Texture in Materials
Prof. Somjeet Biswas
Department of Metallurgical and Materials Engineering
Indian Institute of Technology, Kharagpur

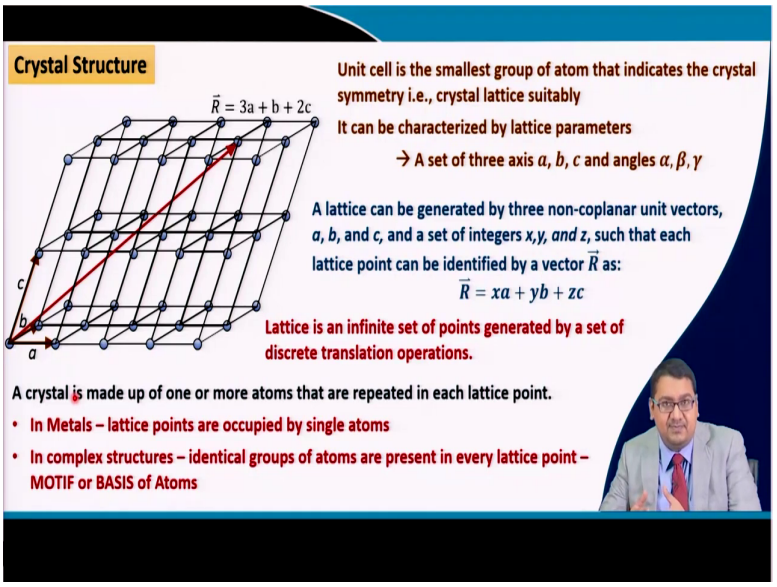
Module - 04
Texture representation
Lecture - 20
Crystal Structures and Symmetry

Good day everyone. Today, we will continue with the module 4, which is basically Texture representation and today, we will be doing the lecture number 20, where we will learn Crystal Symmetry; sorry, Crystal Structures and their symmetry.

(Refer Slide Time: 00:53)

The concepts that will be covered in this lecture are crystal structures; basic crystal structures and the Bravais lattices and we will cover the 7 crystal structure, which contains the 14 Bravais lattices and then, we will go and learn crystal symmetries that is the point group symmetries and the space group symmetry and the Laue groups and the classes.

(Refer Slide Time: 01:23)



So, you see that we already know what is a crystal structure right. A crystal structure is made up of unit cells like this, containing atoms in the sides, right. I have missed one atom so pardon me. Now, this is the most primitive unit cell right. If we define a unit cell, the unit cell is the smallest group of atom that indicates the crystal symmetry that is the crystal lattice and it indicates the crystal lattice suitably right.

So, if we want to characterize this unit cell, it can be characterized by using the lattice parameters a, b and c of the three axis's and these, a, b and c are at an angle alpha, beta and gamma to each other. Now, you see that how the alpha, beta and gamma is related to a, b and c.

So, you see the gamma is angle between a and b; whereas, the angle between b and c is alpha and the angle between c and a is basically beta. So, we should remember this and you see that from this unit cell, a lattice can be generated, you know. And how it is generated? It is generated by repeating this unit cell in translational manner in the three-dimensional space.

So, if this non-coplanar unit vectors, a, b and c and if we know few sets of integers like x, y and z, we can change the values of x, y and z and create this whole you know lattice structure by obtaining lattice points for each of this atoms or group of atoms right. We call it Motif.

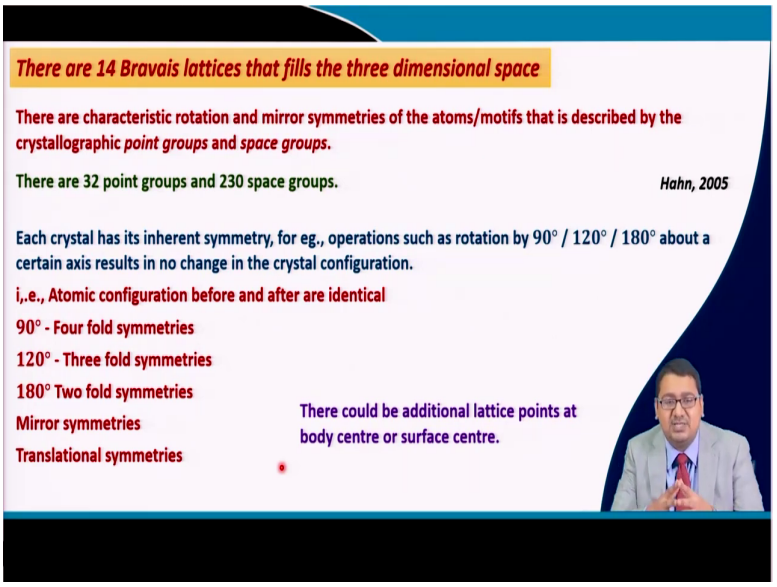
So, you see that an example, so a lattice point can be identified by the vector R bar right. So, R is equal to x times a, y times b plus z times c right. So, for example, if we say that what is

