3D Space Groups III: Bravais Lattices in Trigonal Crystal System
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Lecture 22 c

In this video, I will present Bravais lattices in trigonal system. This is a slightly confusing topic. So, I am specifically discussing this particular Crystal system because it requires some attention.

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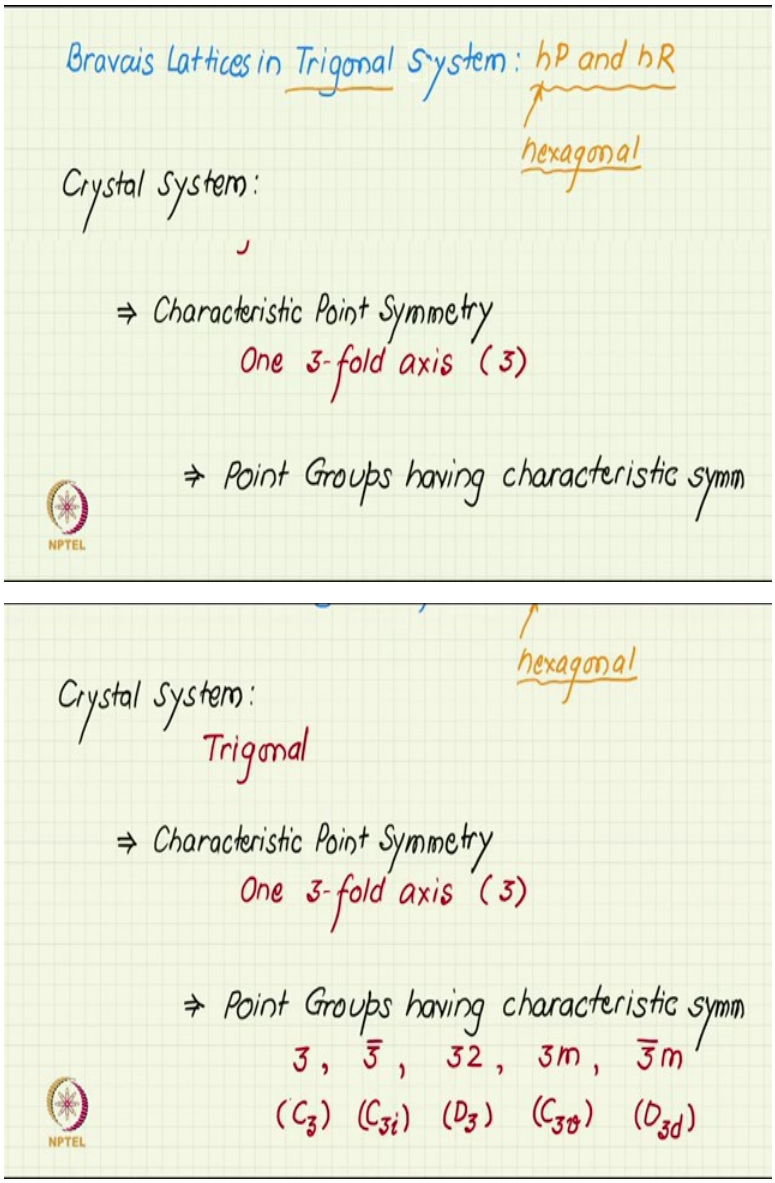

So, there are 2 Bravais lattices in the crystals system trigonal Crystal system hP and hR. So, you can see and this the symbol h stands for hexagonal. So, this itself is somewhat confusing that the crystal system is trigonal, but there are 2 braver lattices which belong to that system

and both are designated with the symbol hexagonal, P of course stands for primitive, and R for rhombohedral.

Now, Crystal system as you know implies a certain characteristic point symmetry. This I keep emphasizing and this is important to keep in mind that a crystal system is not defined by certain relations between lattice parameter but by a crystal having certain characteristic point symmetry. And if you think in terms of the 32-point groups, some of those point groups will have this characteristic point group symmetry. So, Crystal system can also be thought of as classification of point groups having that characteristic symmetry.

So, let us apply this to the example of trigonal system. So, if the crystal system is trigonal, then the characteristic point symmetry is 1 3-fold axis 1 3 fold Axis or in symbol just 3. So, the point groups which will have this 3-fold axis out of the 32-point groups point groups having a single 3-fold axis are 5 different point groups which belong to the crystal system, the trigonal Crystal system. So, these are 3, 3 bar 3 2, 3M and 3 Bar M, that is in the Hermann Mogae notation.

