Foundations of Computational Materials Modelling
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Introduction to Symmetry-1

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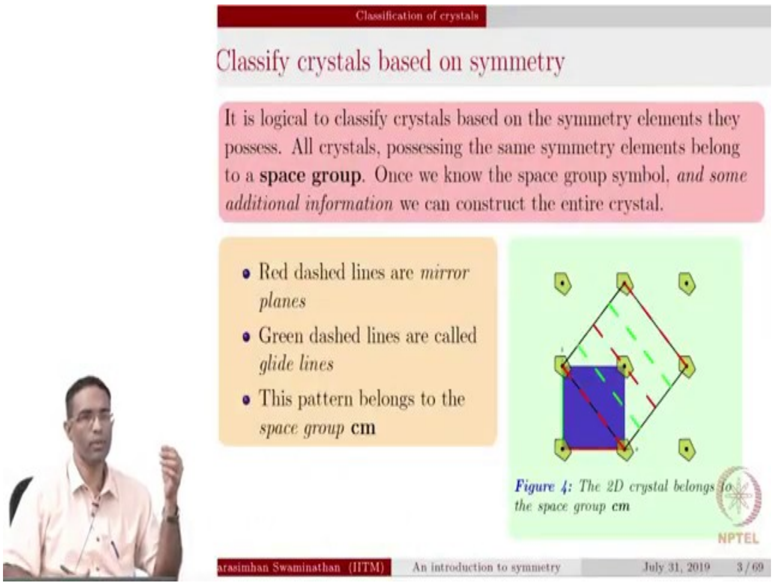

So, now on let us continue and give an introduction to Symmetry. So, I mentioned the word symmetry several times when we were talking about the Bravais lattices. So, actually it makes a lots of sense and it is logical to classify our crystals based on the symmetry that they process rather than the unit cells that is going to be used in order to construct them. Why? Because the unit cells is not necessarily unique, firstly.

Second reason is that properties of that particular material such as elastic constants or thermal conductivity, they all will be reflecting the underlying symmetry that is present in the crystal lattice rather than what was chosen for the unit cell. So, it makes a lot of sense to actually classify this crystal structures based on the symmetry that they possessed. All crystals processing the same symmetry elements we will see what it means to say symmetry elements in a bit, they belong to same space group.

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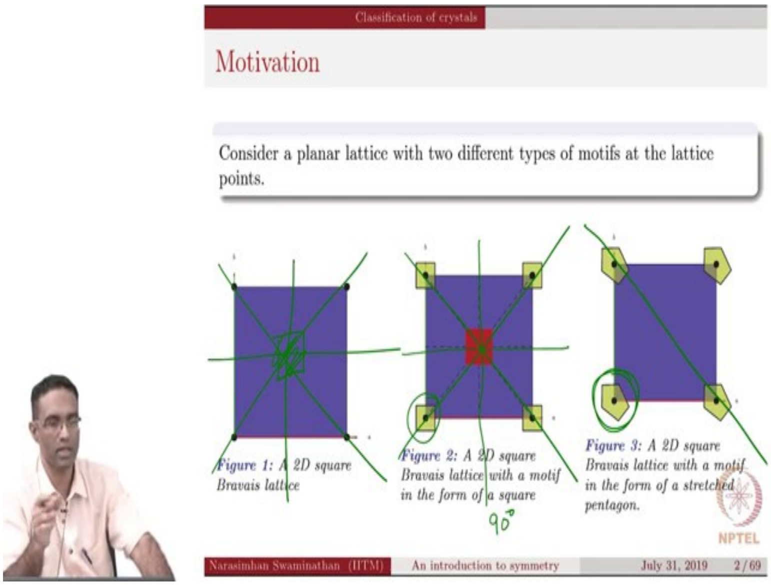

We will be called, so say, so just to motivate the ideas of symmetry, let us take a look at a planar lattice, so this is the planar lattice that we are talking about. So, this is planar, 2D square planar lattice and there are like how many lattice points are there here? One lattice point is there here and at each lattice point I am going place an object that looks like this. Maybe a square, looks like a square. That is the motive and this is going to be repeated in all the three, all the two directions.