the R for this atom or the group of atom, then it is equal to you know a, a, a that is you know 3 times a and then you see 1 times b, if we go parallel to the b and then again, 1 and 2 times c, we reach the atom. So, R bar is equal to 3 a plus b plus 2 c right.

Now, what we understand? We understand that lattice is an infinite set of points generated by the set of discrete translational operations right. So, a crystal therefore, is made up of one or more atoms that is repeated in each lattice point. In case of metals and most usual metals, the lattice points are occupied by single atom right. Each lattice points are occupied by single atoms.

Now, in complex structures, identical groups of atoms are present at each lattice points right. So, you see then, these identical groups of atoms are usually known as Basis of Atoms or it is known as MOTIF.

(Refer Slide Time: 05:31)



So, there are 14 Bravais lattices that fills the three-dimensional space right and there are crystal rotations and mirror symmetries of the atoms or the motifs that is described by the crystallographic point groups and space groups. So, you see what it is meant here is that that there are rotational symmetries, you know mirror symmetries, inversion symmetries that describes point group and there are 32 point groups; whereas, a combination of these point groups with translational symmetry makes up 230 space groups.

Now, each crystals has its inherent symmetries. For example, few have operation such as rotation by 90 degrees and we know that in case of cubic crystal the four-fold symmetry of the axis 1 0 0 or 0 1 0 or 0 0 1 goes along by 90 degree rotation each time to get the identical crystal configuration.

So, by operation such as rotation by 90 degrees or 120 degree; for hexagonal close packed system, the rotation along the basal axis that is the 0 0 0 2 axis is by 120 degree and there could be two-fold symmetries, where we can get 180 degree rotations. So, that the crystal axis results, this rotation results in no change in the crystal configuration. So, that means, that the atomic configuration before and after are identical.

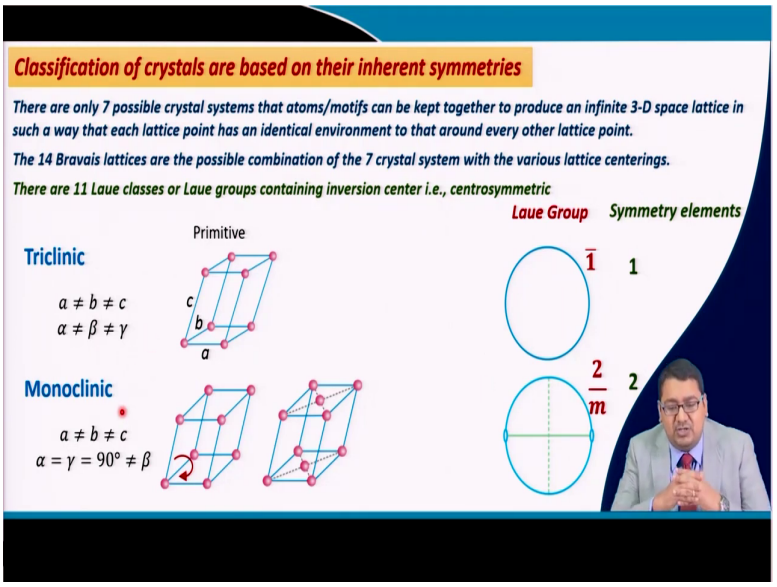
So, what we understood that there is four-fold symmetries and an example is for cubic crystal, for the axes 1 0 0. You know family of axis types and they are rotated by 90 degree each time to get the you know exact same crystal configuration, identical crystal configuration as before and there could be 120 degree three-fold symmetries.

