Foundations of Computational Materials Modelling
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Hernann maugin symbols of space groups

Good afternoon. Let us continue with whatever we were discussing last class. So, basically we were talking about the symmetry of the Bravais lattices, of the space Bravais lattices in 3D.

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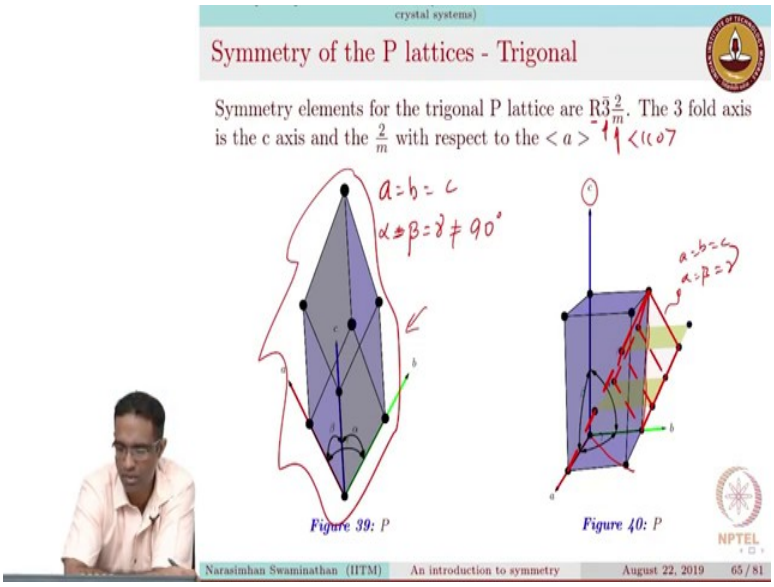

So, in particular we were the, at the last we looked at this trigonal lattice or rhombohedral lattice as it may also be called. And we talked about one specific unit cell that might be appropriated for this particular lattice. We said that it was A equal to B equal to C, alpha equal to beta equal to gamma, but none of them are actually equal to 90 degree, just alpha equal to beta equal to gamma is sufficient.

It so happens that the symmetry of this particular trigonal lattice is represented using R, a 3 bar and 2 over M. Now, it is difficult to see with respect to this unit cell, what these 3 bar and 2 over M actually represent. Because the same unit cell can actually be visualized inside a hexagonal lattice like what is shown right here. We generally use a hexagonal unit cell in order to construct a rhombohedral structure.

It has a 3 fold symmetry and this 3 fold symmetry is about the c axis and the c axis is actually the body diagonal of this unit cell which is marked here, you see the red colour unit cell which is marked here, the red colour which is marked here, that is what this is. That unit cell

here has A equal to B equal to C and alpha equal to beta equal to gamma. So, this is a little difficult visualize and construct, we generally use a hexagonal unit cell in order to construct trigonal lattices.

Here is very important to remember, the 3 bar is with respect to the c axis so as you can see if you rotated it by there is 3 bar symmetry, so that is a 120 degrees plus an inversion that is going to be available about the c axis and the 2 bar M is basically about the 110 axis of the hexagon, so basically this axis, there is 2 fold rotation and a mirror plane perpendicular to it, just like your hexagonal lattice structures.

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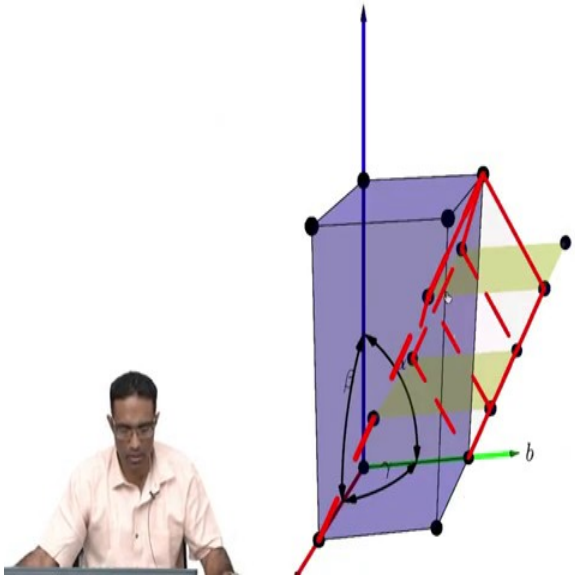

