An Introduction to Materials: Nature and properties (Part 1: Structure of Materials)

Prof. Ashish garg
Department of Material Science and Engineering
Indian Institute of Technology, Kanpur

Lecture – 07

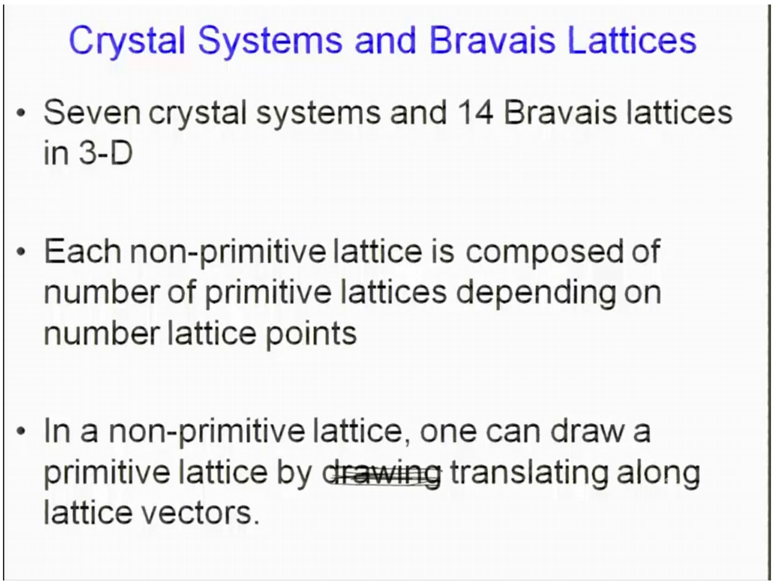
Bravais Lattices

Symmetry in Crystals

So, again, good morning to all of you. So, we will start lecture 7 today, which is going to be little bit based on Bravais Lattices and if time permits, we will start Symmetry in Crystals. So, let me just give you a brief recap. We discussed about primitive non primitive lattices in the last class and what is the motive or basis and how is the relative orientation of atoms and molecules in the motive determine whether you will have a what kind of primitive units that you will have, that 3 thing is that one must follow the definition of the primitive lattice, that is; within the primitive unit cell that it should be a repeatable unit, it should not be there should be no gaps or discontinuities it should be repeatable. So, if you choose a so, smallest possible cell, which must take into account the orientation of molecules with respect to each other, should be such that, so that, it is repeatable and it has identical neighbourhood for all of the species associated.

So, let me now go to the next topic. So, we have seen that, there are 7 crystal systems.

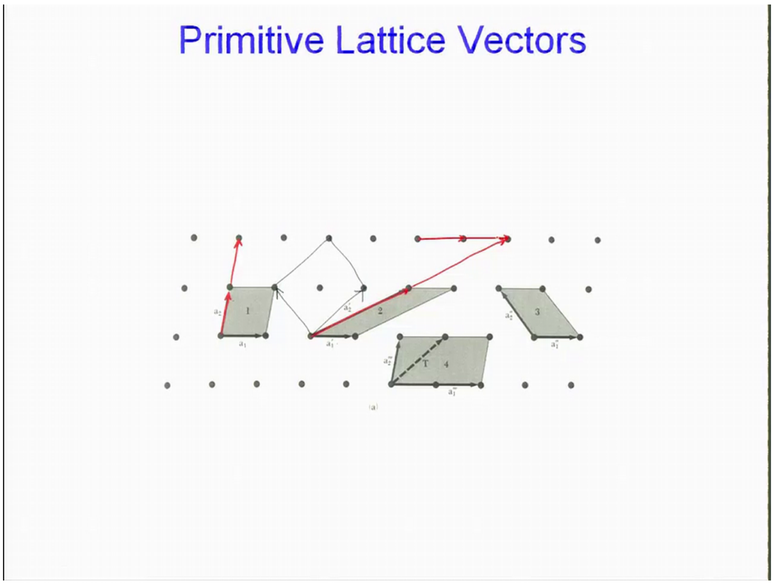
(Refer Slide Time: 01:28)



There are 14 Bravais Lattices in 3-D, and what we also saw that each non primitive lattice, such as face centred cubic or body centred cubic lattice, in case of cubic system is composed of number of primitive lattices depending upon the number of lattice points. So, for example, body centred cubic has 2 lattice points which means it is equivalent to 2 primitive cubic lattices. Similarly, face centred cubic lattice has 4 lattice points; it is equivalent to have it is equivalent to 4 a primitive lattices.