For example, in the hexagonal close packed materials, there could be 180 degree two-fold symmetries like even in the cubic system, the two-fold symmetry exist in the 1 1 0 type family of axes right and you see that the two-fold symmetries could be equivalent to mirror symmetries.

So, you see there could be other symmetries like mirror symmetries that exist. So, there could be a mirror plane and on one side and the other side, it will be the same and this mirror symmetry is equivalent to the two-fold symmetries right. So, a four-fold symmetry may also have a mirror symmetry included in them and then, including all these symmetries, there is a translational symmetry which produces the whole lattice structure and the whole crystal.

So, there are as I said 32 point groups including these symmetries and also including the translation there could be 230 space groups. So, there could be you know in every, we are talking about this primitive you know unit cell, but there could be additional lattice points in the body centre or surface centre and which leads to the creating of 14 Bravais lattices, from the 7 possible crystal structure in presence right.

(Refer Slide Time: 09:37)



So, you see classification of crystals are based on their inherent symmetries right. So, as I said that there are only 7 possible crystal systems that atoms or motifs can be kept together to produce an infinite 3-D space lattice and it is done in such a way that each lattice point has an identical environment to that around every other lattice point right.

So, you see that the possible combination of 7 crystal systems with the various lattice centering, whether it is a body centre or it is at the face centre produces 14 Bravais lattices. On the other hand, the outcome that is the outcome of symmetry from these 14 Bravais lattices produces 11 Laue class or Laue groups containing inversion center and that means, that there are 11 Laue classes which means that 11 crystal groups which are centrosymmetric right.

So, let us start with understanding the various 7 crystal structures that forms 14 Bravais lattices and let us start with the most general, basic one which is the Triclinic system. Now, you see that a triclinic system has a unit cell with a, not equal to b and is not equal to c and you see that this is the primitive unit cell and then, the angle gamma between the a and the b is not equal to the angle beta between the a and the c and is not equal to the angle alpha between the b and c.

And therefore, you see that this triclinic crystal structure which cannot be replicated from primitive to body centred or face centred or you know base centred cubic, triclinic structures has no symmetry at all. And therefore, you see any there is no four-fold symmetry, two-fold,

three-fold, no symmetry along any of the axes even not even in a, b and c; neither in any axis like the body diagonal or the face diagonal.

And thereby, it has no symmetry and so, the Laue group looks like a full circle which indicates that there has to be a 360 degree rotation so that the in any axis, so that the crystal comes identical to the initial circumstances right. So, a Laue class is given by 1 bar right and you see like as you said that if we consider this as a stereographic projection and you can see that in case of you know cubic crystal if you remember, we have 24 symmetry elements right.

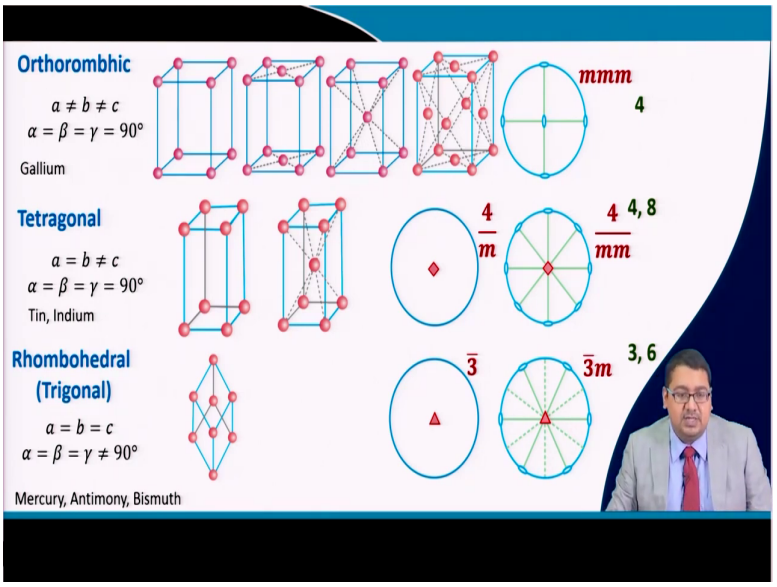
But you see that as because there is no symmetry, there is only 1 symmetry element present in the triclinic condition right, for the triclinic case. Now, the second crystal structure that we need to consider is monoclinic crystal structure. The monoclinic crystal structure also have a is not equal to b and is not equal to c; but in this case, if you see that the beta which is between a and c is not equal to you know alpha and gamma and is not equal to 90 degree.

