Crystals, Symmetry and Tensors
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Crystallographic restriction theorem

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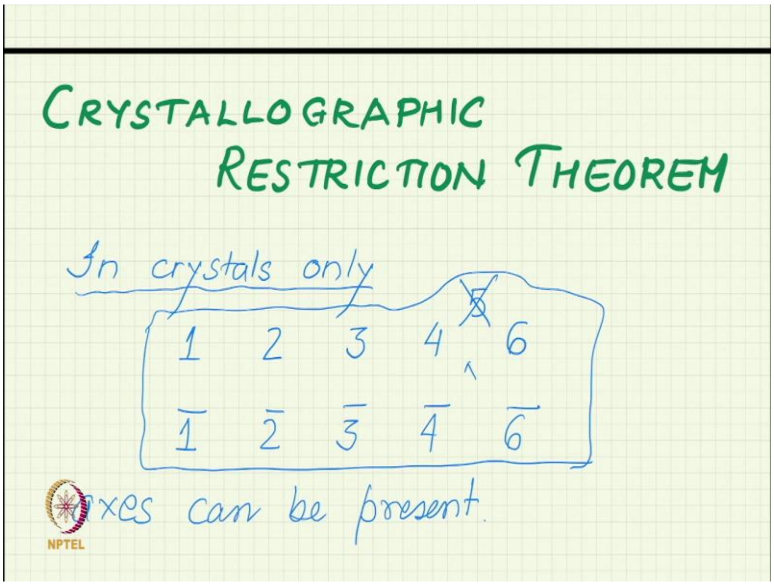

Now, we are ready for our crystallographic restriction theorem, which I said is one of the most beautiful and important theorem of this course. What does this theorem say? This theorem says that in crystals only 1 2 3 4 and 6. I am not making any mistake, 5 is missing and 1 bar, 2 bar, 3 bar 4 bar and 6 bar axes can be present simplifies our life dramatically otherwise, there is no limit on in and goes from infinity.

If there are a finite object, you can have 5-fold symmetry, think of a regular pentagon, 5-fold symmetry in the model making you made icosahedron has 5 bar symmetry. So, all these symmetries 5-fold, 6-fold, 7 fold, 8 fold, regular octagon, 8-fold axis, but you cannot arrange a crystal to have 8-fold symmetry it will not be there. So, in crystals only these 10 possible axes can be there. 5-fold is not there 5 bar is not there how do we prove this?

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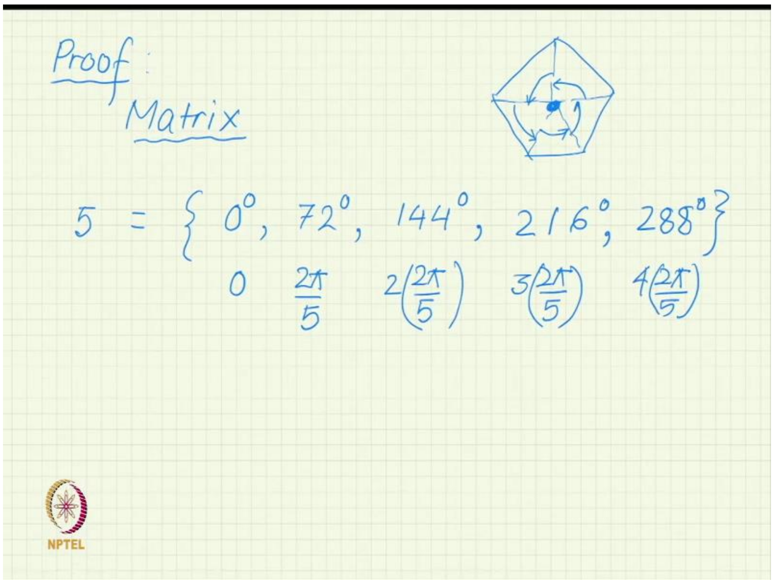