So, I one should be able to draw the primitive lattices within the non-primitive lattices easily. In a non primitive lattice also one so, as a result, what we will do just give a brief flavour of that, that you can draw a primitive lattice by drawing the why I think there is a mistake here? By we should just one second ok, so by translating along. So, let me just cut this word drawing, it should be by translating along the lattice vectors ok. So, let us see how we do that.

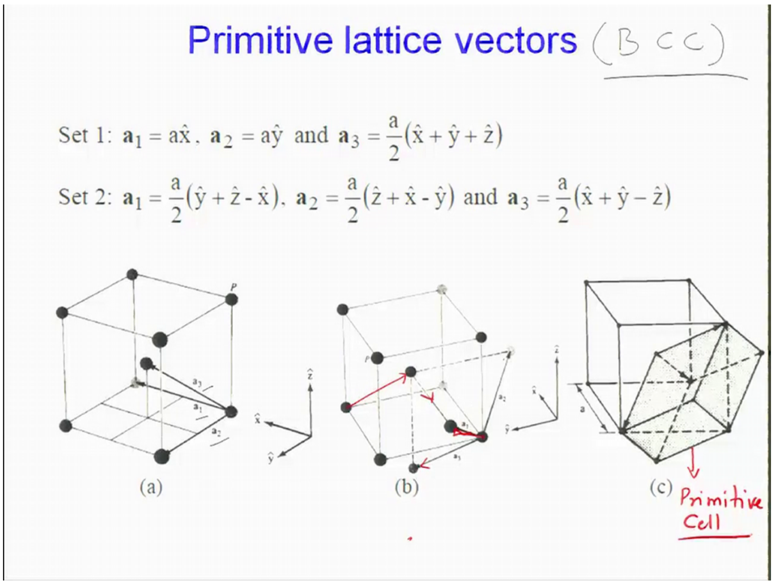
(Refer Slide Time: 02:40)



So, this is for example, a primitive lattice ok, it is in 2D ok. So, this is a 2D primitive lattice. In this, what we have is array of atoms and you can see that ah. So, we have drawn the first primitive unit cell which has this unit cell, this number one and you can see that a1 is a primitive lattice vector; a2 is a primitive lattice, but you see as we said in the beginning the choice of primitive cell is not unique, essentially you can choose any primitive any vector which can give rise to a primitive unit cell. So, you can see number 2, you have primitive lattice vectors as a1 prime, a2 prime, hour is different it is not same as a 2, a 2 prime is from this atom to that atom, but it still gives you a primitive unit cell the area of these 2 cells are going to be equal to each other. You can see in third one, third one you have the say a1 double prime and a2 double prime ok. So, choice of primitive lattice vectors as you can have multiple choices. So, it is it is not a fixed choice as long as you are able to make a primitive units cell out of those 2 vectors or those 3 vectors in 3-D a is perfectly legitimate similarly you can see that, in this case in the case where you have this a1 trip a1 triple primary to triple prime, you can see that this is the unit cell that you are drawing which is a non-primitive unit cell, which is a bigger unit cell ok.

Similarly, there are multiple choices of non-primitive unit cells as well. So, in this case this is one unit cell. You can have one non-primitive unit cell like that this is also non-primitive unit cell. So, this could be lattice vector; that could be a lattice vector. So, basically what I am trying to emphasize upon is when you choose a particular primitive unit cell, the choice of primitive unit cell vectors is multiple ok. Why did those vectors always give you a primitive unit cell of same type of same area?