However, the alpha which is between b and c and the gamma which is between b and a are equal to 90 degrees, which makes it suitable to have you know axis that is the b axis which has a two-fold symmetry or the same axis could be represented by the mirror symmetry. So, the Laue class could be written as 2 which represents two-fold symmetry or divided by the m that is the mirror symmetry.

In case of monoclinic, what we can observe that there is a possibility to obtain not only a primitive crystal structure, but also a base centred crystal structure; base centred monoclinic crystal structure. If we draw, if we draw a stereographic projection like this, we can see the presence of you see two two-fold symmetry and of course, they are identical because they are 180 degree apart.

So, the h if this is h k l, then this is minus h minus k minus l. So, they are both equal. Now, if such a situation exist, then there is a division between in this stereographic projection leading to you know two divisions right. So, indicating two-fold symmetry and thus, it has 2 symmetry elements. It is same like the 24 division for the cubic crystal.

(Refer Slide Time: 15:53)



Now, if we go ahead and if we look into another system, another important system is orthorhombic system and the orthorhombic system is again you see a is not equal to b is not equal to c. However, in this case, the alpha is equal to beta is equal to gamma right equal to 90 degree.

So, each of these angles between a b, b c and c a are 90 degrees. In this case, if you see we can have the primitive cell, the base centred orthorhombic structure, the body centred orthorhombic structure and the face centred orthorhombic structure right and this is just because of the presence of atom or motif in different positions, which are other than the corners of the unit cell at the base centered, at the centre of the faces or in the centre, centre of the body right.

So, you see that if we look closely, as because a is not equal to b is not equal to c in this case, what happens that there is two-fold symmetry or mirror symmetry in all these three axis's right such that we can write the Laue class as m m m m each for each axis and then, the Laue group could be given by this stereographic projection with you know 4 divisions; 4 divisions 1, 2, 3, 4 and therefore, it has 4 symmetry elements right.

Now, one of the example of orthorhombic structure is gallium right. Now, let us go to the tetragonal structure. In case of the tetragonal structure, if you see a is equal to b, so you see that a is equal to b, but it is not equal to c; whereas, alpha, beta and gamma is basically equal

to 90 degrees. It also has a body centred crystal structure. Therefore, body centred tetragonal crystal structure is present.

So, in case, the tetragonal crystal structure contains is complex right; that means, it contains groups of atom at every position. Therefore, it is a motif and under such situation, only four-fold symmetry is possible along the c axis right and therefore, this is the Laue class is given by 4 right and in the same axis, there could be a mirror symmetry, therefore, 4 divided by m.

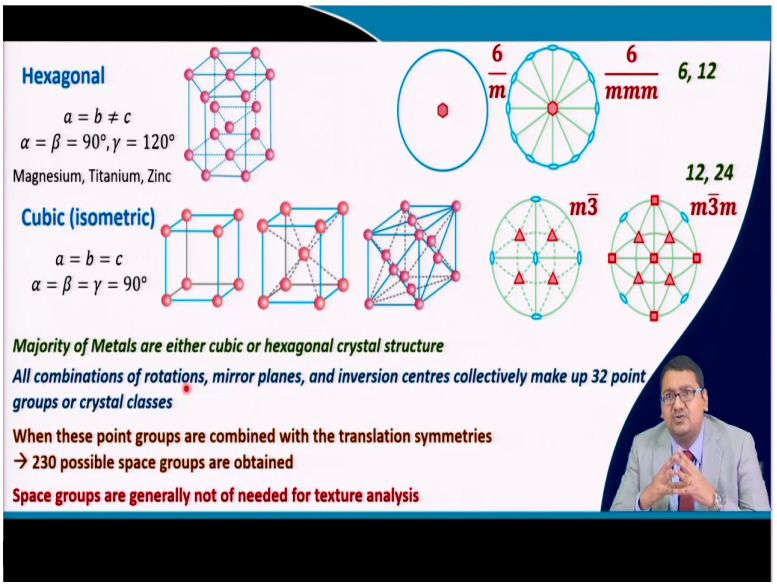
In this case, if we look into this Laue group and we can see that there could be 4 divisions here because of the possibility of four-fold rotations. It is not shown here; but this leads to the formation of 4 symmetry element in case of the tetragonal structure with complex tetragonal structure. But in case of simple tetragonal structure, either it is primitive one or body centred one, one can have four-fold symmetry along the c axis and also, one can have mirror symmetry along either b or c; a or b. So, one can write 4 by mm. In this case, what happens is that because of the presence of two-fold symmetry on the other axes, there is a presence of you know 8 you know symmetry elements.

