Defects in Materials
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Lecture - 02
1 - D Lattice

Welcome you all to the first class on Defects in Materials. In the earlier class, I had given a brief introduction about the syllabus, which is going to be a followed for this course and what exactly will be covered in this particular course. As I mentioned in that class the first thing which one has to understand is that the title itself means that we are studying defects in materials, and mostly we are talking about crystalline materials. If you wanted to study defects in crystalline material, first we should have a referenced standard which is a material which does not contain any defect that is the first criterion which we have to meet it.

So, what we should know is how to generate a perfect material or a perfect crystal which does not contain any defects or it is an ideal crystal. This ideal crystal can be generated by looking into International Unit of Crystallography table which is available, from that if you know the space group of a particular crystal then we can look at it and then try to generate a crystal structure. But if you have to do that what is the criterion we should know first we should know how this table itself is generated, what are the important significance of it, only then we can understand and then utilize it in the best way right.

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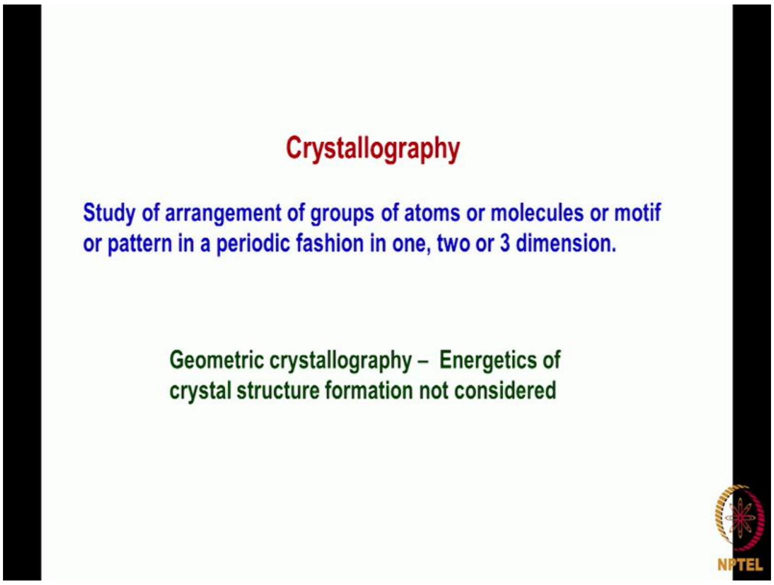

So, this is what will be covered in basically in a lecture which we call it is generally we call this field as crystallography. So, crystallography studies, the arrangement of groups of atoms or molecules or motif or patterns in a periodic way in 1, 2 or 3-dimensions. But what will talk about it is that in generally in crystallography, this is also called as geometric crystallography. The reason essentially is that suppose an element is there; what is the way in which it is going to, which crystal structures it is going to form, that information we cannot get it from a geometric crystallography.

A geometric crystallography it tells what all the options which are available for it if it has to form a crystal what are the crystal structure to which it can form only those information. So, geometrical crystallography is nothing but a sort of a probability of looking at what all the structure which we can form, this comes on the basis of what is the type of symmetry which is associated with the different type of crystals; so what all the possible type of arrangements which we can have. That is what we talk about in this geometrical crystallography.

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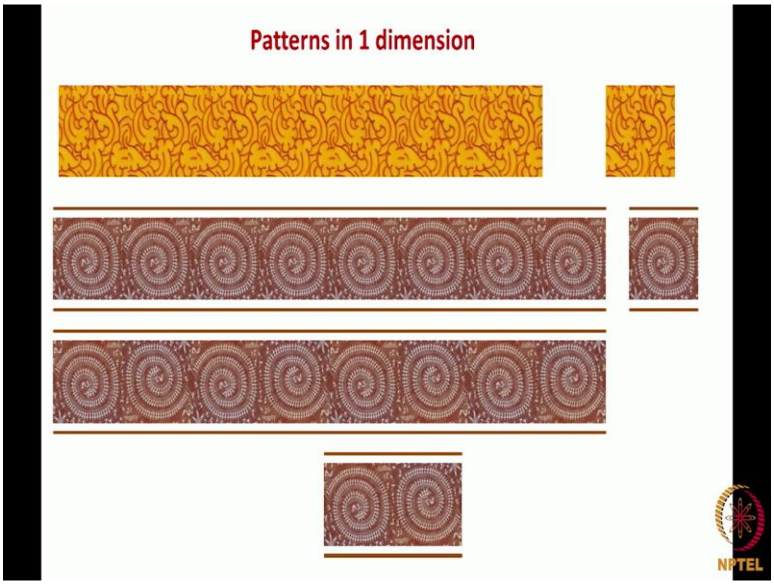