(Refer Slide Time: 04:38)

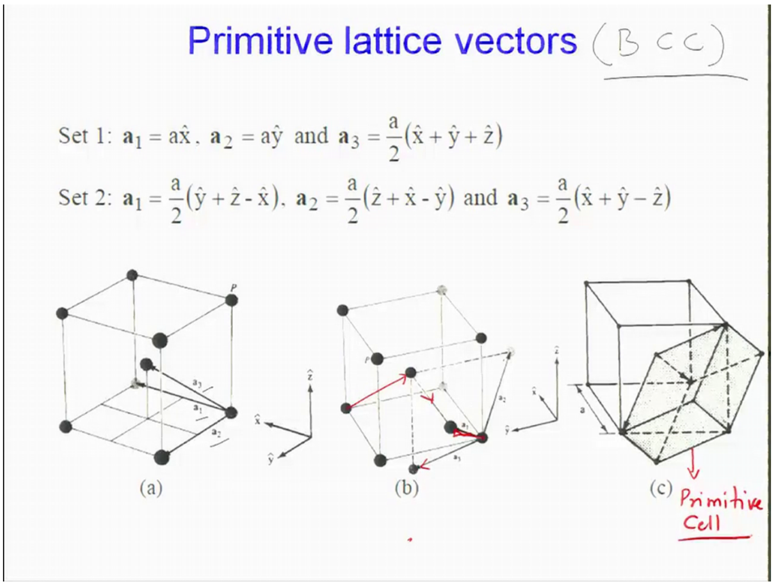


So, in BCC, for example, this is a case of BCC lattice in case of BCC. So, in case of BCC there are. So, I have given you 2 choices, the first set is a1 vector could be a ax hat; a2 could be a y hat and a3 can be a by 2x hat plus y hat plus z hat which means, this is this is a1; this is a2 here and this is a 3 ok. So, a1, a2, a3 this is a set one. You can have this lattice vector, this set of vectors in a still constructed primitive lattice or you can alternatively have rather set of vectors, which is which seems more convenient in BCC see, the what you chooses dependent upon the symmetry, but there are multiple possibilities.

So, this is a1, a1 could be this one, from here to here. So, let me just change the colour of this particular thing. So, this is a1 here; a1 is half of a by 2 y hat plus z hat minus x hat, this is a1, this is for the; so, you can see that, this is a BCC unit cell all right. So, we are checking the atoms which are down there ok. This is the one in the centre, this is on the right side, this is the atom below and this is the atom which is somewhere on the down side ok. So, you can see that, we are going from. So, this is in this case, it is y plus z minus x bar, but you could have very well chosen ah. So, if you if you for example, go from here you could have chosen from here to here, this could be one lattice vector.

So, in this case we are taking this as a origin, that is why we have chosen the atom which is down there. So, there are. So, you can see that this is y, this is x and this is z. So, this is this vector is half of y ok, in this direction; half of z which is this direction and then half of x. So, half of now remember positive x is in this direction. So, we have half of x, negative direction; half of y and half of z and we will reach here. So, this is this is facing you right. So, x is in this direction this atom. So, this is within the cell, this is outside the cell in front of you, this is to the right of the central atom in the unit cell, this is the bottom of the central atom in the unit cell. So, this is a1 vector from here to here, this is a2 vector from here to here and this is a3 vector from here to here. So, you can see that one is half of y plus half of z minus x half of x; this is half of z half of x minus half of y and this is half of x half of y minus half of z and by correcting these vectors, you can make a unit cells something like that this. So, if you if you try doing this exercise using the either of the. So, you have lattice you have the lattice translation. Now you just connect them with each other and you should end up with something like that what you have. So, this is a primitive cell and it is volume is half of the one 20 units of volume.

(Refer Slide Time: 07:53)



This is in case of FCC. So, in case of FCC, you can have vectors. So, this is if choose this as a origin, this is a1. So, this is a1; this is a2 and this is a3. So, basically corner atoms connecting to 3 face centre atoms as a result, a1 is half of y plus z; a2 is half of z plus x and a3 is half of x plus y if you choose your origin differently your vectors signs and they will change. So, if you connect from using these 3 vectors, you get this parallelogram or parallelepiped in the within the cube. This is the primitive cell ok.