And you can see the division of the stereographic projection that is alloy group; 1 2 3 4 5 6 7 8. Now, if we go ahead and then, there is a trigonal crystal structure, we also known it as a rhombohedral crystal structure and in this case, you see it looks something like this. And so, a is not a is equal to b, so a is equal to b is equal to c; alpha is equal to beta is equal to gamma, but none equal to 90 degree.

So, in this case, you can see that if it has a complex rhombohedral structure, then it has only a three-fold symmetry denoted by 3 bar and this because of the threefold symmetry it has you know 3 divisions not shown here 1, 2 and 3. So, there could be 3 symmetry elements written here and if it is having a simple you know rhombohedral structure and no complex structure involved like you know simple metals like Mercury, Antimony, Bismith etcetera.

Then, in those cases, it has threefold symmetry and along with this the other axis, another axis may have a mirror symmetry. Leading to a formation of you know 6 symmetry elements denoted here; you see 1 2 3 4 5 6.

(Refer Slide Time: 21:34)



So, now, we will go to the hexagonal close packed structure. In addition, you can see the typical unit cell of an hexagonal close packed structure. It contains 6 atoms at the corners of the top and the bottom phase; 1 atom at the center of the top and the bottom phase and 3 atoms in between inside the unit cell.

So, in this case, what happens that a which is this one is equal to b and the angle gamma between a and b is 120 degrees and c which is perpendicular to both a and b has as it is perpendicular the angle between c and a and c and b is equal to 90 degree. So, alpha is equal to beta is equal to 90 degree.

There are many elements, which are metals which are, which have the hexagonal close packed structure. These are you see magnesium, titanium, zinc and you can you know that magnesium, titanium are very important metals and are used in industries and in you know biomedical application, aerospace and even in high grade automobiles right.

So, you see that if the hexagonal close packed structure has a complex is a complex hexagonal structure, then it can only have a sixfold symmetry and the same symmetry may have a mirror symmetry too. So, 6 by m and therefore, it can be shown like this for the Laue group and you can write 6 by m in case of the Laue class.

Now, this 6 you know symmetries actually divides this stereographic projection into 6 different areas; not shown here. But it divides, same like this, divides into 6 different areas

and therefore, it has 6 symmetry elements. Now, if it has a simple hexagonal close pack structure, then it not only has a sixfold symmetry about the c axis, but it has mirror symmetries on the other planes too leading to 6 formation of Laue class which is given by 6 by mmm.

And therefore, the Laue groups look like this and you can have you know 12 symmetry elements. Because you can divide the stereographic projection into you know 1 2 3 4 5 6 and like that 6 here, 12 triangles equivalent triangles and you can if you remember that these equivalent triangles will contain in the center 0 0 0 2 or 0 0 0 1.

Here, it will contain 1 1 2 bar 0 for example and then, here it will contain 1 0 1 bar 0 leading to the formation of an you know inverse pole figure right. Can you relate it? So, this is all about the hexagonal close packed system and let us come to the cubic crystal system and which most of the metals that we work on either it is aluminum, which has a face centered cubic system.

We have learnt that this is the FCC crystal structure or if we call out iron or ferritic steel, then it has body centred cubic crystal and then, other elements like copper and you know silver, they have FCC structure and there are many. So, we know a lot about the cubic crystal system and you see this is the one which is primitive and some complex you know crystals may have primitive cubic crystal structure or isometric crystal structure right.

