 sorry this is not point two this is 2 1 0, so 2 1 0 2 1 0.

Student: (Refer Time: 11:07).

2 1 0 intersect is half 1 0 10 reciprocal with begins to 1 0. So, now from here if I draw a perpendicular, this distance is d 2 1 0, I cut it at a point where the distance is 1 by d 2 1 0.

Student: (Refer Time: 11:35).

So, now we see each and every plane in the unit cell is getting converted to a point, where is the point located at 1 by d h k distance.

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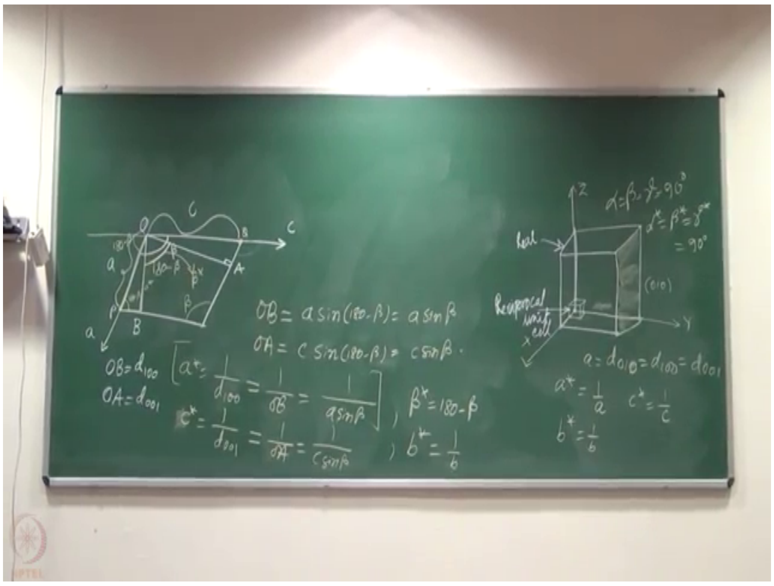

So, if I draw, if I suppose draw a cube, and then suppose from this origin to this distance suppose, this is X, this is Y, and is Z. What is this distance?

Student: (Refer Time: 12:36).

From Y we move that is a, which is equal to this particular plane is 1 0 1 0 plane, so a equal to d 0 1 0, it is equal to d 1 0 0 is equal to d 0 0 1 for cubic system. So, now for this edge length, suppose it is 10 edge form cubic. Where should I cut this point?

Student: (Refer Time: 13:27).

1 by d.

Student: (Refer Time: 13:30).

So, I have it at some point here 1 by d is 1 by 10, where do I have this one is again at 1 by d, this one 1 by 10. So, what I form is a small cube like that which is my reciprocal unit cell. So, the reciprocal unit cell length a star is nothing but 1 by a, b star is equal to 1 by b, c star is equal to 1 by c is a star b star c star are the reciprocal edge lengths.

In case of cube two orthorhombic excluding hexagonal in between cubic, tetragonal, and orthorhombic. When the axes are at 90 degree apart right the angles are 90 degree, this relationship is valid. So, this real unit cell gets converted to a unit cell or reciprocal lattice. So, this relationship of a star, b star c, star is valid for cubic orthorhombic, and tetragonal. When the angels are 90 degree, what happens in case of monoclinic. If this angle is beta, what are these two sides?

Student: (Refer Time: 16:13).

A and c, your b is here. And b is both perpendicular to a and c right. So, now I think this has solid beam following the same rule. What is the distance between these two, what is the distance this perpendicular distance between these two. This plane is parallel to b and c that is 1 0 0. So, this is suppose if I write this as O B, this what is the distance between this and that plane? This plane which is stacking c at 1, but parallel to a and b.

Student: (Refer Time: 17:40).

0 0 1 right. what is this angle inside?

Student: 180 minus B.

Correct, how?

Student: older B and (Refer Time: 18:57) also with the opposite rule yes.

Which angle, this angle you have complete under

Student: Angle (Refer Time: 19:05).

I was coming like that if this is beta that is beta, so this is also beta.

Sin c now this is beta.

Student: Yes, (Refer Time: 19:13).

As these two are 90s.

So, internal angles would be 180 minus theta. So, now my reciprocal lattice of monoclinic would correspond to a star, which is equal to 1 by d 1 0 0 like that. And c star would be 1 by d 0 0 1 done with this like that. a star equal to 1 by a right, a star is equal to 1 by a that is 1 by d 1 0 0 or d 0 1 0 or 0 0 1 it is that is cube.

So, now here a star is 1 by d 1 0 0. Now, you tell me what is d 1 0 0 in terms of a and beta. This length is what a, this length is c. If this angle is beta, what is this angle? If this is beta, this is 180 minus beta.

Student: (Refer Time: 20:54).

So, this is also 180 minus beta. So, now can I write what is O B? Considering this triangle, what is it?

