Crystals, Symmetry and Tensors
Professor Rajesh Prasad
Department of Materials Science and Engineering
Indian Institute of Technology Delhi
Geometric proof of Crystallographic Restriction Theorem

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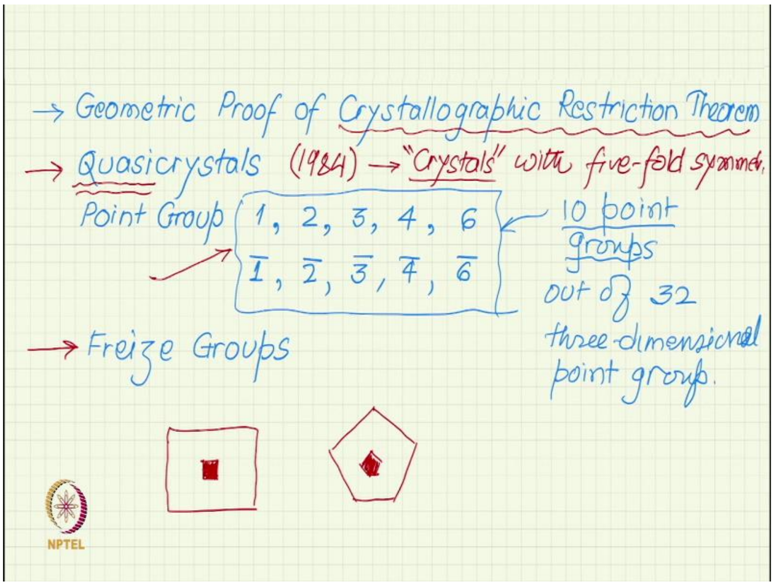

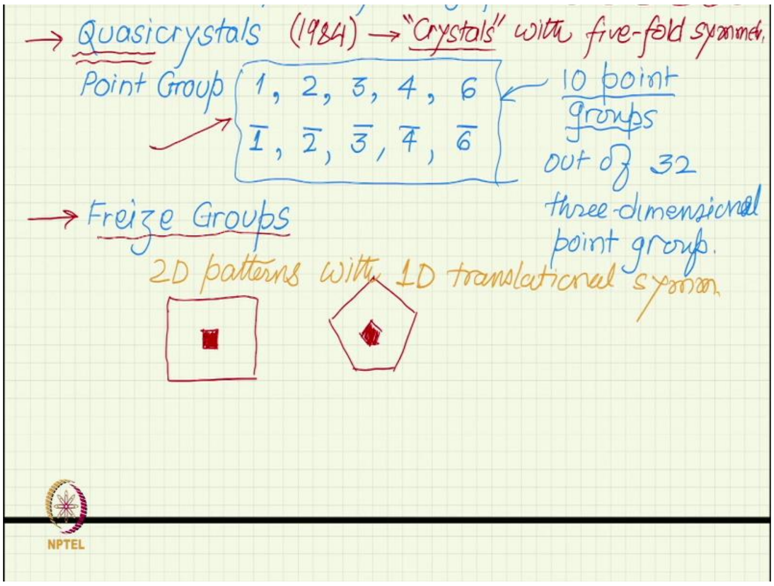

Last class we gave a sort of algebraic or matrix proof of the fact that only these symmetry axes can be part of a crystal. Only these symmetry 10 symmetry axis can be part of the crystal. So, these themselves are 10 point groups, these are 10 point groups because as you have seen that when we say a 4-fold axis, it is actually 4 different operations and identity operation which is a 0-degree operation, then 90, 180 and 270.

So, these 4 operations we have seen form a group. So, 4 means, it can mean it can mean different things, 4 can mean a number 4 or 4 can mean a 4-fold axis. So, that is a geometrical axis or it can mean the point group operation 4-point group 4 which means, the 4 symmetry operations or 4 rotations which are associated with this point group.

So, these 10 symbols 1 to 6 and 1 bar to 6 bar represent 10 different point groups out of 32, 3 dimensional point groups. So, you have already now met 10 point groups as we proceed in proceeding the course, we will try to meet the other 22 point groups which are not in this list. So, that that matrix or algebraic proof we gave this class we will visit a geometric proof for that the same thing.