So, in in case of cubic a is equal to b is equal to c and alpha is equal to beta equal to gamma is equal to 90 degrees right and you know that in case of the cubic crystals, there could be 4, 1 1 1 axis and with 120 degree rotation, it may have threefold symmetry right. It will have some three-fold symmetry.

On the other hand, it will have you know four sorry 3 axes that is 1 0 0 axes which can rotate by 90 degree and have you know fourfold symmetry and it has 6, 1 1 0s which has twofold symmetries. The Laue group and the Laue class basically represents the 1 1 1 axis with the threefold symmetry and therefore, is given by 3 bar.

On the other hand, because of the presence of the mirror symmetries along the 1 1 0 and 1 0 0, it is given by m 3 bar and you can see that if it is having a complex structure, then the other symmetries are less. So, you can see that in case of complex structured cubic crystals, there could be only 12 symmetry elements.

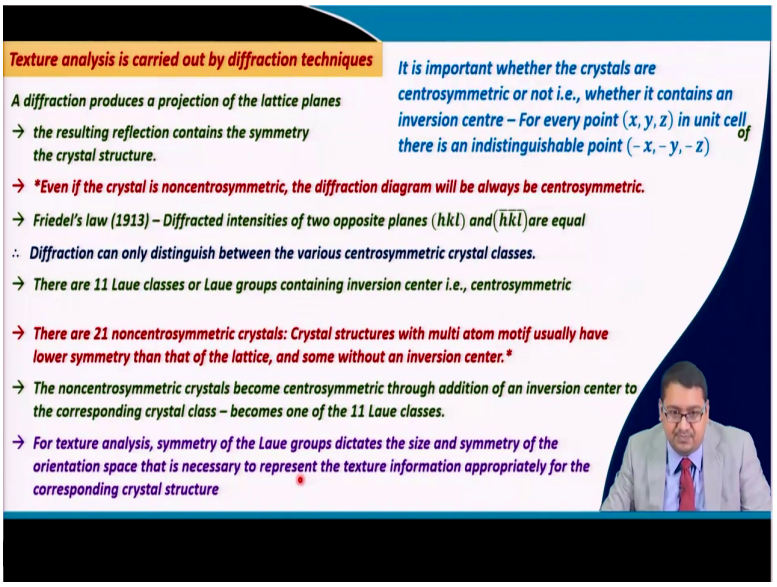
Whereas, in case of simple body centred and face centred cubic crystals like metals for example that I given aluminum, copper, iron, like austenite or ferrite whatever it is. It has all the symmetries that the 3, 1 0 0 axis with 90 degree rotation having fourfold and the 4, 1 1 1 1 with 120 degree rotation threefold and the 1 1 0; 6, 1 1 0s with 180 degree rotations twofold, all the rotations.

And thereby, the Laue group once second, the Laue group and which is basically the stereographic projection could be actually divide itself into 24 triangles with say let us take any one of it with 1 0 0 axis, 1 1 1 axis and 1 1 0 axis and identical triangles 24 triangles and showing 24 symmetry elements.

So, as we can understand that there are seven crystal structures and each of the crystal structure because of the presence of atoms or motifs at different positions could form 14 Bravais lattices. We can go back you see you can go back and count them; you see 1, 2, 3, you know 4, 5, 6, 7, 8, 9, 10 and 11, 12, 13, 14. So, 14 Bravais lattices right. On the other hand, we can again go back and we can see that 1 2, we if we calculate the Laue groups, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11.

So, 11 Laue groups are possible. Therefore, you see what we understand. We understood that all the combination of rotations mirror planes and inversion centres collectively make out 32 point groups or crystal classes. When these point groups are combined with translational symmetries, it forms 232 possible; 230 possible space groups right. Space groups are generally not needed for texture analysis right.

(Refer Slide Time: 29:59)



So, you see a most of the texture analysis, leading to obtain full information of the texture is done only by diffraction techniques; means, either it is electron beam using electron backscatter diffraction or x-ray beam using x-ray diffraction techniques. It is important whether the crystal is centrosymmetric or not. Now, the most crystals as simple crystals are usually centrosymmetric, are centrosymmetric all of them; most of them.