In the show and flies notation, we write them as C3 C3I because 3, 3 bar is a 3-fold with a center of inversion. So, that is what is a recorded or noted in the show and fly's notation that is a 3-fold as well as an inverse and Center. 32 is called the dihedral group D3 3m is a 3-fold with vertical mirrors that is mirrors passing through the 3-fold axis and 3 Bar M is D3d that is a dihedral group of order 3 with diagonal mirrors. So, D 3d anyway. So, these 5, any Crystal having these 5 point group symmetry will be by definition a trigonal Crystal.

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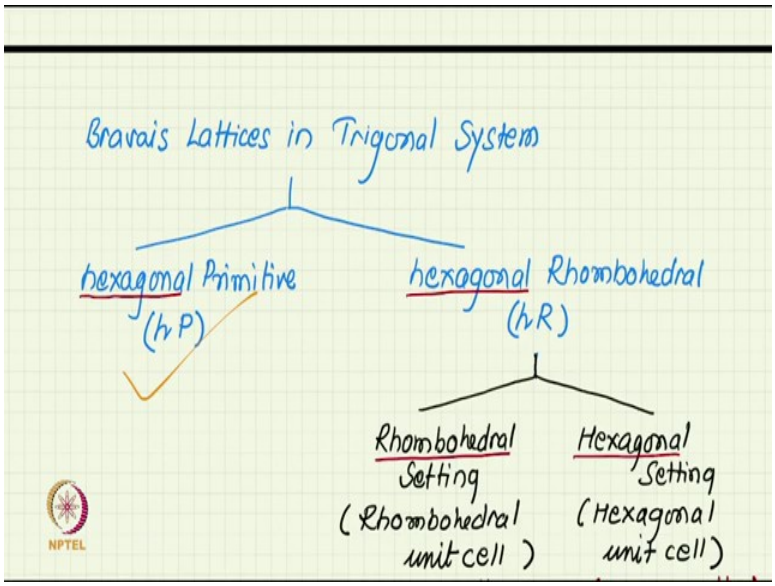

But to denote this trigonal Crystal or to represent these trigonal crystals, we need Bravais lattices and as I pointed out, that the Bravais lattices in the trigonal system, there are 2 of them you have, either the hexagonal primitive or hexagonal rhombohedral hP hR, P of course is a primitive, it is referred to as, referred as a conventional unit cell chosen for this lattice will be a primitive unit cell.

In the rhombohedral, the conventional unit cell allowed are actually again 2. So, these 2 are known in the international table and of course, one confusion also comes because different authors and different books, sometimes use these terms in different sense. What I am trying to do is to stick to what the current International tables published by International Union of crystallography is referring to. So, in this notation, the hex, in the, if you look at the international tables the hexagonal rhombohedral space groups hR space groups are always referred to in 2 different unit cells or 2 different axial systems.

One is the rhombohedral, these are called settings rhombohedral settings, I will call it my rhombohedral unit cell or hexagonal setting which uses the hexagonal unit cell. And in this case, the rhombohedral is actual rhombohedral setting or rhombohedral unit cell is a primitive unit cell and the hexagonal unit cell is non primitive, it is an R-centred cell which is available only in the trigonal system. So, you can see that in the current nomenclature none of the lattice or unit cell in the trigonal system has the name trigonal, there I have name either hexagonal or rhombohedral.

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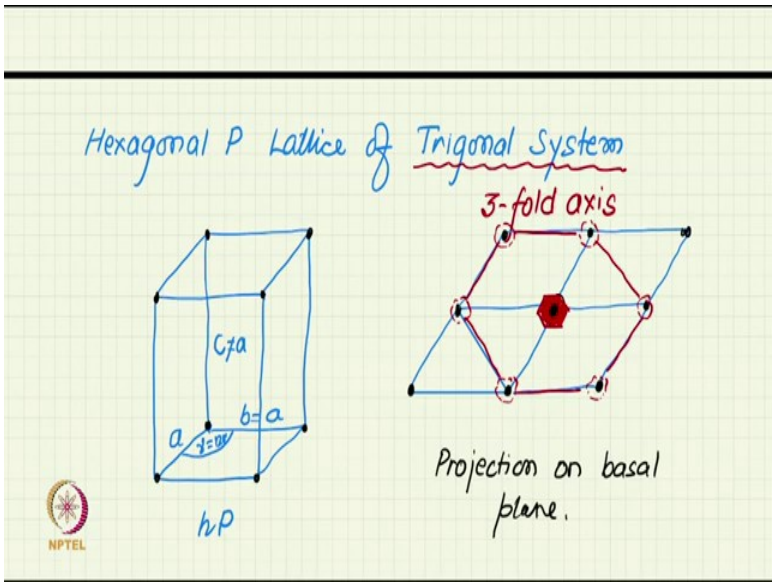