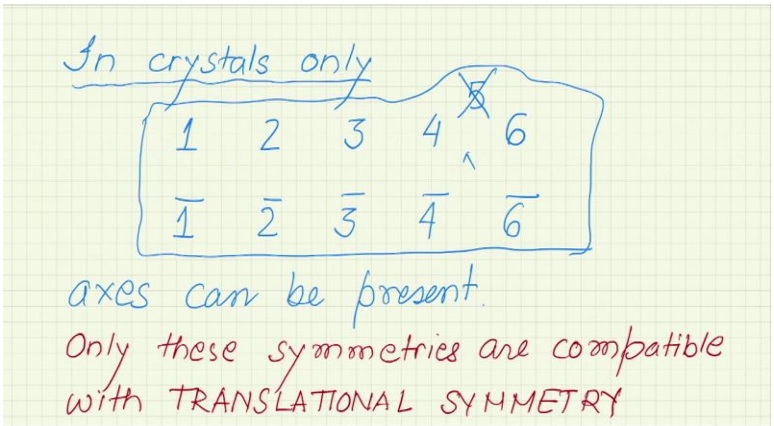

The Matrix proof is very very simple it will if you have understood the matrix method now, the proof will be proof will almost appear to be trivial. So, let us do the matrix proof. Why this is so, why is this restriction is coming? What is special about crystal which is not there in a regular octagon?

Student: Point group has to axes (())(3:05)

Professor: 5 fold is a point group point group 5 fold axes is a point group there are 5 rotations if you consider 5 fold axes. 5 is point group, point group consisting of 0 degree 72 degree 144 degree after this 216 degree, these rotations we will bring Pentagon into self-coincidence if you join the centroid of the Pentagon to the vertices, these are the 72 degree 1 times 72 degree 2 times 72 degree 3 time 4 time and finally 5 time.

So, these 5 elements 0 2pi by 5, 2 2pi by 5, 3 2pi by 5 and 4 2pi by 5 so, these represent the symmetry operation so it is a point group and it leaves 1 point of the Pentagon unchanged the centroid of the Pentagon and change its appointed group proper point group. It is not that 5-fold axis will not give you a point group. It does give you a point group, but it gives you a point group incompatible with crystal.

Where is that incompatibility coming from? One thing which is not the finite object that nothing is repeating there is no unit so there is only one object. So if there is only one no object it can have arbitrary symmetries, but as soon as you demand that object should repeat at equal intervals in 3 directions that repetition, that translational symmetry is actually what is putting this restriction.

So, this restriction comes from the fact that only these symmetries compatible with translational symmetry of the crystal which is the defining symmetry of the crystal, crystal you not have any 2fold 3fold 4fold symmetry if it is a crystal, 1 symmetry which is guaranteed for it to have is that it should be translationally periodic how we define crystal, we did not say a crystal which has a 4fold symmetry with a crystal should be a translationally periodic arrangement of atoms.

When we brought in translational periodicity essentially we are demanding that it is having translational symmetry. So, only these symmetry rotations only these 10 symmetry rotations are compatible with translational symmetry why is that?

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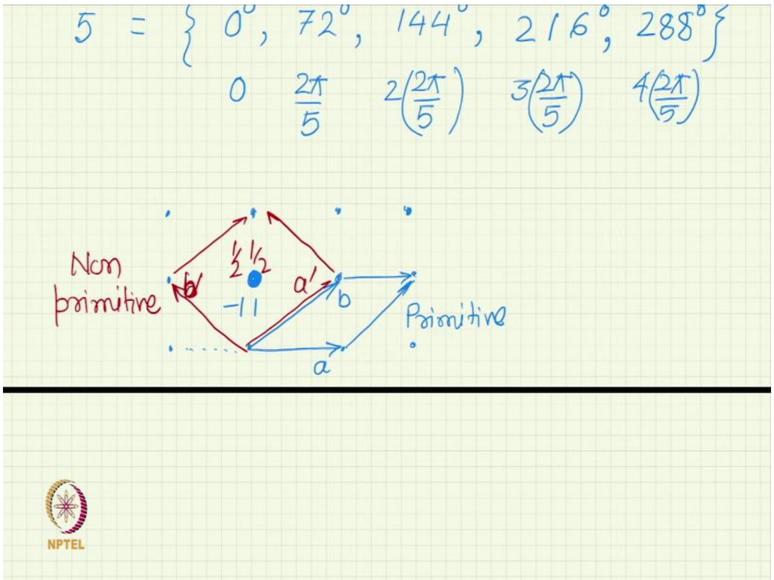