Now, few crystals with complex motifs may be centrosymmetric or may not be centrosymmetric; but whether the crystal is centrosymmetric or not. That means, whether it contains a inversion centre or not, for while doing diffraction for every point x, y, z in the unit cell, there will be an indistinguishable point minus x, y minus y and minus z and this is true for centrosymmetric. However, may not be true and is not true for non the structure having no inversion center and which is not centrosymmetric.

However, you see a diffraction produces a projection of a lattice plane right. So, the resultant reflection, the resultant reflection; the reflection means the diffraction the resultant diffraction may contain the symmetry of the crystal structure. Therefore, even if the crystal is non-centrosymmetric, the diffraction will always be centrosymmetric. This is very important to understand. Now, this occurs because the diffracted intensities of two opposite planes h k l and h bar k bar l bar are basically equal.

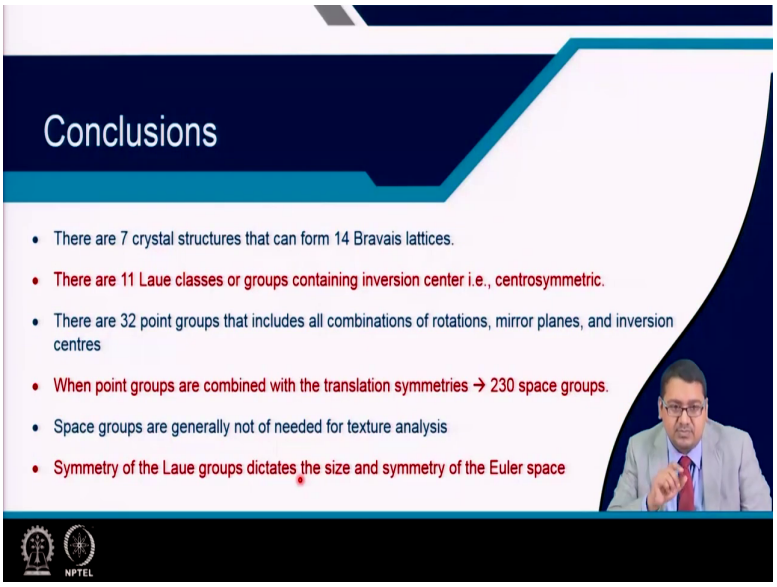
Therefore, you see diffraction can only distinguish between different centrosymmetric crystal classes. It cannot distinguish between a non-centrosymmetric and centrosymmetric class,

which with the inversion symmetry in the non-centrosymmetric case becomes equivalent centrosymmetric because during the diffraction, it gives the diffraction opposite diffraction minus.

So, h bar k bar l bar diffraction too. Now, so there are as we said 11 Laue classes or Laue group containing inversion center or they are centrosymmetric right. Therefore, there are 21 non-centrosymmetric crystals. These crystal structures have multi motif multi atom motifs ok usually have lower symmetry than that of the lattice and some without an inversion center.

I am again repeating, these non-inversion centered non-centrosymmetric crystals, the diffraction always remains centrosymmetric right. So, the non-centrosymmetric crystals become centrosymmetric through addition of an inversion center to the corresponding crystal class and becomes one of the 11 Laue classes. So, for texture analysis symmetry of the Laue groups dictates the size and symmetry of the orientation space. So, why it is important here? Because you see for the texture analysis, you see the symmetry of this Laue group; so, symmetry of tetragonal trigonal orthorhombic cubic hexagonal leads dictates the size and the symmetry of the Euler space that is the orientation space, which is necessary to represent the texture information more appropriately for the corresponding crystal structure.

(Refer Slide Time: 34:34)



So, the finally, we can conclude here that there are 7 crystal structure that by combination and position of atoms or motifs at the centre of the body or the center of the base can form 14 Bravais lattices. There are 11 Laue classes based upon the you know crystal symmetry and

which contains inversion center that is there are 11 crystal structure or you know which 11 type of Laue classes or Laue groups which are centrosymmetric.

There are 32 point groups that includes the combination of rotation, mirror planes and inversion centres, combining the point group with the translation symmetries makes a 230 space groups. Space groups, we do not need it for, need them for texture analysis. Therefore, we restrict ourselves to understanding point group and Laue classes. So, the symmetry of the Laue group dictates the size and the symmetry of the Euler space.

Thank you very much.