So, let us look at this in little bit more detail now. So, let us say hexagonal primitive unit cell or hexagonal primitive lattice. So, hexagonal P you know, the conventional unit cell used will

be a hex, rhombus-based prism. So, you have a rhombus, a equal to b, the angle between them is 120 degree, and you have the height of the prism c which is not equal to a. So, this gives you a hexagonal P unit cell of the hexagonal P lattice. So, lattice point since it is primitive, lattice points will only be at the corners.

You can see it in projection also, you have the rhombus you divide the rhombus into triangle for just for reference and there are lattice points here which are representing lattice point at the base as well as lattice point on the top, 4 of them, because they will project exactly at the same location in the projection, this is called projection on basal plane.

Now, the question is, we are talking of, just now we said that we are talking of trigonal system which is supposed to have a 3-fold axis one of the 5 point groups which have 3-fold access. So, then but this system, the hexagonal P lattice on its own will have a 6-fold axis. So, if I extend the, you can see the 6-fold axis better, if I draw the projection of few more unit cells whether you will have lattice points here, if you look at any given lattice point then let me focus on this one. So, you can see that that is surrounded by 6 lattice points here, the lattice itself will have a 6-fold symmetry.

Then how is it? So, if it has a 6-fold symmetry let me draw a hexagon here to represent the 6-fold symmetry. So, you have 6-fold symmetry axis passing through each lattice point. So, then it is obvious that this can belong to a hexagonal Crystal system, but how does it belong to trigonal Crystal system. It will belong to trigonal Crystal system only if we decide to put a motif of, motif having symmetry of the trigonal system, Motif having one of these 5 point groups. All of them have a single 3-fold access, if I choose any of those point groups and place it.

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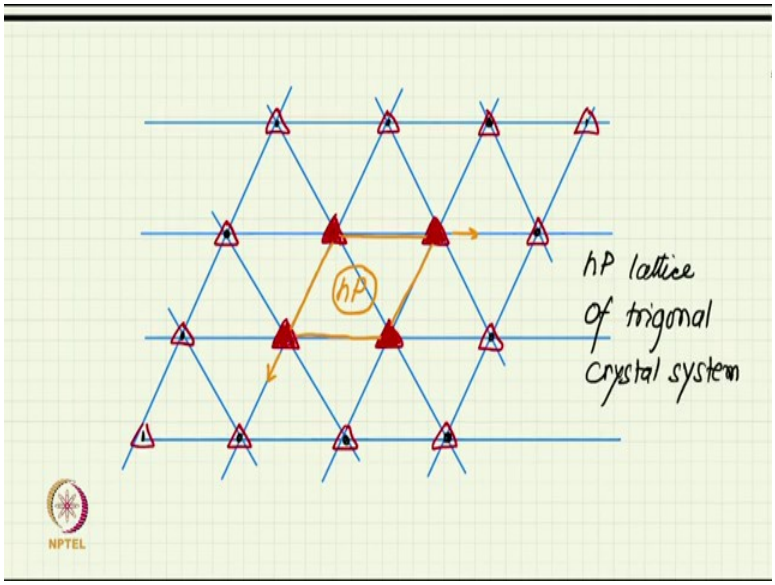

So, let me make another drawing. So, let us look at now I have drawn projection of many hexagonal P unit cell and these are the lattice points, the base of the unit cell of course is Rhombus, but I have divided each rhombus into equilateral triangles and just for visualization. And, if instead of what I told that you have a 6-fold axis passing through each lattice point which is what is also happening here now. But instead, if I decide to place a 3-fold motif one of those 5-point groups having a 3-fold axis and if I align the 3-fold axis parallel to the c axis. So, in this projection diagram let me just try to place a triangle, if I place a triangle, then the 6-fold is Disturbed and all the 6-fold is converted into a 3-fold.