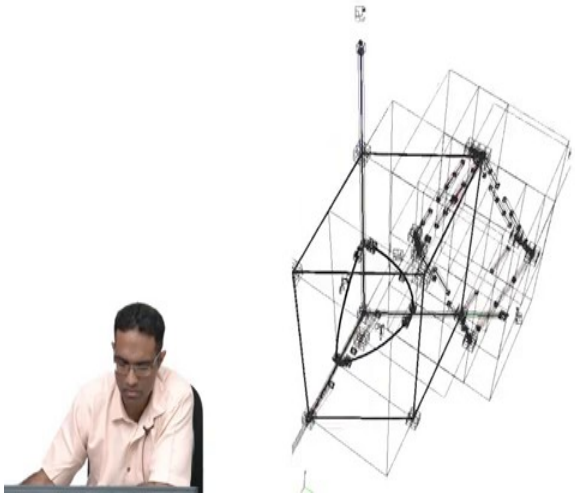

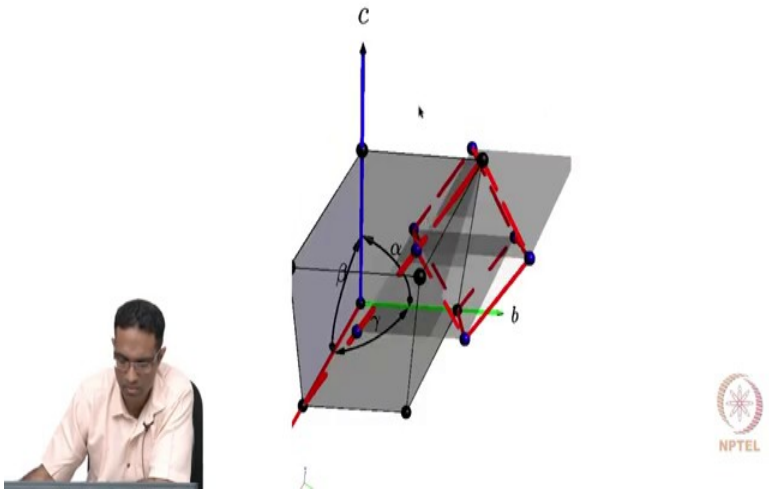

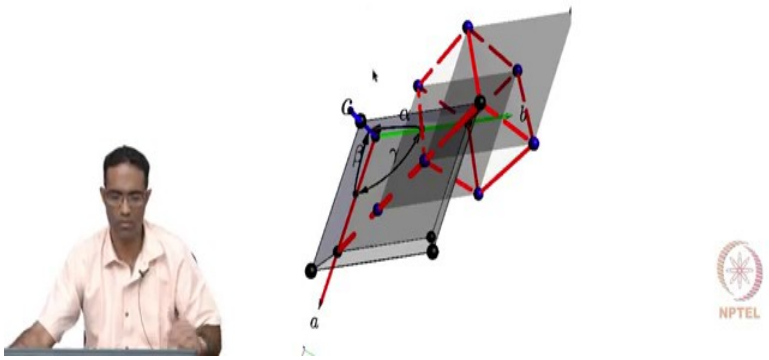

So, we can take a look at it in a little bit more careful manner if I am able to show you the 3 dimensional image. This is sometimes important to understand well because it is not very clearly explained in some of the books. So, what the cell basically consist of, so you will have a basis, I am sorry I am not able to...