Now, if you look at it what are the kinds of symmetry that you can actually see. Like for example, if you take, if you put a mirror here, the right hand side is being reflected on the left hand side. If you put a mirror here, the top is being reflected with a bottom and if you a mirror here, this is being reflected like that and so on. Like so many mirror planes so to speak. Then there are also appears to be a 4 fold, let us not use the word fourfold, there are also appears to be a, if you rotate it by 90 degrees, the object coincides with itself.

You can do it four times and you will look get exactly the same lattice or same 2D crystal, correct? Now, what I am going to do is I am going to take this out and replace it with a stretched pentagon. And it is somewhat oriented in a weird manner. Now, this was, this the first square lattice that we talked about also had the same symmetry as here. It has all the symmetries in the planes, it also has a 4 fold rotation, correct?

But the second we put the pentagons here, we lost the fourfold rotation, but this still seems to be having some symmetry. There some symmetry associated with it. There seems to be one mirror plane like that, that's it. There is no mirror plane in this way. There is only one mirror plane that is reflecting this part to the other part. The second I put a different motive, the symmetry of underlined crystal lattice went away as we saw for several, as we saw for the 3D example when I was explaining what a crystal is.

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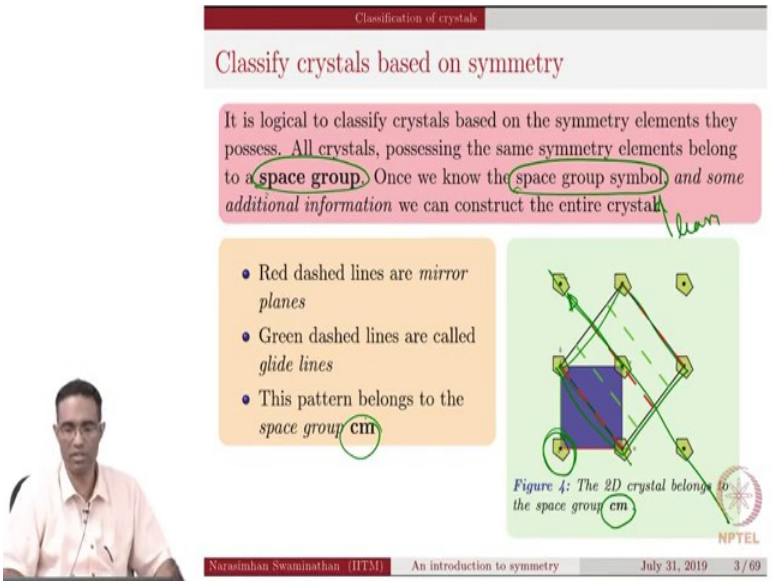

So, depending upon what you put there, the symmetry of the crystal structure of the lattice basically changes. The symmetry of the lattice changes, depending upon what you put at the lattice point. All crystals which process the same symmetry elements are supposed to be in one group called as a space group. We will deal with that in detail as we go along. Once we know something about the space group symbol, which we will learn, we will learn and some additional information we can actually construct the entire crystal. So, remaining couple of lectures are going to be focused on see actually how we can do that.