Student: (Refer Time: 08:36) vectors (Refer Time: 08:39).

Shortest Lattice translation that is a basically, it is a lattice translation.

Lattice translation is you go from one point to another then from. So, for example, if I go to previous slides; so, lattice translation you choose this as the origin ok. Now, if you go from here to here; you get a point lattice point, you go from here to here; you get a lattice point. Similarly, in this case also you went from here to here; you got a lattice point, you go from here to here; you get a lattice point. In this case, you go from here to here; you get lattice point that again you go from here to here; you get a lattice point. So, Lattice translation Vector. So, choices are unique, you go from one lattice point to another lattice point.

Student: (Refer Time: 09:25) FCC in BCC.

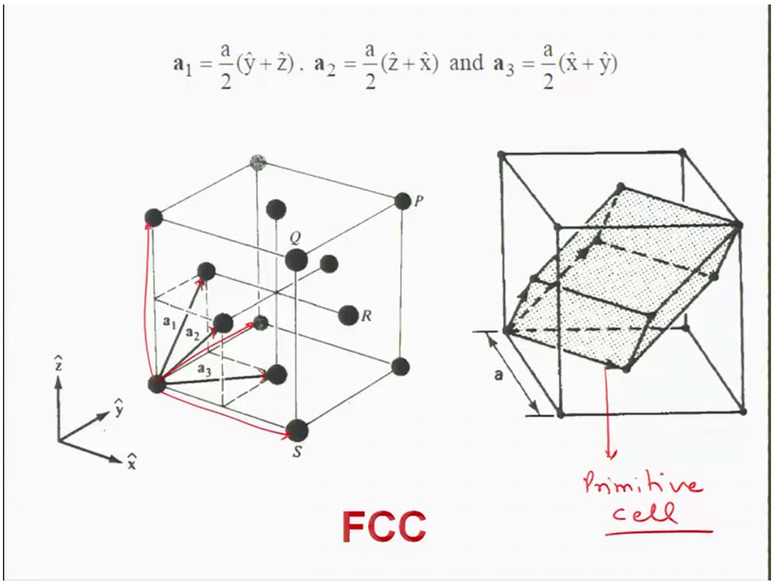
Yeah.

Student: those are non-primitive.

Non-primitive unit cells, but non-primitive unit cell is consists does consist of student: primitive.

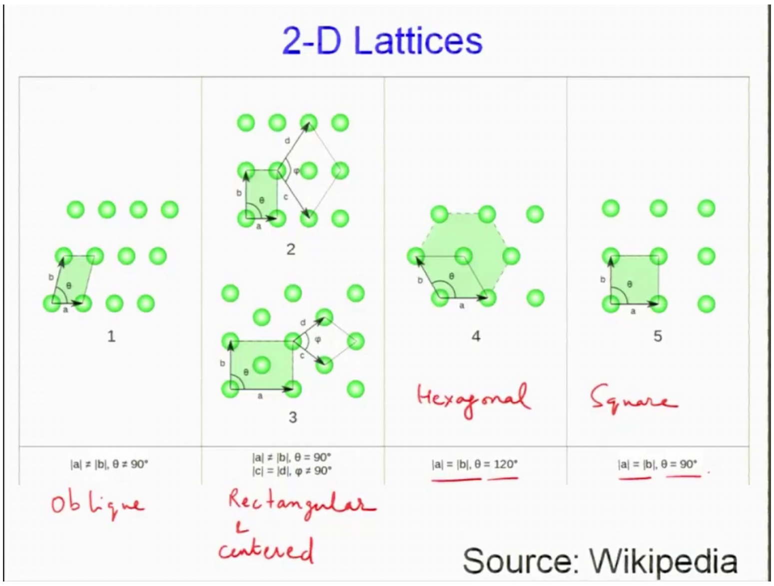
Primitive. So, in this case, in this case, what is a shortest lattice translation vector? That is what we look at. So, that is the primitive lattice vector ok that is the primitive lattice vector because 1 primitive cell is made up of 2 primitive cells right. So, you can always choose a primitive lattice vector within the non-primitive cell.

