Chemical Crystallography
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Basics, Symmetry and Equivalent Points in Crystallography
Lecture - 05
5 Fold Symmetry and 2D Lattices

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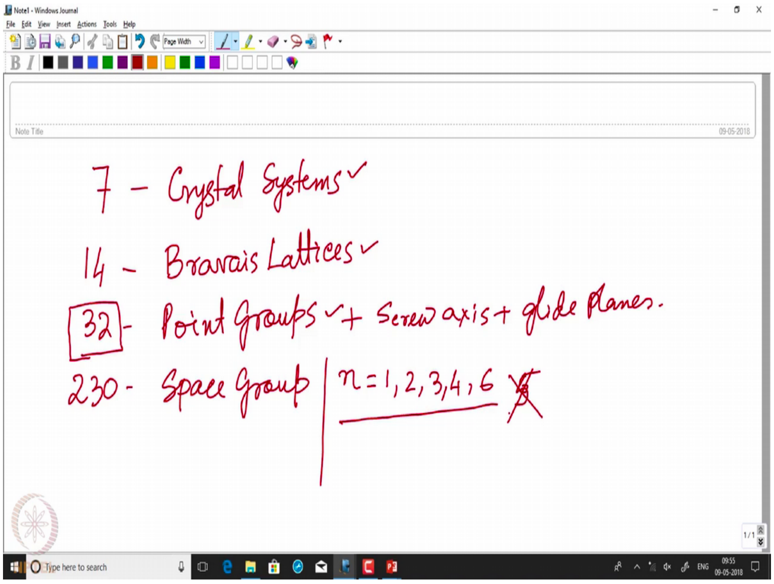

Welcome back to the course of Chemical Crystallography. In last 4 lectures, we have learnt some of the basic aspects. So, what we learned is to remember a few set of numbers. For example, we have discussed about 7, which indicates 7 crystal systems. We have learned about 14 Bravais lattices, 32 point groups. And we just indicated that there are 230 space groups which utilizes these 7 crystal systems, 14 Bravais lattices and the symmetry elements that are present in 32 different point groups and in addition we have two types of symmetry elements screw axis and glide planes.

So, now as I indicated the number 32 is restricted simply because the crystallographic symmetry elements, the principal axis of symmetry which we identified as n has a restriction of 1, 2, 3, 4, 6 only. And there is no say chance of having a 5 fold symmetry. So, today we will start by doing a simple geometrical derivation to identify why we do not have a 5 fold symmetry in three-dimensional lattice.

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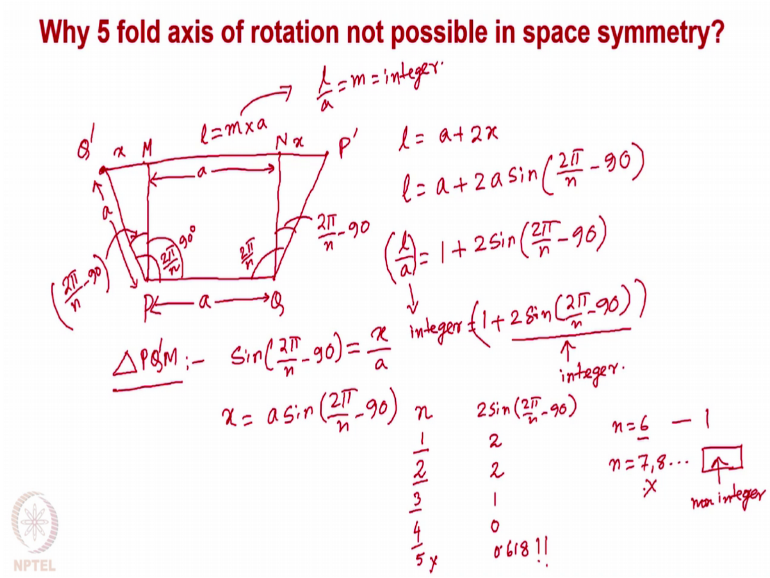

So, what we know is in a crystalline system in a periodic arrangement of atoms or molecules, we have two atoms located at unique edge length; and those two atoms are repeated in along x, y and z following a particular translational symmetry. So, if we take two lattice points for example, two lattice points P and Q are two positions of two objects at a distance of unit cell length a. Now, if we rotate the line P Q in the left side so that we end up reaching another lattice point Q prime somewhere else in the lattice. And the angle that we travel is designated as 2 pi by n; n signifies the n fold rotation of about a particular axis, so that we can reach another lattice point equivalent to Q at Q prime.

Similarly, Q P we are rotating in the opposite direction; and reaching another lattice point similar to that of P prime by rotating about the same and a 2 pi by n. So, obviously, the distance from Q to P which is l should be some integral multiple of the unit cell edge length a, because these two points P prime and Q prime are representative of two lattice points at a given distance. And as we know P and Q are at edge length a, so the distance between P prime and Q prime has to be integral multiple of a.