So, if you start with a hexagonal lattice but use a trigonal motif, motif consistent with the trigonal symmetry you will get a crystal which is trigonal, but you will still use for your reference you will use a unit cell which is hexagonal. So, that is what is meant by a hexagonal p unit cell for a trigonal lattice. This triangle I have, use this as a triangle but it can be motive with any of those 5-point groups but finally since that their 3-fold is along the c axis these axis will get converted into 3-fold, etcetera. It is an hP lattice of, we can call it an Hp lattice of trigonal Crystal system. So, that is that is this branch that is this branch. Now, let us look at the other branch, the other lattice which is possible in the trigonal system, and that is hexagonal rhombohedral.

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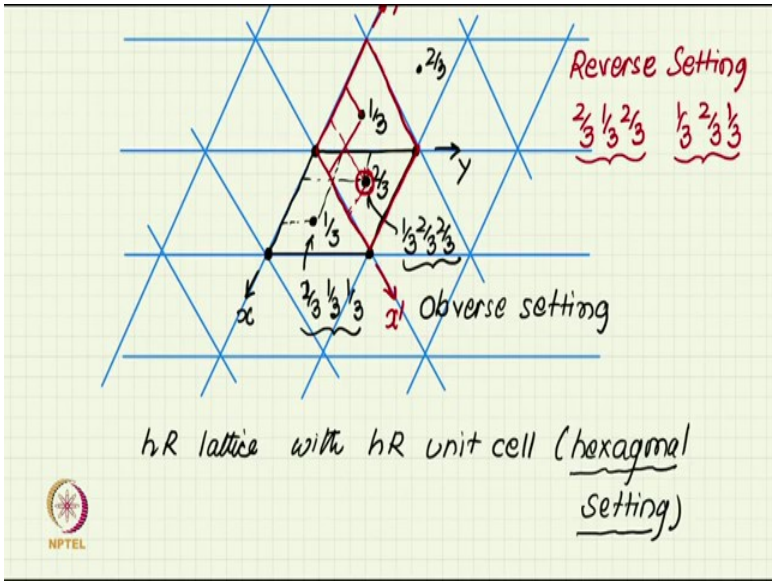

Hexagonal rhombohedral, again we start our starting point is again the hexagonal primitive lattice. So, let me outline the rhombus, this will be the rhombus unit cell. However, the lattice point now instead of the corners will be lattice point but we have 2 more additional points which correspond to the centroids of these 2 triangles, but their c height, the z height is one third here and 2-thirds there. So, this is your new unit cell and this one third and 2 third points are also lattice points. So, there are effectively now, this is your hR lattice when hR unit cell, this is the hexagonal setting known as hexagonal setting. A hexagonal setting just to confuse you okay.

So, this is an hR lattice hexagonal rhombohedral lattice, lattice is rhombohedral but the setting still is hexagonal, you will see what is the rhombohedral setting soon. And here also, you can have in this hexagonal setting, you have what is called the obverse and reverse settings. So, what is shown here is obverse setting. But if you choose, let me mark this one third point, in another unit cell that will be one third, this will be 2 third.

Suppose, we choose our axis. So, let us let us write down the coordinates, the full coordinates of these 1 third and 2 third points. So, the one third point, if you look at the coordinate along x and y axis. So, this is 2-thirds in the x-axis, one third on the y-axis, and one third on the z-axis and this point is one third along the x axis, 2 third alongs y, and 2 third along z.

So, this black unit cell is what is called the obverse setting lot of jargon, lot of terminology to confuse you. But obverse setting, but we could choose our x and y axis differently rotated by 60 degree so, to say let me highlight this red unit cell x Prime and y Prime. So, now the red one is reverse setting, where if you now look at the coordinates.

So, this coordinate now, the one which I am outlining in red at the moment becomes if you look with respect to the x Prime y Prime axis, the first one is 2 third x coordinate, this red point, the current red point is 2 thirds one third and then the height is 2 third and the other point if you look at its coordinate is one third 2 third and one third. So, you can see that these coordinate the red coordinates or coordinates of internal points with respect to the red axis and coordinates of the internal point with respect to the black axis are slightly different, the way 2 thirds and 1-thirds are distributed along x y and z. So, these 2 settings are known as obverse and reverse setting for the hexagonal setting, for hexagonal are lattice.