Because algebraic proof we never drew any lattice or vector or anything, there was just a matrix and we decided that the matrix is made up of integers and we decided that or not we decided we proved that and the trace of the matrix is 2 cos theta plus 1 and since 2 cos theta plus 1 became integer. You found that only these 6 symmetry these 5 symmetry rotations are possible or 5 symmetry axis are possible.

1,2,3,4 And 6 we did not prove 1 bar 2 bar 3 bar, but that is left as a simple exercise for you the prophage simple because all you have to do is to multiply that matrix with the matrix representing inversion which is which will multiply all the diagonal terms by minus 1. So, you will again get the same result instead of saying 2 cos theta plus 1 is an integer now, you will say negative of 2 cos theta plus 1 is an integer.

But finally, you will get the same axis but of course, there is one new thing which came in 1984 crystallography is much older than that, more than 100 years old. So, this theorem and all are more than 100 years old. But in 1984 there was some sort of revolution or shaking a foundation of crystallography. That is what the kind of news which was coming it was nothing like that, but it was a new discovery and where they were finding that there are crystals with 5fold symmetry.

That was the original discovery later on. 10-fold symmetry 7-fold symmetry various kinds of symmetry groups started coming in. So, I put crystals under inverted comma, because they are not really crystal. And that is why the objective quasi was prefixed to crystals to distinguish them from true crystal, which we are discussing in this course.

So, they are not true crystal, and if they are not true crystal, then they are not restricted by this crystallographic restriction theorem. So, that is why they can have so called non-crystallographic symmetry like 5-fold axis or 10-fold axis 7-fold axis and all. We will also discuss the Freize group in freize group which is the first group now, we will start where we will start thinking of combining translations with points symmetry because after all periodicity or translational symmetry is the essential symmetry for crystals.

So, unless and until you have the translational symmetry, you do not make a crystal. So, point groups only give you symmetry of finite objects. So, square for example, is square is not a square crystal. But a square has a 4-fold symmetry. So, it has a point group 4. So, the symmetry of his square is more than 4 we will see, because it has mirrors also, but not thinking of mirror if you are only thinking of rotation.

So, it is not right to say that the symmetry of the point group symmetry of a square is 4. But the rotational point group symmetry that is ignoring mirror reflections, and so, is 4, but it is a finite object, it is not a crystal, crystal can also have 4-fold symmetry as we are seeing because this was obtained by combining them with translation, this restriction came because only these symmetry operations are consistent with translation.

Otherwise, this restriction is not there, I can finite object Pentagon is there you know that you can draw a regular pentagon it will have a 5-fold symmetric. So, it that nothing can have 5-fold symmetry is not what we are proving nothing which has translational symmetry can have 5-fold symmetry. So, it is the translational symmetry which is putting this restriction.

So, the freize group is objects which have 1 dimensional translational symmetry. So, we will see that crystals have 3-dimension translational symmetry, we are looking at tiling 2 dimensional tiling also which have 2 dimensional translational symmetries and we can limit to 1 dimensions then you will get a freize group. So, freize group if you define these 2 dimensional patterns. So, pattern in 2 dimensional, your drawing in 2d by the translational symmetry is 1 dimensional. 2d patterns with 1d translational symmetry.

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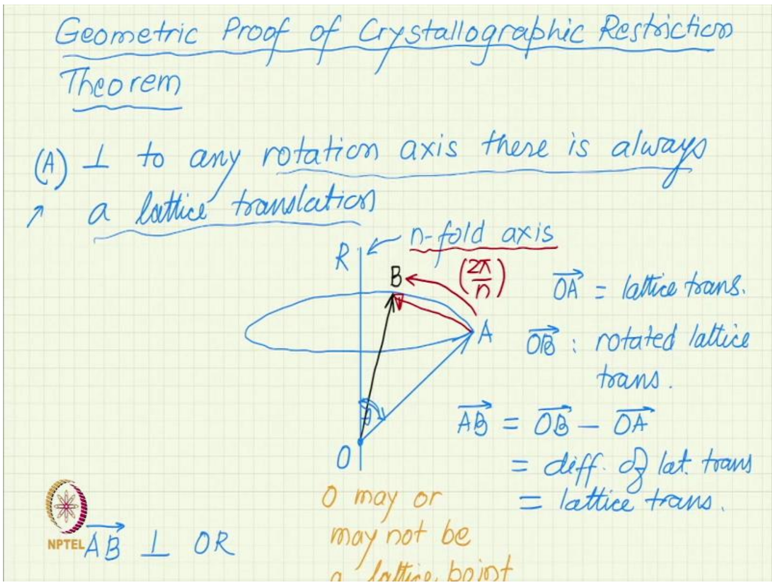