Student: A sin.

a sin.

Student: 180.

180 minus beta is equal to.

Student: A sin beta.

A sin beta. Similarly, if I take this point as Q, can I write what is O A? O A is c sin 180 minus beta is equal to c sin theta. So, a star is 1 by d 1 0 0 that is O B that is equal to 1 by a sin beta, and this equal to 1 by O A, which is 1 by c sin theta. And this angle is the reciprocal lattice angle between d 2 reciprocal lattice axis, so that angle should be termed as beta star, so that beta star is equal to 180 minus beta.

Here since alpha equal to beta equal to gamma equal to 90 degree. Alpha star equal to beta star equal to gamma star, once again equal to 90 degree. Here in this case we did not have to change the angle, because they are mutually perpendicular. Here the angles are not mutually perpendicular. So, now in monoclinic system a star is 1 by a sin beta not only 1 by a. c star is 1 by c sin theta not just 1 by c. What is b star? What is b? B is here b is perpendicular to both c and a. So, a situation is like cubic.

So, beta star b star is just 1 by b right. So, now you can imagine, if I have to do it for triclinic, what will happen? The angles are alpha beta and gamma. So, each of these terms will have at least 2 sin terms sin alpha, sin beta, sin beta, sin gamma, sin sin alpha, sin gamma. And also two about a and c and gamma.

So, I would like you to go through the textbook and see these are formula, we get a better idea. I do not want to be rewrite those, but we have to do something else in the class. So, this is how one can derive the reciprocal lattice constants for different unit cells is there any question at this point. We are dropping a perpendicular cutting the particular at a distance 1 by d of that I am placing a point that is not we are doing.

Student: (Refer Time: 25:36).

Student: (Refer Time: 25:38).

Student: (Refer Time: 25:42) we have to intersecting b (Refer Time: 25:43) around a and c.

So, what we are talking about b star if the plane, which is like this and from here I drop a perpendicular that anywhere since it is perpendicular here, because this axis is 90 degree here, 90 degree there. So, will you talk a perpendicular here, it is already 90 degree. So, one it is a 1 by b is transacted right that means, this a case which your cubic, tetragonal, orthorhombic system.

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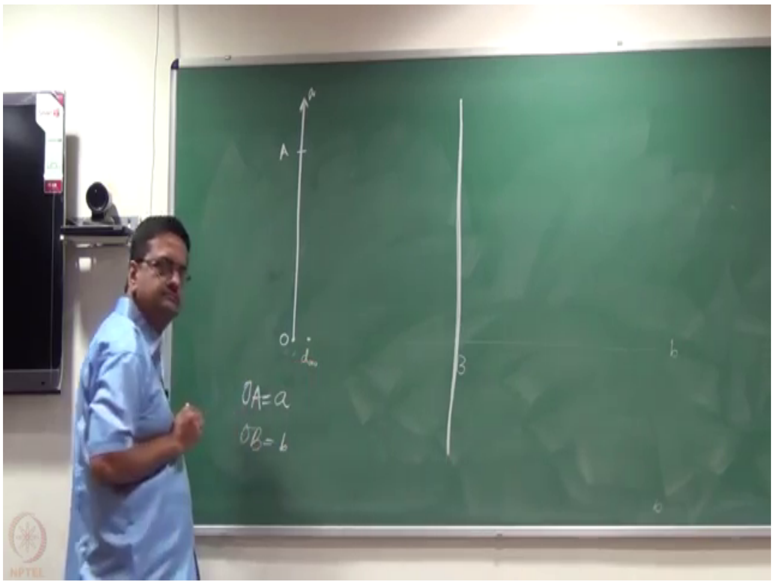

Now, I am going to draw only one axis instead of three. Suppose, this is my a direction, and I am starting from this origin O. And my page length A is here. So, O A is equal to a. So, now if O A is like this, I can have planes parallel to O A like that. All planes parallel O A can be like this, all planes parallel O A can be like that, all planes parallel O A can be like this right. In any way, parallel planes are going to be like that.

So, what does it indicated from this point if I drop a perpendicular to this plane, and I cut it at a 1 by d distance it falls here. A plane which is here I drop a perpendicular distance is smaller, so 1 by d is larger falls here, and so on. So, the plane which are like this. All the reciprocal lattice points will fall in this length. If I have the plane like this, the reciprocal lattice points will fall in this length.

So, as a result all these reciprocal lattice points that are going to be formed, we will form a plane, where I will have points equidistant from you are is it like not equidistant, and it will form a new lattice. It will form a three-dimensional video distinct.

How get a c with 1 set up planes ? Suppose, this is a, and this dimension is suppose my b direction, and this is where it comes one. So, this OB is the edge length b suppose. So, the plane which start this at that point as a distance d equal to 1 by b. Suppose, that b is 10, then it a chop it at a distance 1 by 10 at move this point that is my reciprocal lattice point corresponding to d 0 1 0.