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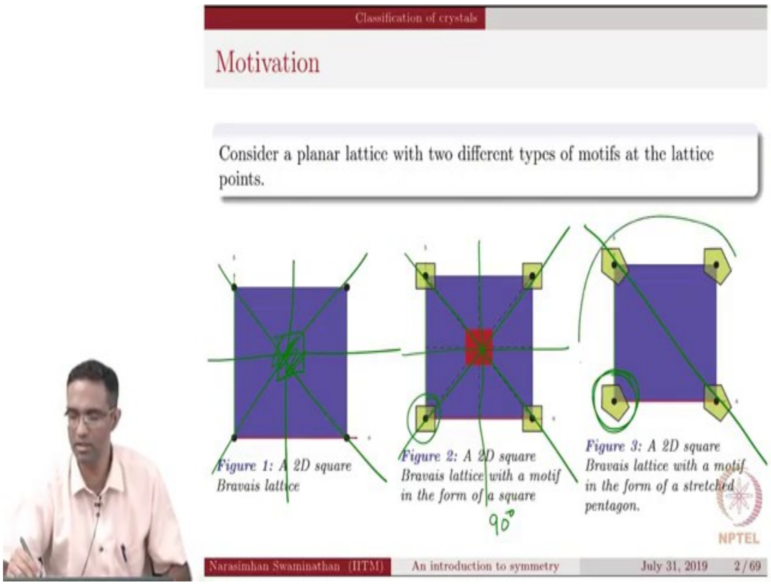

Now, what was the, what other symmetry elements are present in this plane crystal.

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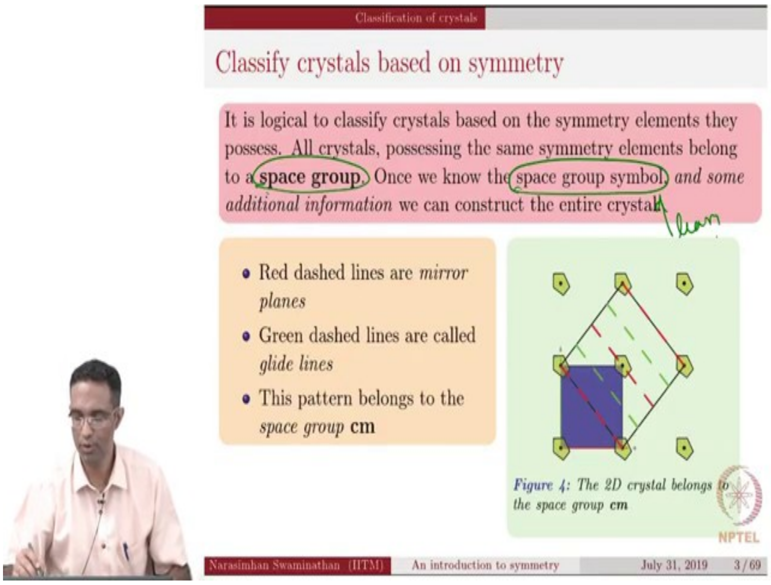

If you take a careful look at, if I repeated in all the, like a couple of more, if I add couple of more like that, then you see additional symmetry elements basically appearing, so obviously you have a mirror plane like this, but then you have something else also . You have this element being reflected about this line and then being moved forward a bit. This pentagon is being or is being reflected and being move forward.

So this, if you take this as a unit cell and repeat it in 2 dimensions you would be able to generate the entire crystal structure. This 2D crystal actually belongs to what is referred to as a space group cm, we will see what those things mean, I just want to introduce you to the kind of stuff that we will be looking at. So, this is belongs to the space group cm, centred, c for centred, m for mirror, but what do, with respect to what is the centring, with respect to what the mirror exist something we will see in a couple of lectures.

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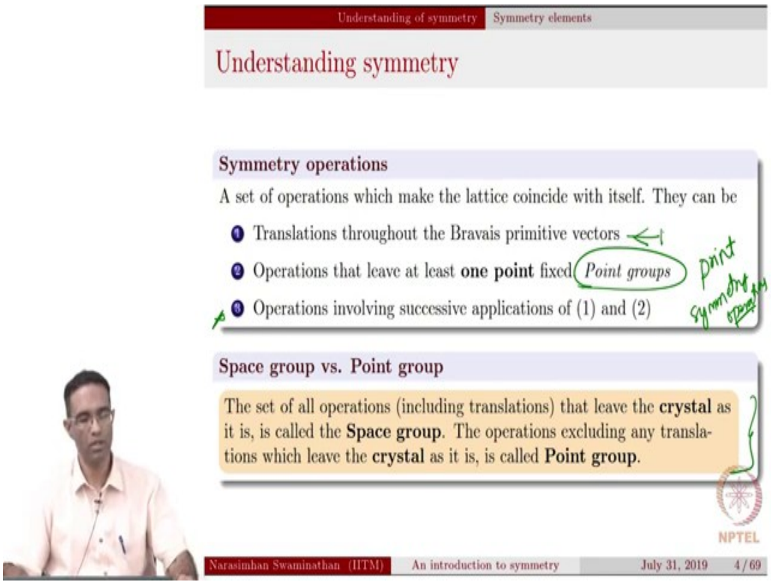