So, let us look at first the geometric proof of our crystallographic restriction theorem, we will first prove that perpendicular to any rotation axis. That is in a crystal if you have a rotational symmetry axis. Now, you have already seen that no you have not seen you do not know because we will not use the matrix proof now, we do not know the proof. So, we do not know that 5-fold does not exist. We want to come to it another way.

So, we know that some symmetry axis can be there in a crystal. So, let us say that this is some rotation axis and if it is a crystal it will have some lattice translation. So, let us draw that lattice translation so, I am trying to be general the lattice translation could be parallel to the axis or perpendicular to the axis or at an angle if it is perpendicular to the axis then there is nothing to prove, if you assume that there is a translation perpendicular to the axis.

So, that is why I am making an inclined translation not assuming that this is perpendicular, but later on we will say that it will generate or show that it will generate a translation which is perpendicular also. So, OA is a translation OR is the rotation axis and since it is a rotational symmetry axis, it will rotate things around it. So, if OA is 1 lattice translation to maintain the symmetry there should be another if I rotate this by whatever n fold it is, I should get after 1 operation I should get another lattice translation OB.

So, A to B you are going by the rotation of 2pi by n because that is what is meant by the -fold axis. So, if OA a lattice translation OB is also a lattice translation but then if you have 2 lattice translations then if I join the vector A to B what is A to B that also has to be if 2 endpoints have 2 lattice translations are joined that is also some are differences of all lattice translations will be lattice translations.

So, OA is a lattice translation, OB rotated lattice translation, AB is OB minus OA, which is a difference. So, that is also a lattice translation. Means, they will OA take you from a lattice point to another lattice point all vectors do not have this property. So, we are talking about various special vectors which if I if I put the tail of any of these vector at a lattice point the head will also be at a lattice point.

Now, what can you see say about is relation of AB to OR, is AB orientation of AB related to OR it has to be perpendicular in any rotation because it will form a surface of a right circular cone of half angle theta. So, the circle which I have drawn the rotated vectors have to be on that circle. So, that is on the base of this cone and OR is the axis of the cone.

In many ways means I am just giving you a hint many ways you can show that AB we will be perpendicular to OR. In 2d pattern, this was trivial, because your rotation axis were OA perpendicular to the plane of your drawing. But in 3d this was not obvious. But in 3d also now, you know that whatever orientation your rotation axis is, if it is a symmetry rotation axis, there has to be some translation vector which is perpendicular to that axis.

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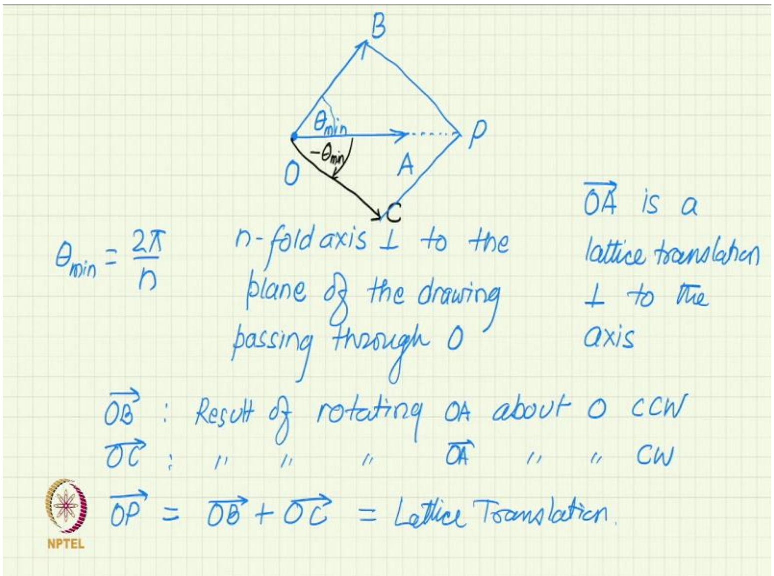