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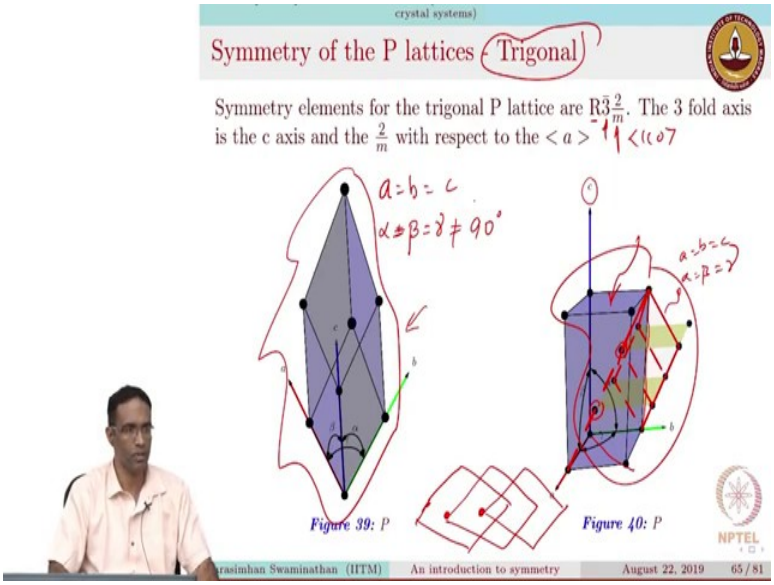

So, what this, how this looks from the top views as follows. So, you will have a rhombus, so you are looking at the thing from the top, so from above the c axis, and then you will have a corresponding point here at 1 by third the height and then another point here, which is present at 2 by thirds the height, so, and they will keep getting stacked in this particular manner.

So, it so happened that you know there are 2 unit cells are possible when you have such a symmetry, one is this one which is obviously not primitive, it is not primitive because there is going to be one lattice point right there and the other lattice point right there, both of which are inside the unit cell. However, this unit cell, which is marked in red colour is a primitive unit cell because it contains only one lattice point.

So, for trigonal structures we generally use the hexagonal unit cell in order to construct, this is something you might want to remember. So, even when they have given the other coordinates, other unit cell dimensions it is possible for us to find out what would be the dimensions of the hexagonal unit cell through geometry? So this is what I wanted to mention before we started off with the next topic.

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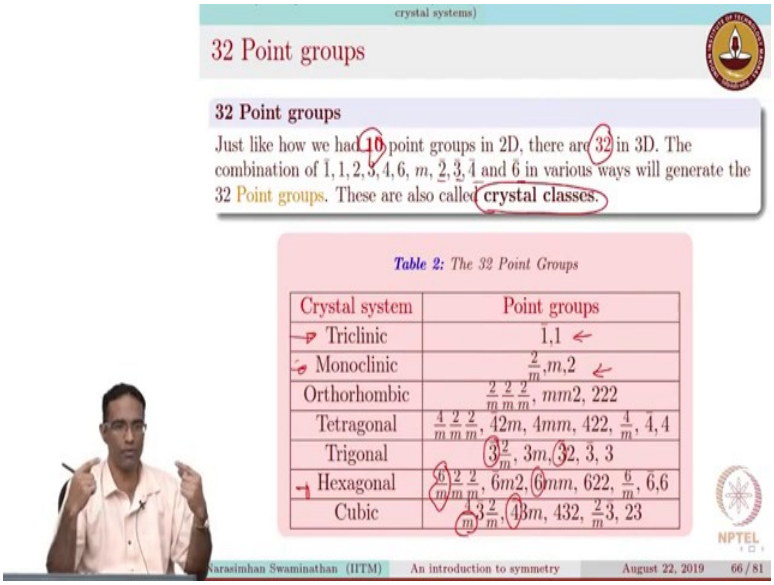

So, what happens is just like how in case of plain groups you have about 10 point groups, in 3D you have a total of 32 point groups. Basically, the combination of 1 bar 1, 2, 3, 4, 6 mirror, 2bar, 3bar, 4bar and 6bar in various ways is capable of generating these 32 different point groups. So, these 32 different point groups are also called as crystal classes. If you say crystal class it essentially means these.

