Characterization of Construction Materials
Prof. Piyush Chaunsali
Department of Civil Engineering
Indian Institute of Technology - Madras

Lecture 13
X-Ray diffraction Introduction to X Rays and crystallography Part 2

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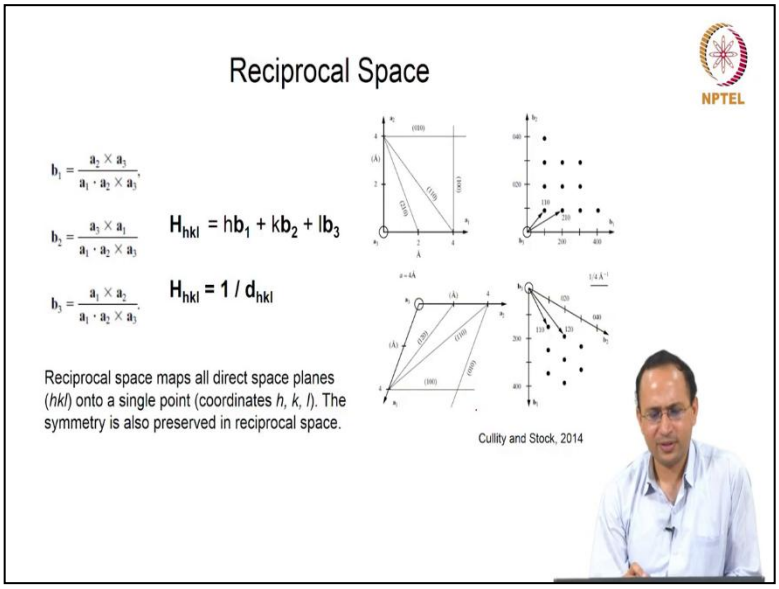

It is very important to look things in reciprocal space. So, far we have been looking at the direct space. We will learn how to construct a reciprocal space. So, for an example we take the direct space on the left (in slide). So, let us see direct space here we have a_1, a_2, a_3 which are the three crystallographic axis.

We do not plot a_3 assuming it to coming out of board. So, you have a_1 and a_2 which are the two crystallographic axes and considering the plane 1 1 0 it will have one intercept with a_1, one intercept with a_2 and 0 as it is not cutting a_3 in reciprocal space. So, when (1 1 infinity) is reversed we get (1 1 0). Similarly 2 1 0 are known as the Miller indices.

We know that a_1, a_2, a_3 are the vectors in direct space. We can say that the b_1 vector in reciprocal space is expressed as

$$b1 = \frac{a2 * a3}{a1.\, a2 * a3}$$

Hence, b_1 will be perpendicular to a_2 and a_3

b_2 and b_3 in reciprocal space is written in the similar way as mentioned below

$$b2 = \frac{a3 * a1}{a1.a2 * a3}$$

$$b3 = \frac{a1 * a2}{a1.a2 * a3}$$

So now you understand how these this is in the reciprocal space. The benefit of reciprocal spaces maps all direct space planes on to a single point. So, in this case we want to map all 1 1 0 planes and points in reciprocal space which represents corresponding to 1 1 0 plane. So, you get the b1, b2 and which gives 2 0 0, 3 0 0 and 4 0 0.

The distance from origin of reciprocal space to the particular point is half of the inter planar spacing. Inter planar is the distance between the planes in direct space and it is shown as d_{hkl} The length of the vector (H_{hkl}) will be the reciprocal of d_{hkl}.

In reciprocal space distances are expressed in Angstrom inverse. This vector on the plane 1 1 0 will be perpendicular to the plane. So, the advantage is that you can map the planes to a point.

So, if there is a point 1 1 0 it will tell you all about 1 1 0 planes. Also there is a periodicity in reciprocal space which makes things easy to visualize and simpler. So, mainly reciprocal space maps all direct space planes onto the single point. The symmetry is preserved in the reciprocal space. Now same thing if we apply two different system.

Now we are talking about the perpendicular axis in direct space and we have to construct the reciprocal space by referring to the basic principle. So, b_1 is a_2 *a_3 hence b_1 has to be perpendicular to both a_2 and a_3. For b_2 is a_3 *a_1 so it is perpendicular to both a_3 and a_1.
Because a 2 it has to be perpendicular to a 2 also it has to be perpendicular to a 3. So, the b 1 direction is this, b 2 should be perpendicular to both a 3 anyone now a 3 is again coming out of the slide and a 1 is this direction so it has to be perpendicular that means this is the direction it has to be perpendicular to both a 1 and a 3 see the difference. Now once you have constructed the space; you can put the points in that.

The points will be like1 0 0, 2 0 0, 3 0 0 while considering the b_1 axis and for b_2 axis it will be like 0 1 0, 0 2 0, 0 3 0, 0 4 0. For points like 1 2 0 means there will be 1 intercept along b_1 and 2 along the b_2.