Let us look in some patterns in 1-dimension, 2-dimension, see what we can understand from this. So, though we wanted to construct cells in 3-dimensions, it is better to start from because there are some crystals which are there in 1-dimension also, 1-dimensional periodicity. There are like if you look at surface of a material surface of a material. A surface of a material is a 2-dimensional crystal, and then bulk crystal is a 3-dimensional crystal. So, it is important and in our interest to know what are types of periodicity mixes in all this 3-dimensions. Let us just look at this pattern. When we look at this pattern can you make out whether any periodicity is there in first pattern, what do you see?

Student: Yes, there is.

Yes, there is some periodicity is there. So, some pattern is getting generated is there and that pattern repeats itself correct. In the second one and the third one, if you look at it the second one it is very easy to make out.

Student: Yes.

That what is the pattern but in the first one it is a little bit difficult; the third one if you look at it the type of pattern which is getting repeated is not one because like here it is a, this is the motif which is getting repeated or the pattern which gets repeated. In this particular design, there is only one which is getting repeated, so that means that the pattern which repeats itself we call it as the motif. So, this is the motif in these two cases these are asymmetric motifs. When we say something is asymmetric; that means that there is no symmetry which is associated with that motif, correct.

Now, if you look at the second one - the motif, which repeats that motif itself has got some symmetry associated with it. So, what we can have is that motif itself can have symmetry or the motif itself can be there without any symmetry we called as an asymmetric motif. Using an asymmetric motif, using some symmetry operations we will come to know later, the different types of motifs could be generated.

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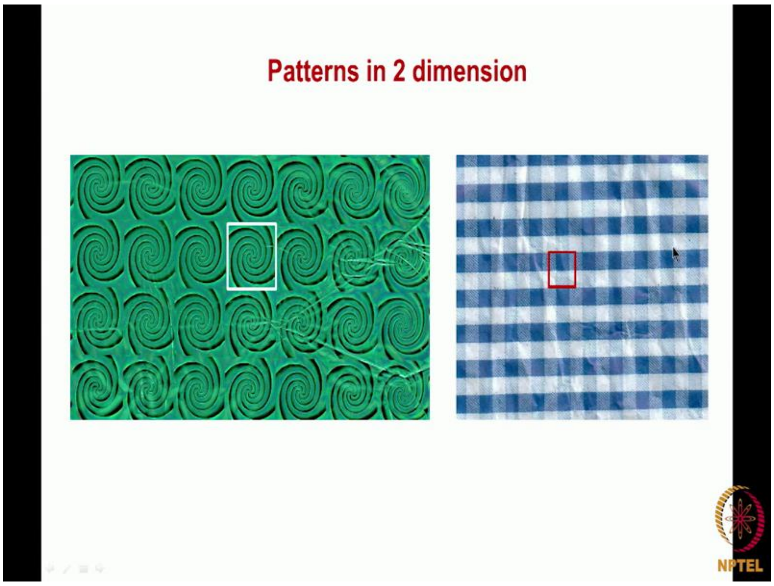

Now, let us look at this pattern, so pattern in 2-dimension. This design if you look at it the first one is taken from wallpaper or a design packing paper design. Here if you look at it the pattern which generates or the pattern which repeats itself is essentially the one which is shown in that white square. How, is it getting repeated by keeping one on top of the each other, we can generate it; it looks like a square pattern. This is one which is taken from a cloth. Here again you can say that this is the one which is a motif which is getting repeated again and again.

In both the cases, what we have is a square type of pattern, but the motifs are two different types of motifs. So, it looks like a two different types of a design. So, in nature if you look at it, even when we look at various types of a designs, but when we look at it for especially if we take with this example itself that though different types of designs we can see that what is getting repeated is many of them are common.