So, now let us draw a perpendicular from P to P prime Q prime, and another perpendicular from Q to P prime Q prime, and we identify those two points as M and N. So, now, the distance m, n is nothing but a; distance M Q prime is x, and N Q prime is also x, which indicates that l equal to a plus 2 x. So, now the point here is 90 degree which indicates the outer angle here is 2 pi by n minus 90. The same is valid on the other side.

So, now if we consider a particular triangle P Q prime M, in that particular triangle P Q prime N M, we can write sin 2 pi by n minus 90 equal to x by a, because P Q prime is also a, is that right. So, now, if we try to see what is the value of x, x equal to a sin 2 pi by n minus 90. So, now, from the expression that we have on the left hand, on right hand side here, l equal to a plus 2 x, which means 2 a sin 2 pi by n minus 90. So, if I now rearrange, l by a equal to 1 plus 2 sin 2 pi by n minus 90. So, now, this l by a from this expression turns out to be m which is an integer. That means to have an integral value of this l by a the right hand side which is 1 plus 2 sin 2 pi by n minus 90 has to be an integer which means this 2 sin 2 pi by n minus 90 has to be an integer.

Now, let us see what happens, we are going to write the values for n and corresponding 2 sin 2 pi by n minus 90. For n equal to 1, it is 2 pi minus 90 which means 270. So, n equal to 1, the value of 2 sin 2 pi by n minus 90 turns out to be 2. For n equal to 2, this number once again turns out to be 2; n equal to 4, this number turns out to be 0, if you see then this comes out to be a non-integer. For n equal to 5 this number turns out to be 0.618. And once again for n equal to 6 the number turns out to be 1. And any value for n equal to 7, 8 or whatever, the number does not turn out to be non-integer. So, it is a non-integer, so that indicates that in case of three-dimensional periodic systems, we can only have values of n as 1, 2, 3, 4, 6, and not as 5 or anything higher than 5. So, this puts a restriction on the number of principal axis that 1 can think of in crystallography.

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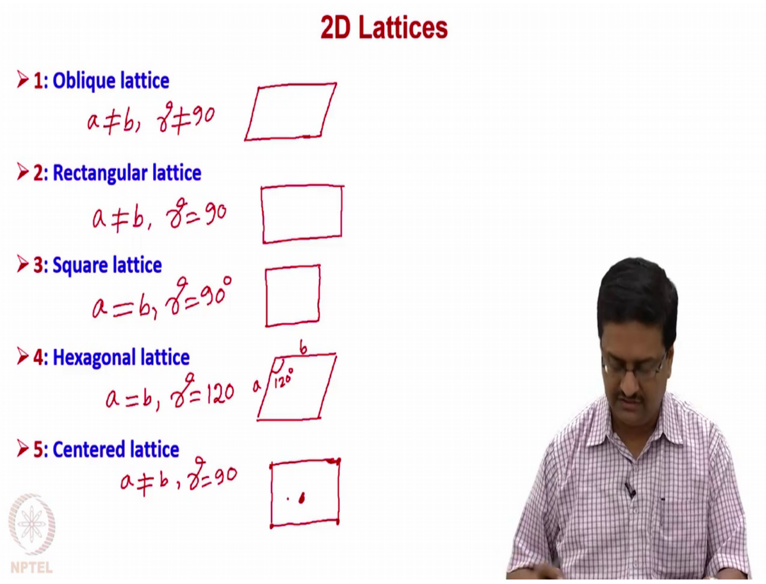

So, now depending on this understanding that how many different types of symmetry elements are possible, let us try to consider different two-dimensional lattices. In the previous class, if you remember, we have discussed about one-dimensional lattices; and there were 7 of them. So, now, here we will talk about these two-dimensional lattices which are five different types. So, when we say it is an oblique lattice the restriction is like a not equal to b; and the angle between a and b gamma which is not equal to 90 degree. So, an oblique lattice should look like this. When we say it is a rectangular lattice, it actually means a not equal to b, and gamma equal to 90 degree which means we should draw a rectangle. So, the angles between the axis are 90 degree.

Now, the third type of lattice is a square lattice where a equal to b, and gamma equal to 90 degree, what we get is a square. The next one is hexagonal lattice where a equal to b, and gamma is not 90, but it is 120 degree. So, in that case, the lattice would look like this where the two edge lengths are same and the angle between the two is 120 degree.

Now, the last type of lattice is a centered lattice where a is in general not equal to b, but gamma is equal to 90 degree; in that case what we see is we draw a rectangular lattice and we have a centering at the middle. So, what does it mean that we have atoms at 8 corners or lattice points at 8 corners and at the center. So, this particular lattice is called the centered lattice, f s centered lattice, one face is centered.