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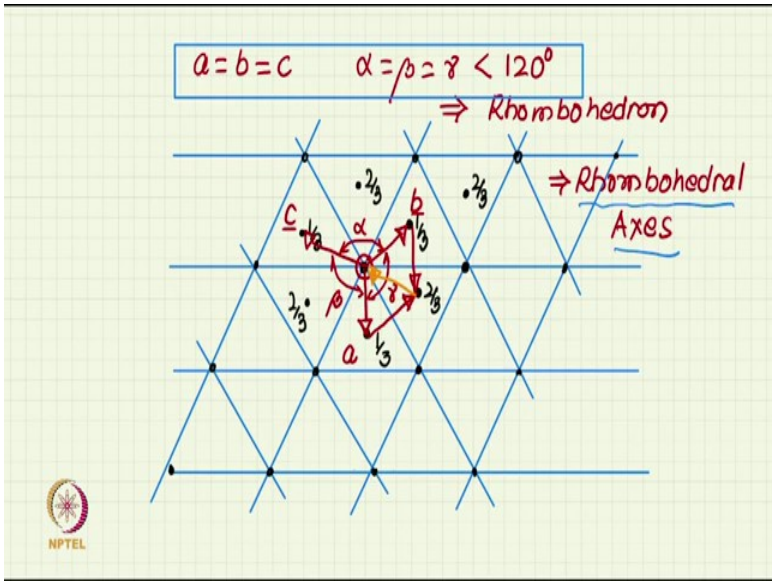

Now, let us come to the rhombohedral unit cell choice for hexagonal setting. So, I again start with the lattice points, these lattice points are at 0, 1, and all other integral values all will project at the corners of this hexagonal or triangular Network, as you may please to call it. And these points are now one third, 2 thirds, let me mark some more points.

Now, suppose I start at the 0 level with that lattice point and join 3 of these lattice points which are at one third level above this point and call these as my basis vectors, you can see that these 3 vectors will have equal lengths because all of them are equally distributed symmetrically distributed about the central point. So, and, means if you so, if you can use trigonometry and geometry to show that these vectors are of the same length. So, we have a unit cell in which a equal b equal c, and you can also see that these angles.

Now, there are no more 120 degrees because of the z coordinate which is one third. So, there will be 120 degrees only in projection if one third was actually 0, but now since these points are above the centroid. So, these 3 angles between a and b you call that gamma b and c Alpha

and a and c beta. So, these 3 angles are also equal but they will not be 120 degree there will be less than 120 degree.

And any 3 vectors define a parallelepiped , they will define a parallelepiped, which will be a rhombohedron. So, parallelepiped defined by these lattice parameters or the 3 vectors is a rhombohedron, and this is then called the rhombohedral setting or rhombohedral axis. And this is quite often in many textbook you will find this unit cell as the definition of the trigonal lattice, but you can see that the trigonal… this is only one of the possible choices for one of the possible types of lattices.

So, 2 lattices hexagonal P lattice and hexagonal R lattice, in hexagonal R lattice you have centred cell with the 2 lattice points inside and one lattice point at the corners. And in the hexagonal R lattice there is another choice of unit cell, which is the rhombohedral Axis or rhombohedral choice. So, you can if you so wish you can, show this in 3 dimensions but I do not want to venture into that I leave it to your imagination that what you will be getting here.

So, if these 2 vectors for example if you join you will reach the next level 2 thirds. So, that also will be a vertex of your parallelepiped and then finally, on the 2 thirds if you join add the vector c you will head towards the centre again. But since you are starting with 2 third and c Vector further raises you by one third you will come to a height one above the original Centre or original origin.

So, that will, if you do this you will get a rhombohedron or a parallel piping when one 2 vertex along the c axis 0 and 1 and then 3 vertices at 1 third, 1 third, 1 third, and 3 vertices at 2 thirds high. So, that gives you the 8 vertices of the rhombohedron. So, I hope I have made an attempt to clarify the situation a bit, but if I have confused you even more, I am sorry about that. Thank you very much. Bye bye.