So, let us look at that since, since you have a crystal since you have a crystal and since we have a translational periodicity and you have a choice to select some crystallography coordinate system which will be some lattice translation suppose this so, this is 1 possible basis vector you can have what is the difference between the blue bases and the red bases Blue is primitive. Red non-primitive what is the difference in the coordinates which these bases will give to the different points.

For example, this point, this point will have coordinates what in the blue system minus 1 suppose if this is my a, and my b, this is my a prime and this is my b prime. So, in the blue system it is minus 1 1 in the red system will primitive ever give you a fractional coordinate that is the beauty or that is the advantage or that is the power or that is the excellence of a primitive system.

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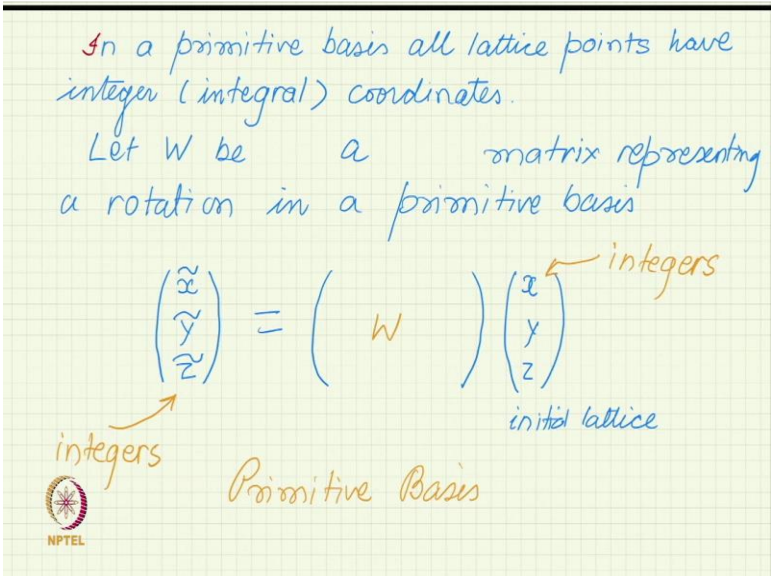

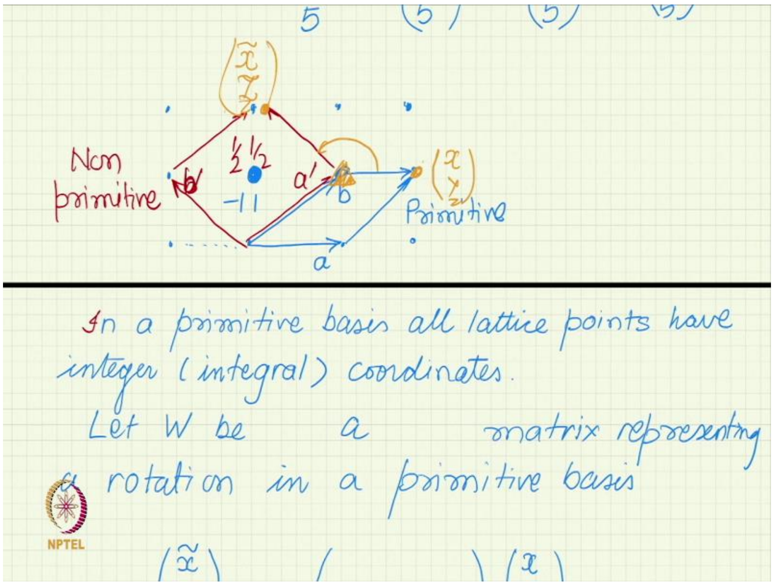

Primitive assures you that all lattice points will have integer coordinates integer or sometimes it is called integral but it has nothing to do with the definite or indefinite integral, integral here is adjective of integer. So, now, let us write suppose W is the rotation matrix, matrix representing let W be a matrix the presenting a rotation in a primitive basis. So, you have some coordinates some starting coordinate of some lattice point xyz coordinates of the rotated point remember we decided that not to write prime for rotation but the till day.