(Refer Slide Time: 10:01)



Non-Primitive Lattice Vector would be you have a cube. So, Non-Primitive Lattice Vector would be this, that and that, but these are shortest Lattice Translation Vector which has primitive lattice vectors.

(Refer Slide Time: 10:18)

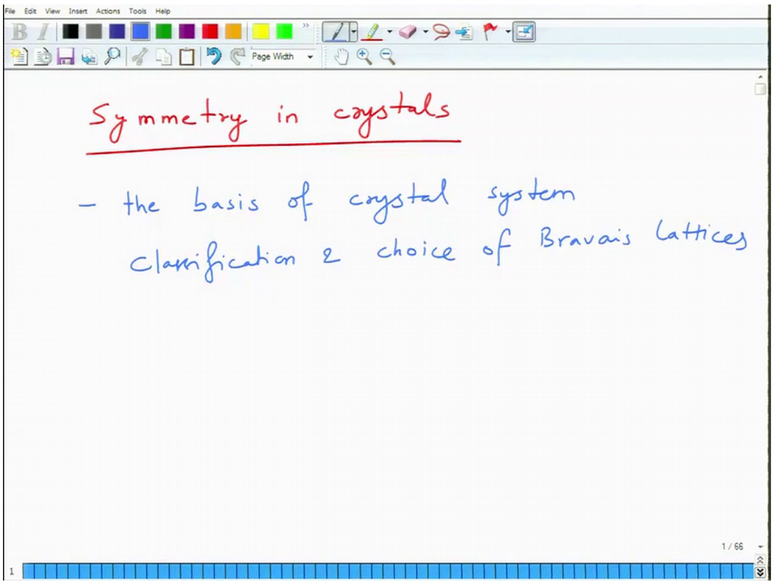


So, I think in one of the earlier classes I asked you to draw 2-D lattices which are possible. So, there are few possibilities you can see the first one is a is not equal to b and theta is not equal to 90. Other 2 possibilities are a is not equal to b, but theta is equal to 90 and third one is a is ah. So, in this case you can have, a is this is centred Lattice ok. So, a is not equal to b theta is equal to 90 degree, but you have a atom in the centre. So, this is a Rectangular Centred Lattice. So, this is a Oblique Lattice; this is a Rectangular and Centred one; this is hexagonal in which a is equal to b ; theta is equal to 120 degrees alright and then you have a Square Lattice where, a is equal to b and theta is equal to 90 degrees.

So, these are the possibilities which exist in 2D. 5 possibilities of Bravais Lattices all right. So, now we been talking about Primitive and Non-Primitive unit cell and we have also said key that there are multiple possibilities of primitive unit cells. One can have a square depending on type of arrangements; you can have a parallelogram; you can have different shape parallelogram. So, multiple possibilities are there provided they have only one lattice point per unit cell. The question was, how do you define a criteria? So, that you do not end up with multiple possibilities. How you fit them into certain criteria and that is where the system of this crystal system came into being. So, crystal system is the classification according to crystal system you could see that there are certain criteria based on lattice parameters and they are correlations.