Now, the question, which arises, is that is there in restrictions or how many types of periodicity, which we can have in 1, 2, and 3, dimension that is the information which we require. So, just suppose we will have to represent this; a pattern which is getting repeated, how can we go about and do it. Because the patterns itself are different designs are if you look at it is an asymmetric pattern in this particular case, it is a pattern which is very complicated. The best way to represent it is if you wanted to look at periodically, and look at the periodicity and work on it, the best thing to do is to represent it by some point.

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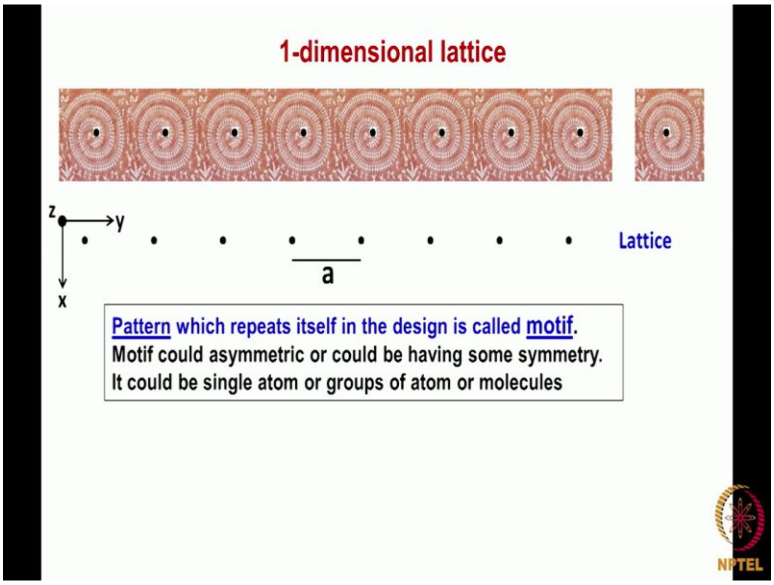

So, that is what we have done is represented with a point correct. This is the point which repeats itself this point could have been placed anywhere it does not matter, but it will show the same. And if you place at particular point at this corner everywhere it should be placed as it particular corner that is how the lattice has to be generated. Now, we can look at the periodicity of the lattice because that is much easier because we have removed the pattern. Once a pattern has been removed, we can very well see only what is getting repeated. And when we look at this periodicity, and when we look at the periodicity in the pattern, one thing which have to if 2-dimensions or 3-dimension, we have to use coordinate system to represent the axis.

So, the conversion which is followed in crystallography, I thought that write it the first instance one should understand how what is the international convention which is being followed in the books and crystallography. If you follow that convention, it becomes much easier to understand the books. So, what essentially is done is that from top to bottom is how the x-axis is defined, y-axis is from left to right and the z-axis is coming out of the screen. This is the convention, which is being followed to represent the origin and the different axis.

Now, if you look at it when the pattern gets repeated, what is the shortest vector which is getting repeated that is from one lattice point to another lattice point, and this is the distance which it is getting repeated. So, if you represent it by a vector a, so this is the lattice parameter correct. So, the pattern which is getting repeated is what we call it as the motif. The motif could be asymmetric or it could be some symmetric motif. So, motif itself could have symmetry we will come about symmetry little bit later. And this motif could be essentially in an art form, it is a pattern in solid state physics, if you look at if we look at position of atoms single atoms or groups of atoms. Then in chemistry if you look at it we talk about molecules various types of molecules, the molecules itself will have some symmetry associated with it. Then this motif gets repeated or the motif which is getting repeated, when we have a presented by a point we call it as a lattice point.

What is the periodicity which is underlying this lattice is what is described by the lattice. In the pattern, what is the periodicity, which is getting repeated that we can show it by essentially the lattice? Then lattice point generally we assume to have zero-dimensions and infinite symmetry associated with it; and lattice is supposed to be infinite in all directions. So, surface-surface do not come in the lattice, but in real crystals always that will be there surface, surface are very important. And the shortest translation vector in different coordinate axis directions we call them as the lattice parameter.