So, if it is one or 1 bar you know that the unit cell is basically triclinic, if it is just having 2 fold symmetry, it is basically monoclinic, if it is having 2 fold symmetry mirror in sub-sequence slots with this combination mm2 or 222, then it is orthorhombic, if there is a 4 fold rotation and in the next sub-sequence slots you have a 2 fold rotation it is tetragonal.

Then if you have a 3 bar that is present in the second slot and the first slot has a mirror or a 4 or a 4 bar, then it is a cubic system. In the first slot if you have a 3 bar, then it is trigonal and if the first rotation axis the 6, then it is nothing but your hexagonal unit cell or crystal system can be used in order to generate the crystals with the point group.

Student: Can we use the trigonal and rhombohedral interchangeably?

Professor: Actually, no. One of them is called trigonal the other one is called rhombohedral, I actually forget which one is called what.

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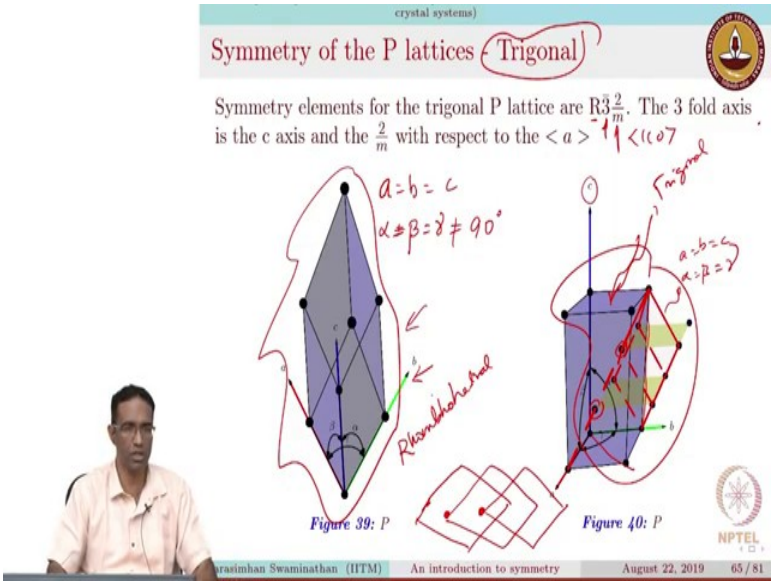

But I think this one is called trigonal and this one is called rhombohedral, okay, you can correct me if I am wrong, it is just a…

Student: Other way round.

Professor: Or let us switch it. Somebody says I switched it.

Student: rhombohedral has equal sides?

Professor: What is that?

Student: equal sides

Professor: Rhombohedral is the one which has equal, a equal to b equal to c, alpha equal to beta equal to gamma, is that right? Or you do not remember?

Student: Yeah, in the tables it is written like that for Rhombohedral.

Professor: Okay. So, this one is trigonal and this one is rhombohedral, that is a question of names. So, as long you understand what it means, I think it is more than sufficient.

Student: R represents what?

Professor: R represents rhombohedral just for that particular space group alone we use R. So, whenever we have a space group R, you will find out that it is rhombohedral. That means it is having this 2 units cells and other things can be identified from the presence of this R.