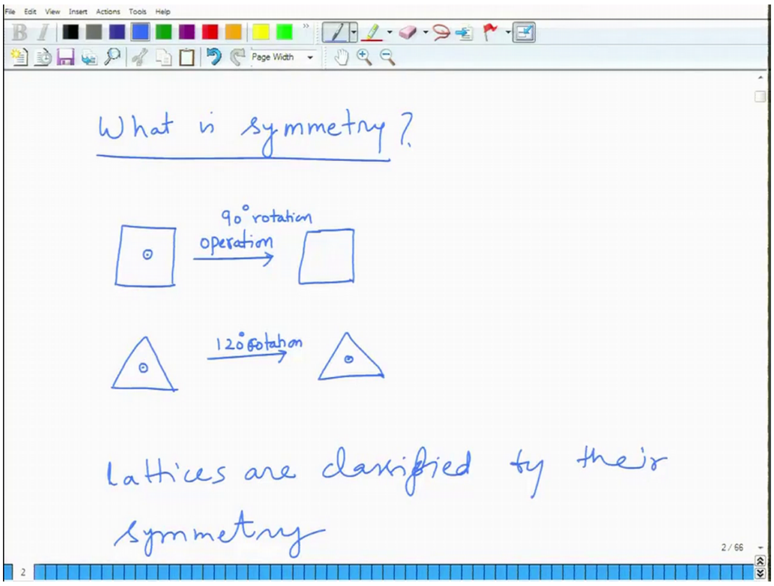
So, how do you get this criteria? This is as you can see this based on Symmetry right. So, you can intuitively that are cube is more symmetric as compared tetragon right, because cube has 3 sides which are equal, it has all 90 degrees angles and tetragon has all the 90 degree angles, but it has one side which is different as compared to other two. The question arises is what is this criteria adhoc or is there is there some scientific basis surrounded and we will see in the coming few minutes that, the area the there are certain Crystallography Symmetric considerations which have to be followed, to evolve this criteria and we will now take up those Symmetry criterion in next few minutes.

(Refer Slide Time: 13:10)



So, what we now start with this called as Symmetry in Crystals and why do we need to understand is. So, that we can understand the logic behind, the basis of crystal system classification and choice of Bravais Lattices. This is a very complicated topic. So, unfortunately in this course we do not have enough time to get around complete aspects of crystallographic, but we will try to just establish a bi[g]- simple basis how to deal with it. So, what is symmetry?

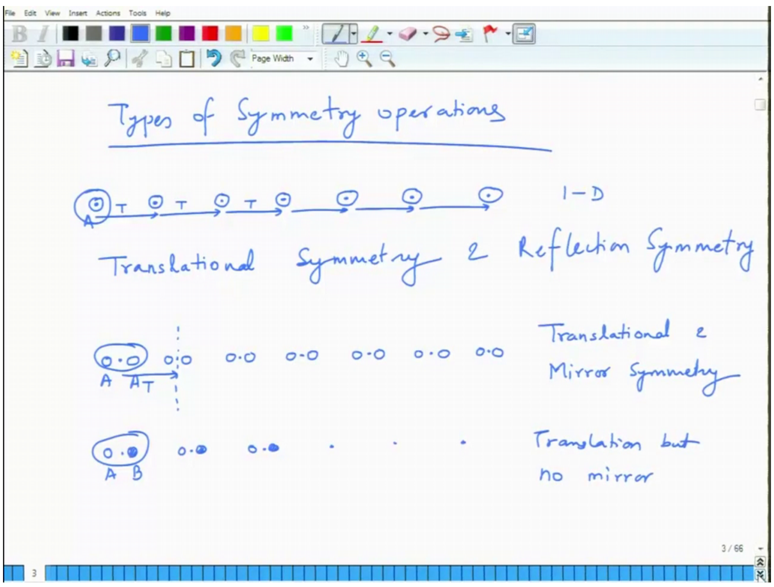
(Refer Slide Time: 14:09)



That is the first question. So, the answer of this question is, symmetry is an operation, which brings an object into it is original state. So for example, if I take this Square ok. So, what is the symmetry operation I can perform on perform on it? So, that it remains it looks a same. One possible option is, if I choose this as a centre of square and I turn it by 90 degree rotation around this axis. So, the axis is perpendicular to the plane of the paper. So, if I apply 90 degree rotation then this again looks the same right, it comes back to square shape. So, this is 90 degree rotation. So, this is called a Rotation Symmetry. Similarly, if you take a triangle, equilateral triangle, what operation do you need to perform on it? So, this is a centre of the triangle, let me say centre of the triangle and I degree I provide a 120 degree rotation. So, it appears in the n shape. So, these are. So, these are just examples of operations which you can perform to bring the object into the same shape. So, why we need to understand is because lattices are Lattices are classified by their symmetry.