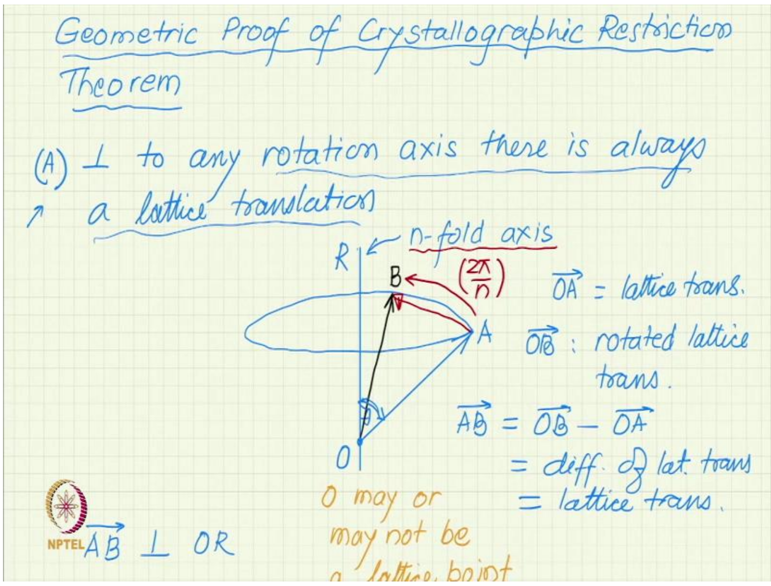

This part is usually missed in books. So, that is why I gave you to lose because most books will start with this part B, but this part is A required because they assume so, they will say that, now assume that O is my n-fold axis and let OA. So, with now OA is n-fold axis perpendicular to the plane of the drawing.

So, I am not drawing the whole axis, I am only drawing the intersection of the axis with the plane of my drawing. So, the axis is going through O and is perpendicular to the plane of drawing. Since it is a lattice from our earlier proof from part A, we know that there will be a lattice translation in the plane of the drawing. So, that lattice translation we are calling OA.

Because the plane of the drawing is perpendicular to the axis and we have just seen that perpendicular to the axis you are assured to find a lattice translation. Now, if it is n-fold axis, then you will know that theta min is 2pi by n. So, n-fold axis will rotate this lattice translation by this theta min to give you vector OB, it can rotate both clock, when there is a n-fold rotation you can rotate plus 2pi by n or minus 2pi by n.

Because anywhere there is a symmetry group and rotation can act both ways. So, you can go the other way around also. Now, you can add these 2 vectors counter clockwise and then we are having OP which is some of OB and OC and again by the same understanding since OA was a lattice translation OB is obtained by a symmetry rotation to symmetry rotation. So, take a lattice translation to another lattice translation.

So, OB is a lattice translation OC is the lattice translation and OP which is sum of 2 lattice translations is also a lattice translation. And again I leave some geometrical steps for you. It is easy to show that OP is what is the relation of OP to OA it they have to be parallel. Prove that geometrically.