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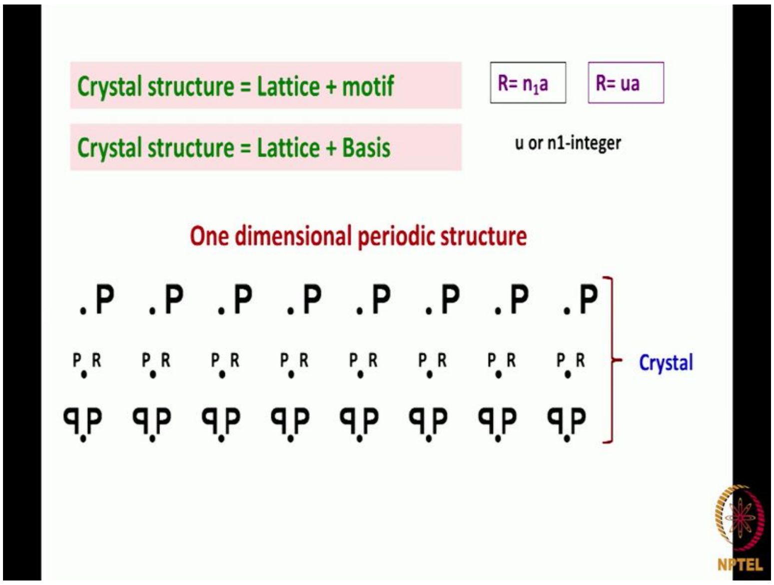

Now, from this what we can understand. When the pattern which is there, which is getting repeated we can call it as a design that is the terminology which I am using it. In crystallography, we will call it as some crystal. The crystal itself when we are trying to represent it we have a lattice, and around each lattice point we have a motif which is a input around it. So, lattice plus a motif is what crystallize. In some books, you will find that instead of motif that terminology basis will be used, and it can be represented by a vector R equal to u into a it is written, a is the shortest lattice translation vector, u is the number of times it gets repeated to reach a particular lattice point, this is the 1-dimensions. Similarly, we can write it for 2-dimensions as well as 3-dimensions.

What I had given here is that instead of a pattern which is an art form, we can use some symbols also like generally in books if you will find, they will use a letter like P R R to represent an asymmetric motif. In this case, I had use P, and I can represent it P by a lattice point that some dot and this repeats itself this is one way to look at it. Another if you look at it there are two types of asymmetric motifs are getting repeated in the next one, next crystal structure which I had construed P and R. But these two are 2 asymmetric 1, they have close each other, but if you look at it you do not see any asymmetric between them in the motif.

The next one is one where I have a P and the inversion of, not a inversion a mirror of P is also there these together constitute the motifs that repeats itself, this is an another type of a structure which we are looking at it. From this itself, we can understand that even in 1-dimension, we can have some symmetry around the motif which can repeat itself, but what are types of symmetry which we can have which can repeat itself we will see shortly.

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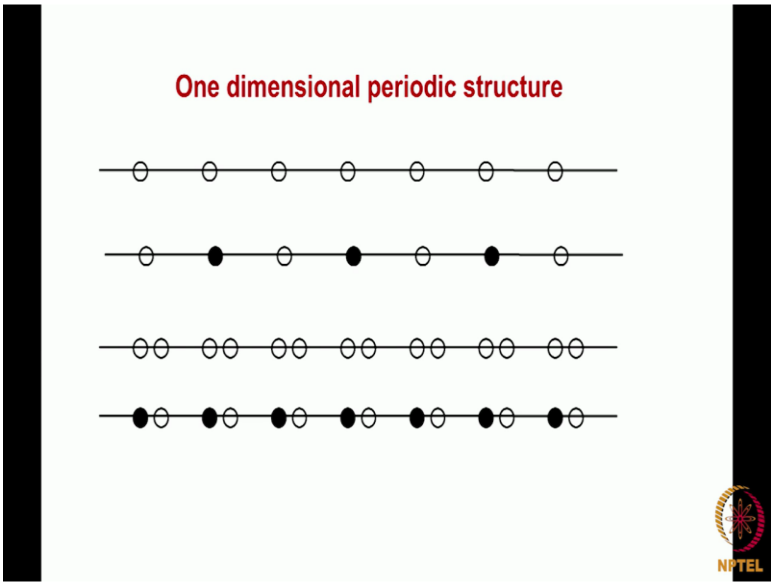

Before going further first let us look at periodicity in 1-dimension. So, what I have done it is I had given some more examples here 1-dimensional lattice where I had taken an atom two types of atoms one with open circle represents, one atom close circles represents another atom. Then different ways in which it is getting repeated this I had just generated, so that one can work out and find out what is the lattice parameter, what is the motif, which is associated which is repeating itself all these information one can work out.