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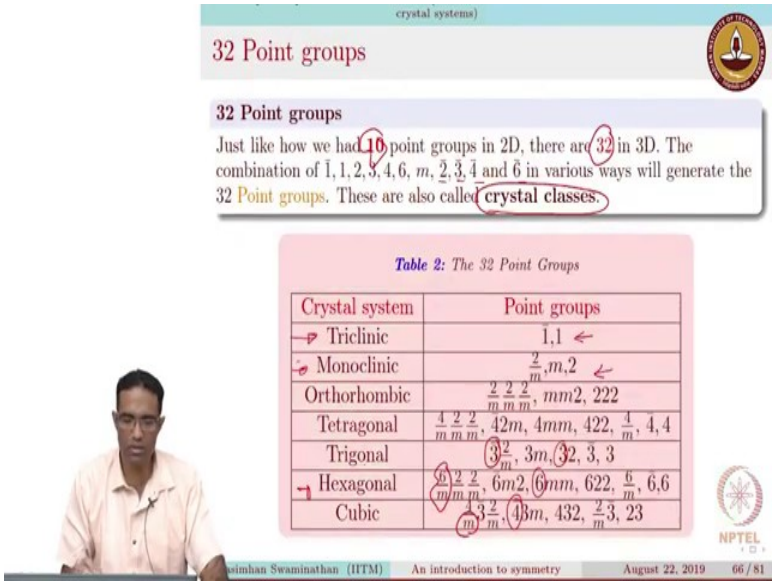

So, these are various point groups are present in 3 dimensions.

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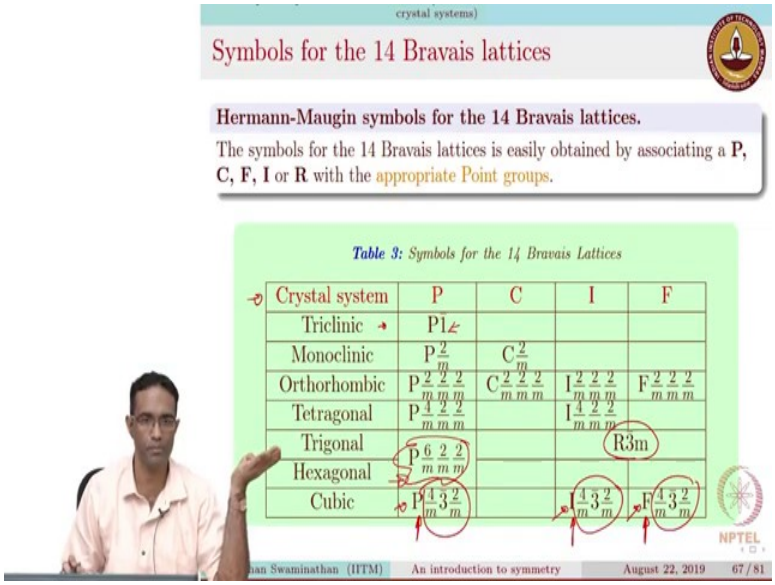

Now, we can also talk about the Hermann maugin symbols for the various Bravais lattices, for all the Bravais lattices. So, for the crystal system, triclinic crystal system you have P1 bar, which is basically the space group to which the triclinic Bravais lattice belongs to. There was no other symmetry elements that was present there. For monoclinic you can have P and C, that is a primitive 1 with only 1 lattice point at all of the corners, and then you can have a centered unit cell.

For, orthorhombic you can have P, C, I and F, so P stands for Primitive, C centered, I is body centered, and F is face centered. For tetragonal you can have only primitive and the body centered version and we talked about how if you have a face centered version it turns out to be the body centered version. For trigonal you have R3 bar M and then obviously this represents hexagonal, this is written like this because you know you can use hexagonal unit cell in order to create the trigonal lattice as well.

Like what we discuss a couple of minutes. For, cubic you can have a primitive version, you can have a body centered version and you can have a face centered version and notice that the only thing that is difference, that differentiates between these individuals space groups is the translation operator P or I or F. Otherwise, the point group is essentially the same, correct? Like we discussed previously if you want to know what is point group that is associated with a crystal you just have to remove all its corresponding translational symmetry operators and you will get the corresponding point group. Is it right?