So, initial because if it has a rotation suppose this was your rotation axes or this is some sort of rotation axes then it will rotate some lattice point to some other lattice point. So, this lattice point is being mapped to that this lattice point is what I am calling xyz after rotation I am calling it x tilde, y tilde, z tilde and the matrix is doing that transformation for me.

So, the matrix is W and my basis is primitive bases in the primitive bases what is xyz what is the form of xyz, integers so, each x y and z are integers after rotation the new lattice vector which you get is also being represented in the primitive bases. So, what will be the form of these integrals? Now, if you have a matrix which on multiplication gives you from an integer column vector to another integer column vector all wedges.

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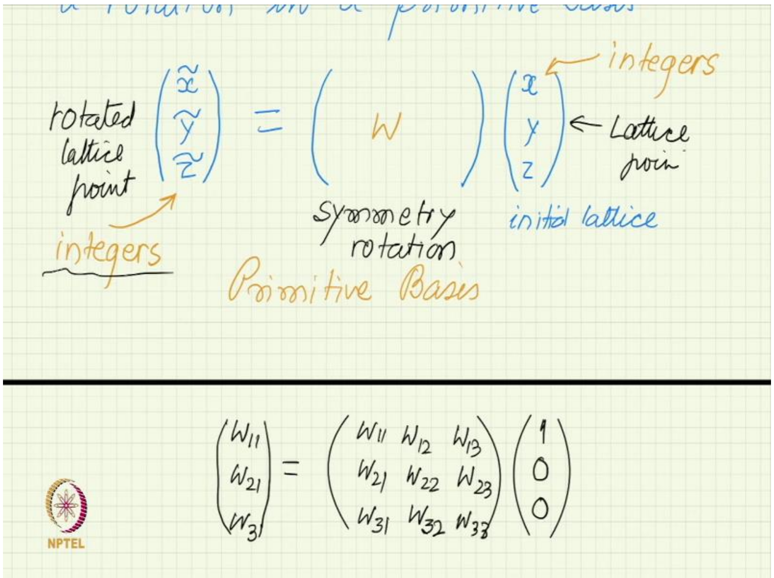

What will be the form of W? So, let us do it one by one any rotation not symmetry rotation because it takes a lattice point to another lattice point. So, this is also a lattice that is why they are integers. So, this is a lattice point the lattice point and this is a transform lattice point or rotated lattice point and this is the symmetry rotation, the rotation will act on all vectors all lattice point one of the lattice point has to be 1, 0, 0 and of a vector the first basis vector 1, 0, 0 multiplied by W will give you what?

That is the first column any matrix if you multiply by 1, 0, 0 you pick out the first column 1, 0, 0 was integer. What do you say about W11 W21 and W31? each of W11, W11 is an integer W21 is an integer W31 is an integer, if they were not then the relationship it a lattice point goes to lattice point and in primitive bases they are integers will be violated.

So, if this W is a symmetry rotation and I am working in a primitive basis then W11 W21 and W31 have to be integers if I multiply by 0, 1, 0. What will I get? The second column and what will we claim or what we will decide about these numbers in integral. So, all elements of this matrix integrals. So, this matrix itself is an integral matrix.