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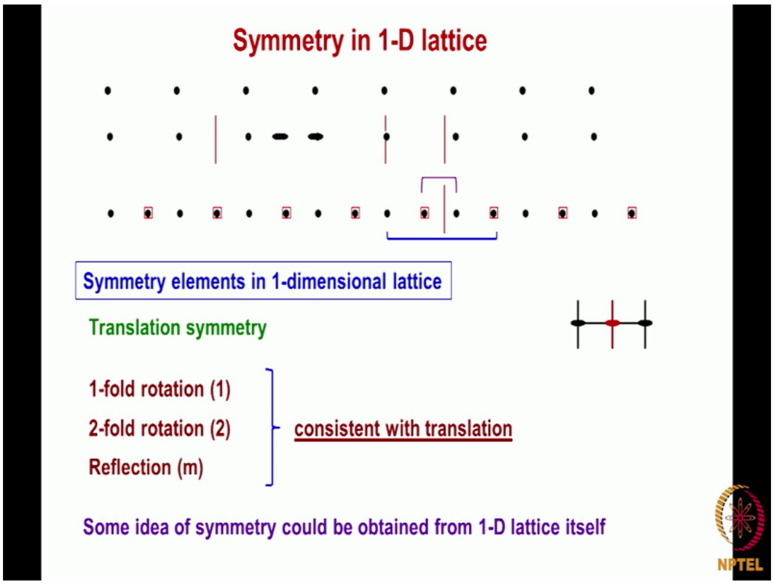

Now, let us look at the symmetry in a lattice. Just if we look at this lattice itself, the first thing which we see it is that there is a translational symmetry which is associated with it. If I move from one point here to another point here; after the movement, it set an identical position. So, in an infinite lattice, we will not be able to make out that we have moved it correct. So, this symmetry we call it as a translational symmetry. Suppose, around this point, I just try to rotate it by some particular angle, what will happen, it will come to a position, which will be inclined with respect to this, but it is distinct.

So, it is not coming to position which is identical with itself. So, then that point have do not have any symmetry. Suppose, I rotate it around this by 360 degree it comes back again to a original position. Though we have given a 360 degree rotation the present position and the earlier position, we are not able to distinguish them; that means, this is a mathematical attempts we called a something which is invariant whatever you do it, it is the appears the same.

And similar to 1-fold around this, if I give a 180 degree rotation also then what will happen it will just come back again to the same position. I can give an 180 degree rotation with respect to midway between the two lattice points then again what is going to happen is that 180 degree this point will be moved to here this point will be moved to here from one position to another. So, essentially again if you look at this as a 2-fold symmetry which is associated with it correct.

So, now, we can see a 2-fold symmetry. Is there any other symmetry which we can see in this pattern? No, we just see this. What have done it is here now I had how this symmetry is represented a 2-fold symmetry is represented with an ellipse. So, I had just marked it at this lattice point and another one which come it in between. Now, you see this is the one which is a symbol for showing a mirror. If you put a mirror like this then this atom position it will be getting reflected here, and this position gets reflected here that means, they are coming back to a identical position. So, we can have a mirror passing through the lattice point. Now, is there any other position we can put a mirror?

Student: (Refer Time: 17:21).

Like in between if I put it now you see that it is again getting reflected. So, these are all the two positions we have, one at the lattice point one in between; similarly for rotation also, one of the lattice point one in between we have a 2-fold rotation. Let us consider this particular case, which I put a mirror somewhere else in between arbitrarily. Then if I look at it then this atom position will be getting reflected from here to here, which is not a lattice point and these position will get reflected from here to here which is not a lattice point.

So, if we put a mirror plane at some position arbitrarily it does not that means that from this we can understand that once a lattice is fixed, where all we can have the symmetry elements also is decided. We cannot have everywhere anywhere we can put an axis and different points in the lattice we have different types of symmetry that is the apart from these particular one mirror symmetry we can have it at the lattice point and the midway between. Similarly, what is true for 2-fold rotation in between regions whichever we take it there is no other symmetry is there?