So, now before going into further details of two-dimensional space lattices, once we have talked about lattice centering now if you remember I had asked you to solve a problem by a tetragonal lattice does not have a tetragonal lattice does not have a face centered lattice. So, let us try to understand why we do not have a face centered tetragonal lattice.

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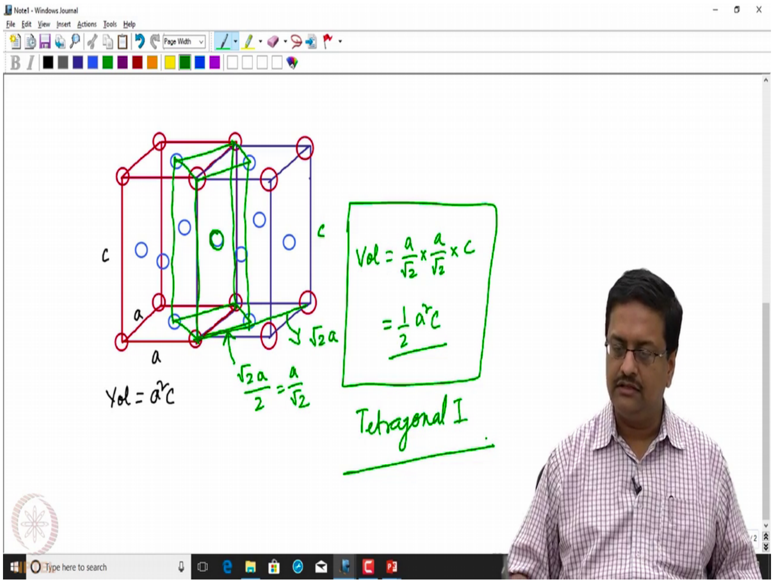

So, suppose I am drawing a tetragonal lattice here. This is the tetragonal unit cell and then I am putting corner atoms in red and placing them at all 8 corners. And then I will draw the face atoms with blue sorry; we will draw the face atoms using a different colour. So, this is a face centered tetragonal lattice, but as I say a face centered rectangular lattice does not exist. Before we go further let us determine the volume of this lattice this is a. This other side is also a, because it is tetragonal a equal to b and not equal to c. So, the volume of this lattice that we have drawn is equal to a square c.

Now, I want to extend this lattice on the right hand side and join it with the previous one. This is the adjacent tetragonal lattice. And I will once again draw the corner atoms in red; and the face atoms as it was blue we will add those face atoms here as well. So, now we have two adjacent face centered tetragonal lattices. Now, see what I am going to do, I am going to draw a different lattice using green colour by joining the face atoms to the corner atoms and joining the atoms placed in on two faces and then the green line indicates a new lattice.

So, now you see what has happened the green lattice has atoms at 8 corners and a lattice and a lattice point or one atom at the center of this green lattice which means it is in the body center of that particular lattice. Now, why should we consider this as the correct Bravais lattice, let us see the volume of it. See the diagonal here is root 2 a. So, the edge length that we have here is root 2 a by 2 which is a by root 2. So, the corresponding volume of this green lattice is a by root 2 into a by root 2 into c, because the height has not changed. So, what we have is half a square c. So, the volume of this green lattice is half that of original red lattice which we had drawn at the beginning.

So, to explain this three-dimensional figure which we have drawn as face centered tetragonal lattice, it can be described as a body centered lattice having half volume. So, when we have possibility of representing same crystal structure using a smaller volume, we should use that as the basic lattice instead of the one which has a higher volume. And this question arises every now and then when we try to index a crystal system. We should always look at the unit cell parameters and the volume of the lattice that we are getting from a crystal data and see which is giving you the lowest volume with highest symmetry.

So, suppose if there are choices between two different tetragonal lattices, we should choose the volume choose the lattice which has the smaller volume. If we have a choice between two different symmetry lattices, then we should choose a lattice of higher symmetry than a lower volume. So, this is where we need to make a decision what lattice should be chosen at the beginning of any crystal data collection.

So, in this particular case, what we saw is that tetragonal I has a volume which is half compared to that of tetragonal f lattice. And hence we consider this as the Bravais lattice tetragonal I. So, in these few lectures, what we have learned our basic aspects of x ray diffraction we have talked about the different crystal systems 14 Bravais lattices, the origin of 32 point groups. We have discussed about different symmetry elements like screw axis, glide planes and things like that. So, in the future lectures, we will utilize these basic concepts to draw 2D space lattices with their corresponding symmetry elements, symmetry operations incorporated. So, when I will be drawing those 2D lattices, I will be using the symbols and notations that has been taught to you in the previous lectures. So, it is used, it is going to be useful. If you look at the textbooks and come prepared for the next lectures.