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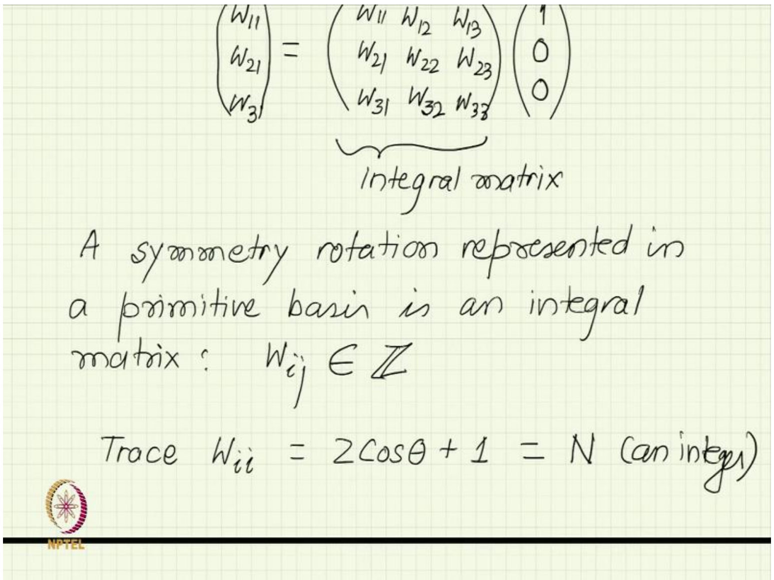

So, any symmetry rotation represented in primitive bases is an integral matrix. Integral matrix means all W ij for all values of i and j they are integers. If that is true and if this is representing a rotation what can we say about the trace but 2 cos theta plus 1 should be integer it is an amazing result.

Just think about it 2 cos theta plus 1 cos theta is a fraction and theta an arbitrary angle rotation angle with an arbitrary rotation angle theta cosine can have any value I am multiplying it by 2 adding 1. So, it can have any arbitrary value. But, if this theta is part of rotational symmetry of a crystal, then only those thetas will be allowed for which 2 cos theta plus 1 is in integers.

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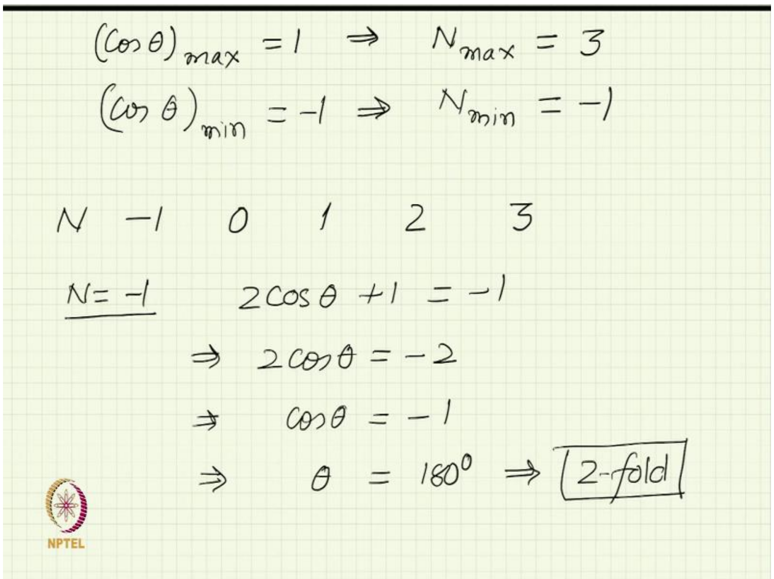

Welcome to this very, very said this is what you are already seen that the translational symmetry is restricting theta is not letting you have arbitrary theta because arbitrary theta will give you a non-integer but if it is part of crystal symmetry our analysis demands that 2 cos theta plus 1 has to be an integer. What will be the maximum integer for 2 cos theta plus 1 what will be the minimum value of n.

So, what are them all possible integers n, minus 1 0 1 2 3 What are the axes we are saying that are allowed 1-fold, 2-fold, 3-fold, 4-fold and 6-fold 5, 5 different axes, 5 different integers between minus 1 and 3 beautiful result, you can just now simply work out that what do these n stand for. So, n is equal to minus 1, 2 cos theta plus 1 is equal to minus 1, 2 cos theta is equal to minus 2 cos theta is equal to minus 1 theta is equal to 180 degree.

180-degree rotation 2-fold axes. So, we are happy 2-fold axes is allowed for a crystal any existence of n equal to minus 1 is telling as that 2-fold access is allowed for a crystal.