So in order to get this you should first traverse along b_1 and then you go parallel to b_2. Therefore it translates all the planes to single point

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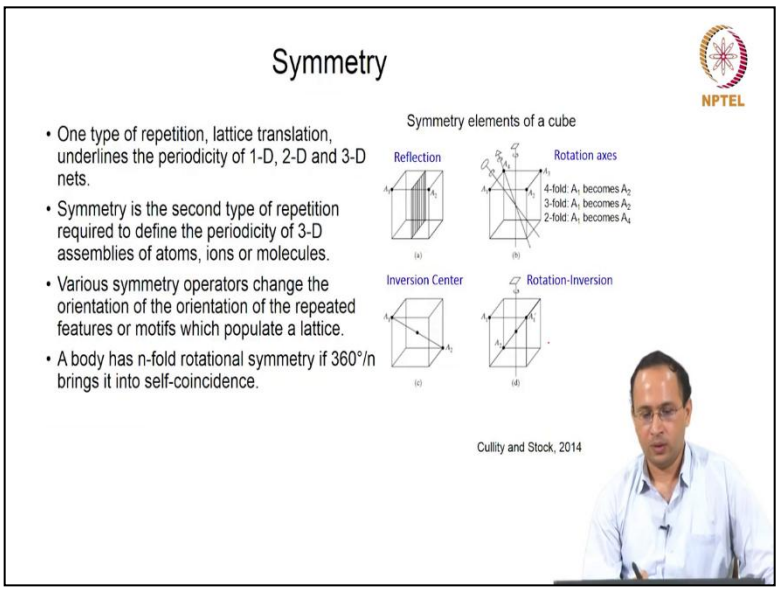

Now we look into symmetry, symmetry is one type of the repetitions in crystals. So, one of the repetition is lattice translation where you simply translate the lattice in one direction which gives periodicity. Symmetry is the second type of repetition required to define the periodicity of 3-D assemblies of atoms ions and molecules.

Various symmetry operators change the orientation of the repeated features or motifs which populate a lattice. For example, we are looking at the symmetry element of a cube so we have reflection symmetry in this case where a_1 axis becomes a_2.

Now we talk about the rotation of the same cube in terms of 4-fold symmetry.4 fold symmetry means if you rotate the cube by 90 degrees it brings self-coincidence which means this node at a_1 after 90 degree rotation becomes a_2. Similarly a_2 becomes a_3 in four fold type of symmetry if you rotate by 90 degree.

Also there is threefold symmetry which means you have to rotate by 120 degrees along the marked threefold and we see that a_1 becomes a_2 . Now for twofold symmetry, cube is rotated by

180 degrees. Also there is a symmetry operation called inversion centre, so you can see that a_1 becomes a_2 which is centre inverted.

There is a rotation inversion operation where when you rotate for example there is a fourfold rotation a 1 becomes a 2 and then there is the inversion where a_1 becomes $a_{1'}$ and thereafter $a_{1'}$ becomes a_2 which is combination of rotation and inversion.

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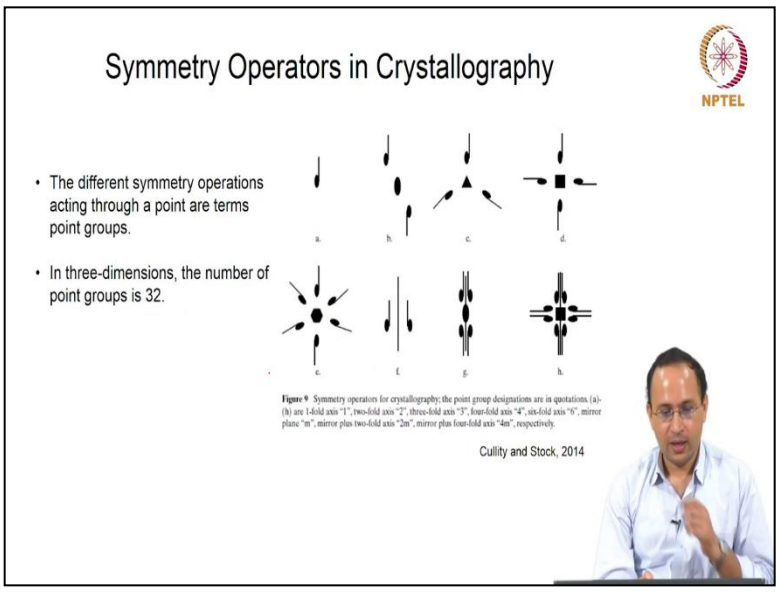

The different symmetry operations acting through a point are termed as point groups. Now in the plot above what you see are the symmetry operators for crystallography with the point group designation in the quotation. So, a is one fold axis which means you have to rotate it by 360 degree to come to self-coincidence.