So, it is not only this rotation which is one Symmetry Element. There are multiple symmetry elements. So, what are these Symmetry Elements? So, as I said Symmetry is an operation, which you perform on a when which when you perform on a on an object you bring into the position of self-coincidence. So, let us now look at what are these symmetry operations types of Symmetry Operations?

(Refer Slide Time: 16:31)



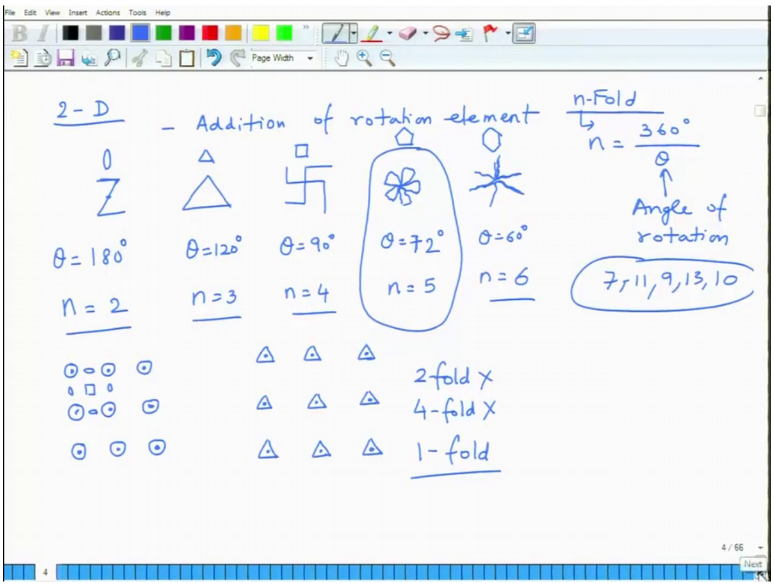
So, Types of Symmetry Operations, actually first one we should call as a translational because if you start just from 1-D Lattice. So, let us say, if you have this case of 1-D Lattice and you just put an atom here. So, you can see that, if you move from this point to that point by a vector T, in an infinite array of points in 1-D, then this Lattice

Translation Vector T, brings me into the position of self-coincidence because if this point is identical to that point, then this is a Translation. So, this is a case of what we call as a Translational and this is a defining symmetry in 1-D ok, in 1-D, you must have Translational Symmetry.

Now, let me do one more thing, if I change the motif around it. So, this is again in 1-D. Instead of keeping motif as one atom there, I keep motif like this ok. So, what I have here? I have Translation T, but I also have a, what is it? Mirror. So, I have Translation as well as. So, I have Translational and Mirror Symmetry ok. You can make this little worst. You can make the mirror disappear if you make this. So, let us say this becomes dark. So, mirrors disappeared now right, but it still has because the motif now is. So, motif initially was A now it is AA now the motif is AB. So, motif this is the motif in this case, this is the motif in this case, this is the motif in this case, but now you have translation, but no mirror.

So, in 1-D, you can have operations which are called as Translation and Mirror Operation Reflection, we call it Reflection. So, Translational Symmetry and ok. So, these are two Symmetry Operation; Translation, Reflection. They apply to 1-D, 2-D, 3-D, all of them, but they are so, but the only two cases which are possible in 1-D are these 2. So, let us move to little bit more complicated.

(Refer Slide Time: 20:18)



So, let us now go to let say 2-D ok. So, we have seen two of them, Translation and Mirror. Their applicable is starting from 1-D to 3-D ok. 2-D there is addition of what we call as rotation element all right. So, for example, if I take this Lattice Z, what is the rotation I need to provide on it to make it to bring it in self- coincidence? I need to rotate it by. So, theta is 108 degree. So, if I rotate around this point by 108 degree, it will become it will it will come into same shape so. So, now, in case of Rotational Symmetry, we define this as Fold n-Fold Symmetry.