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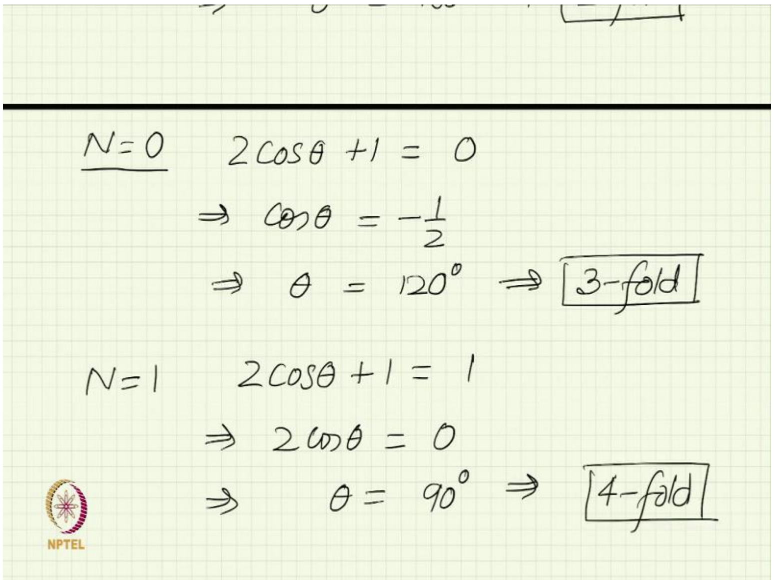

N is equal to 0 the main thing is done the rest is just algebra and identify what these numbers are representing in terms of the angle cos theta is minus half, theta is 120-degree fold 3-fold n is equal to 1, 2 cos theta is 0, theta is 90 degree.

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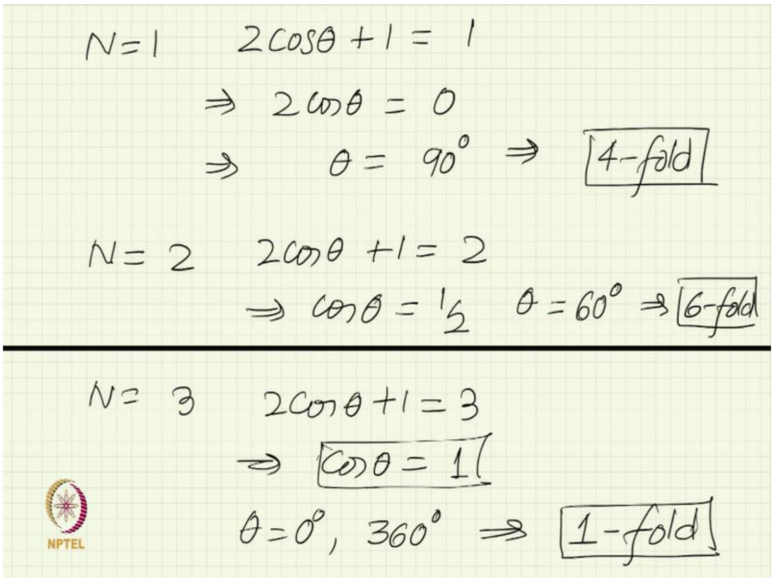

Finally, n is equal to 2, is not final, n is equal to 3 we have to go up to n is equal to 3, 2 cos theta plus 1 is equal to 2, cos theta is equal to half, theta is equal to 60 degree, 6fold. We have exhausted everything what will 3 give. So, n is equal to 3, 2 cos theta plus 1 is equal to 3, cos theta is equal to 1, theta is equal to 0 degree which is same as 360 degree, which is not symmetric, but we do not like to be negative.

So, we see we have 1-fold symmetry saying 1-fold symmetry saying that there is no symmetry any arbitrary any odd object if rotated by 360 degree or if not rotated at all by 0 degree it will be in self-coincidence. So, symmetry is not required for that. But if there is no symmetry we take a positive attitude to life and say it has 1-fold symmetry. So, thank you very much.