In this case b, it shows twofold axis which means you have to rotate it by 180 degrees to get self-coincidence. The case c has three fold symmetry which means you have to rotate by 120 degrees. Now for case f is mirror plane where it is just the mirror image of plane.

Now this case g is a mirror plus twofold axis where you see the mirror image and when you rotate by 180 degree you get the same. So, in three dimension the number of point groups is 32. So, these are the different symmetry operations acting through a point.

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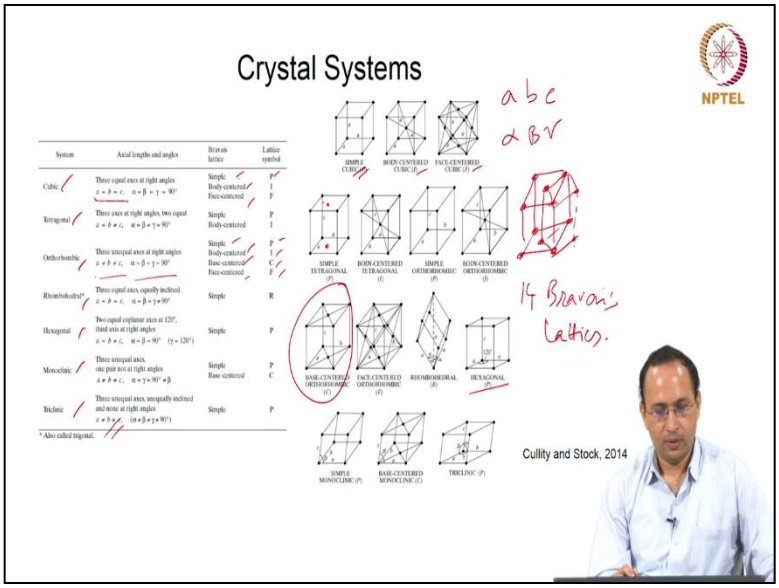

Now we talk about the crystal systems. So, there exists 7 crystal systems namely cubic, tetragonal, orthorhombic, rhombohedral, hexagonal, monoclinic, and triclinic. a, b, and c are the length of the axis and α, β, and γ are the inter-axial angles.

For example, cube has 3 equal axis which means a = b = c and angles $\alpha = \beta = \gamma = 90$ degrees which defines cubic system. So in total we have 7 crystal systems and 14 bravais lattices. So, in cube we can have a simple cubic structure for the aforementioned arrangement and you can also have a body centered cubic system, where we have an atom at the center.

You can also have a face centered system where you have atom on each face. So, a simple cubic is designated with letter symbols P, I, and F. In case of tetragonal system a equals to b but not equal to c. It can have body centered tetragonal system too. Similarly for orthorhombic all 3 sides are not equal.

For hexagonal, a equals to b but a is not equal to c, c is different and two angles are 90 degrees and one angle is 120 degrees. In case of triclinic all sides and angles are unequal.

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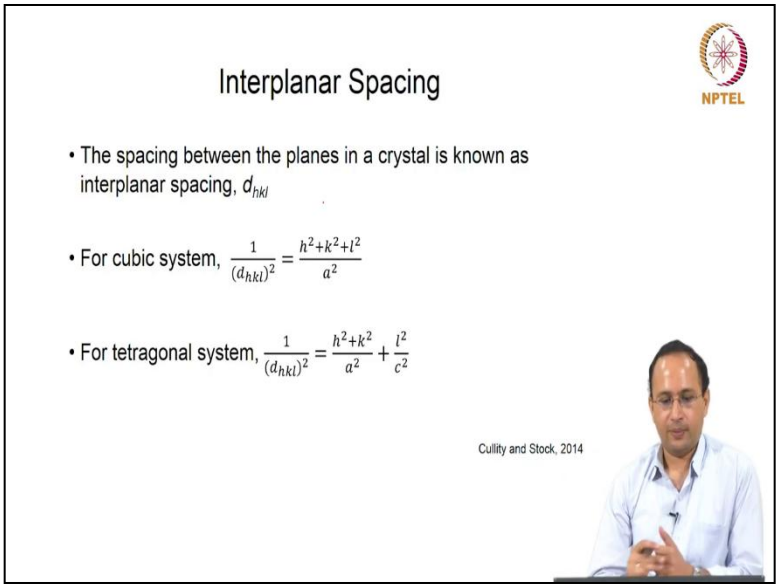

Interplanar spacing is the spacing between the planes in a crystal. For cubic system the inter planar spacing is given by the relationship

$$\frac{1}{(dhkl)^2} = \frac{h^2 + k^2 + l^2}{a^2}$$