So, n is number of Fold of Symmetry and what is this n ? n is basically 360 degree divided by theta angle of rotation ok. So, this is the angle of rotation. So, in this case what will n will what will n be? It will be 2. Now, how can you make a 2-D Lattice out of this? Let us say I have made a 2-D Lattice like this. If I make this as an object or basis. So, let me first complete this part ok. So, this is 2-D object in this case if it is a equilateral triangle it will be, theta will be equal to 120 degree, n will be equal to 3, in case of let us say this symbol, which you all familiar of. So, this is theta is equal to 90 degree, n is equal to 4 and if you look at some flower, let me it is not very symmetric, but. So, some flowers have 5 petals better right. So, you have 5 petals here.

So, here you need to provide a rotation of 72 degree, 5 fold. If you look at the ice flakes or if you look at things like this, their ice flakes are something like that they are sort of 6 fold symmetry. So, here you need to provide a rotation of 60 degree and this n will be equal to 6 and you can also have things like 8 fold symmetry if you have 45 degree rotation in case of certain objects. So, there are no 7 fold symmetry, you can see there is no 13 fold; 11 fold; all those are absent here. So, and there are mathematical there are mathematical basis that why I cannot go get into details of that, but 7, 11 you can see that here, 9 is missing, 9 fold is not there; 13 fold is not there; although all these are missing here 7, 9 10 fold, all of them. In fact, even 5 fold is not permitted in Crystallography because it does not fill the space.

See the point is, you can have a rotation of that degree, but if object does not fill the space. In crystallography, the important thing is, in crystal crystalline materials the that operation must fill the space ok. So, 5 fold object do not fill the space. So, as a result as a result crystalline materials do not show 5 fold Symmetry. There is another class of material, which show 5 fold Symmetry are called as Quasi Crystalline Materials, but they are non-equilibrium materials.

So, similarly, other Symmetries are also shown by those materials 10 fold Symmetry or 9 fold Symmetry, they could be shown by some materials, but there are seen in Crystalline Materials normally. So, in case of Crystalline Materials, what we are interested mostly in is in 2 fold, 3 fold, 4 fold and 6 fold and 1 fold symmetry folds. So, here and the graphics symbol for these symmetries is, this is shown like this, this is shown like this, this is the symbol for 4 fold symmetry, this is the symbol for 5 fold symmetry and this is the symbol for 6 fold symmetry ok. So, now, let us come back to this Lattice which I have drawn. So, you can see that in this case in this Lattice.

So, if I provide a rotation around this point then even a 2 fold rotation is possible, is there are 3 fold possible? There is no possibility of 3 fold. 4 fold is possible. 6 fold, 5 folds are not possible. So, this has 2 and 4. So, of course, around this point it will have 4 fold, but 2 fold you can also have at these points right. So, basically you define each of the point by maximum possible symmetry. So, this centre here, this can provide you 4 fold. So, although it can also provide you 2 fold, you depicted by 4 fold, because 4 fold is the higher symmetry that you can achieve by to trigger around this point. So, similarly around these points; so, these are depicted as 2 points because cannot give you 4 fold. They can only give you 2 fold. So, you depict these symmetry points rotational symmetry point in the Lattice in this manner.

Now, you can see that, if you if you have you can have a Square Lattice and if I choose a motif which is symmetric enough or which is circular you get 2 fold and 4 fold, but now let us say, the Lattice is a Square, but I replace the motif by these triangles. So, I have changed the motif now. Does it have 4 fold or 2 fold symmetry.

Student: (Refer Time: 27:15).

It does not have 2 fold, no it has no 4 fold. So, so what I mean to emphasize here is, we cannot go by the conventional definition of what looks symmetric. We have to go by these definitions symmetry, which make it very specific. So, although it looks like a Square grid, it is actually not a Square Lattice because it does not follow 4 fold, it does not have a 4 fold symmetry, it does not even have 3 fold symmetry, because if you perform 3 fold symmetry operation, it does not remain the same the only operation you can perform on this is, it has only 1fold symmetry. You can see that it has only 1-fold symmetry, rotational symmetry. So, this is why, in Crystallography, a cube may not be a cube; if it does not have elements of symmetry that are specific to cube which I will to come in a in a short while ok. So, let us let us wind up here and we can now take to the next lecture.