So, symmetry operations or set of operations which make the lattice coincide with itself that is the definition of symmetry. A set of operations that you can do on this lattice, so that is appears exactly the same after you do this operations. You cannot find out the difference, that is, those are the symmetry operations. So, there are basically translations throughout the Bravais primitive lattice. So, basically we have already seen that if you translates a lattice point along the lattice vector it will coincide with itself. So that is a translational a symmetry operator moving along the lattice vectors.

In addition to that you have something called point symmetry operators, which leave at least one point fixed when you are actually performing this operation and then you also have operations which might involves successive applications of both 1 and 2. So, these are different kinds of symmetry operations that are possible which essentially make the lattice coincide with itself. So, we will look at these definitions a little bit later when we actually have covered, Points Groups and Space Groups.

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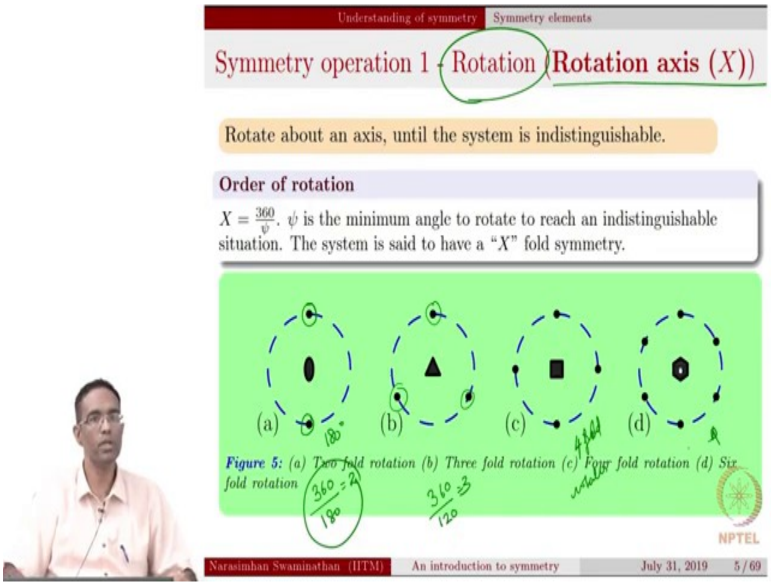

So, we will now talk about various symmetry elements that actually exists, that actually we can work with. The first one is called as the Rotation, rotation. So, rotate about an axis until the system is indistinguishable. For example, if you take this molecule, so there are two atoms here, so by how much, what angle should I rotate it so that this is indistinguishable?

Student: 180.

Professor: 180 degrees. So, 180 degrees if I rotate it becomes indistinguishable. So, this is called as a 2 fold rotation because 360 divided by 180 is 2. It is called a 2 fold rotation so this object possesses as a 2 fold rotation symmetry, right? and once again if you rotate it, it is the same thing again, there is no difference between what you started out with and what you end with. So, this is a 2 fold rotation.

Now, this object here possesses a 3 fold rotation, if you rotate it by 120 degrees, the object appears indistinguishable. This one is 4 fold rotation and this one is a 6 fold rotation. What is missing?

Student: 5 fold.

Professor: 5 fold rotation is missing. What about 7 fold rotations, 8 fold rotations? So, the question is what happens to these rotations? Where are they? Why I did not talk about them? We will continue in next class.