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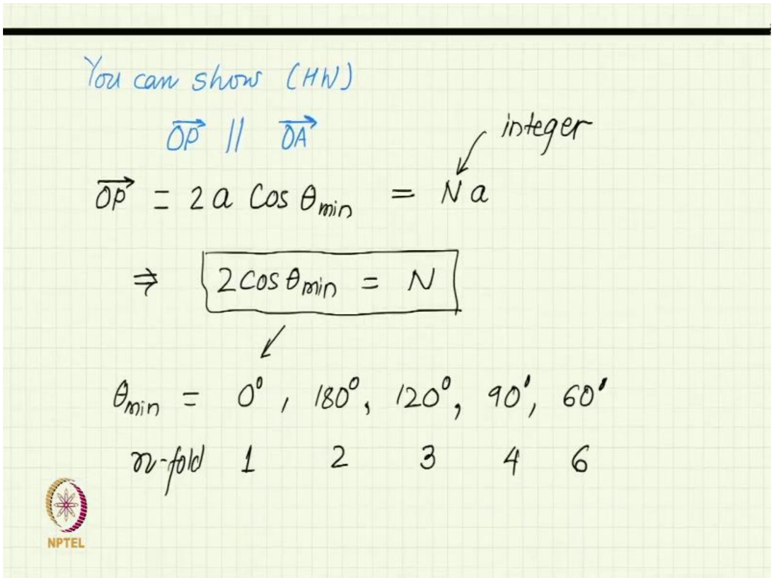

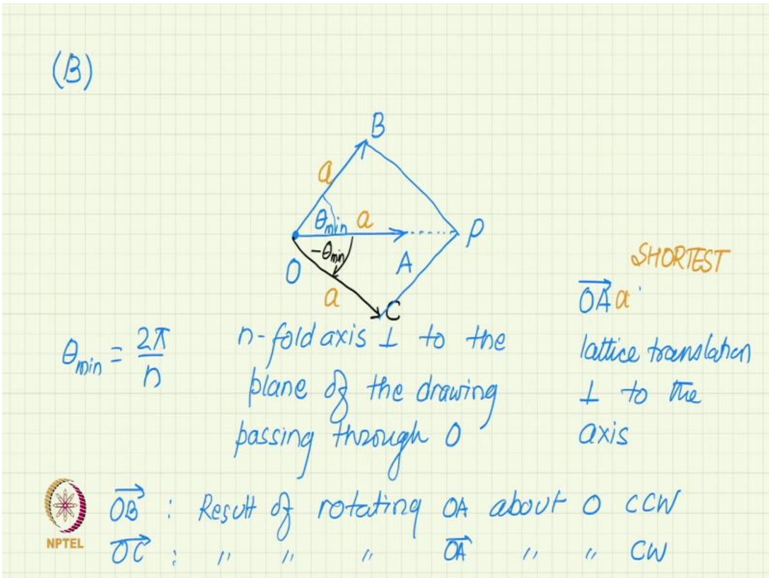

Now, we have not made 1 assumption that is make 1 extra assumption that OA is shortest lattice translation if you have a lattice translation perpendicular to any given axis some of those lattice translations will also be lattice translation. So, actually there will be infinitely many lattice translations are long there, but since it is a lattice translation there will be a minimum lattice translation in any given direction, because you cannot have a smaller and smaller and smaller going to 0.

So, there will OA be a shortest lattice translation. So, we should pick that particular lattice translation we are assured here that there is lattice translation perpendicular to the axis among those lattice translations I choose the shortest 1. So, OA my shortest lattice translation. Now, can you find OP, so, let us say the length of OA was A. So, OB will also be A, OC will also be A, and how can I write OP in terms of A n theta min 2 a cos theta min.

But, if A was the shortest lattice translation, what should OP be n times the shortest because you can only add the lattice translation if you have the shortest lattice translation A, the next lattice trans next larger lattice translation will be 2a, you cannot have 1.5 A. So, 1a, 2a, 3a that is where that is how you will go. So, OP also has to be equal to n times A where n is integer.

So, again you have you can see now, you have a restriction non cos theta coming from a different way of analyzing. So, you have 2cos theta min is equal to n slightly different formulation you will see there we got 2 cos theta plus 1 is equal to n. But if 2 cos theta plus 1 is equal to n, will not 2 cos theta will also be another integer only have to subtract 1.

So, this will also give you exactly the same 5 axes as the previous 1 gave. So, again theta min will be either 0 degree or and 180 degree, 120 degree, 90 degree, 60 degree, that is all no other values of theta will satisfy this equation they will not give you an integer value. So, that is in terms of the fold of the axis 1,2,3,4 and 6. So, that whatever proof satisfies you mode, you can look at it but it is nice to look at it in more than one way the same result.