This is what I have done it is just taken across from one lattice point to an adjacent lattice point, here I had shown the various symmetries which are same. One is a 2-fold symmetry that is around each lattice point, we have a 2-fold; we have a mirror 2-fold rotation and a mirror. And then if you look along this if you take a mirror then also it appears to be the same, so that will be there. Then in addition to it at the center we have a mirror, which is a generated, and similarly a 2-fold rotation, this is all which we have. We extend the usage of how we talk about in terms of 2-dimensions and 3-dimensions unit cell, then we can call this as from one lattice point to another adjacent lattice point is a unit cell in 1-dimension, and these are all the symmetry which are can be seen in unit cell in 1-dimension correct.

What are all the symmetry elements even in this 1-dimension now we have seen in the lattice there is a translational symmetry, there is an 1-fold rotation there is a 2-fold rotation then we have a reflection. And these rotation rotational symmetry and reflection symmetry are consistent with the translation, because then only the invariance will come. So, just looking at this slide, from whatever I have explained, I hope you are got some idea about symmetry, what symmetries are which we will consider later in detail in 2-dimensions and 3-dimensions.

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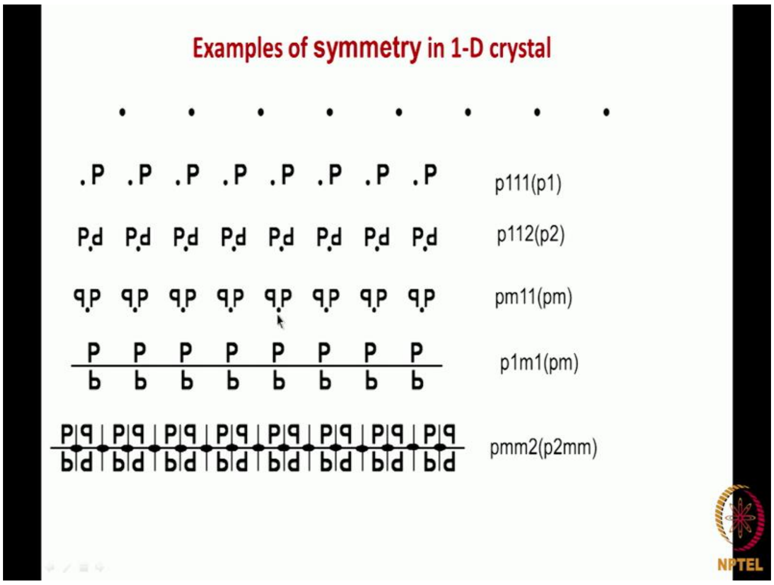

Suppose, we wanted to construct a crystal what should we do, the best way to do it is to put a asymmetric pattern or an atom or a group of atoms around each of these lattice point. Let us do that. If you put an atom an asymmetric pattern around each of the lattice point, now if you look at it this is becomes a crystal, in this crystal only 1-fold rotation is there along the x-axis, y-axis as well as the z-axis. So, this is written as a primitive lattice with 1 1 1, there is x y and the z-axis, they are symmetry and it is represented as P 1. Now, if I take a motif, which has got a 2-fold rotation, and then I place it around each lattice point, now a crystal which has been created. Now, this crystal what is the symmetry which it has, it has got a 1-fold along x-axis because if you rotate it by 360 degree only it will come back along y-axis again an another 1-fold rotation; along the z axis that is perpendicular to a screen you have a 2-fold rotation right. So, this is represented as P 1 1 2, this way and short form which is used as P 2.

Suppose I take a mirror image of this asymmetric motif, and make that as a motif and put it around each of lattice point. Now, we can see that along x-direction, we have a mirror; y-direction there is 1-fold, z-direction there is only a 1-fold. So, now, what we have is that P m 1 1, so it is represent as P m. Suppose, we take the same this lattice and put a mirror along this lattice direction and then what is going to happen is there every lattice point every motif. Now we gets I can see that a mirror image is being formed. We assume we consider these to be your motif which repeats itself correct.

So, this if you represent it, x-direction there is no mirror symmetry only 1-fold; y-direction there is a mirror is z-direction only 1-fold rotation. So, this is what we represent as P 1 m 1. This is also if you look at the general symbol, which is used P m because only one mirror symmetry is there. Now, if you look at it here, here what we have done it is this motif which we have taken, we have taken along the lattice plane along the lattice direction, we have put a mirror and then when we have created. Now, we can see that we have two mirror planes are there perpendicular to each other, and then you along the z-direction, there is a 2-fold rotation is also present. So, this is around every lattice point it is there in addition, in between also a similar type of symmetry which gets repeated.

So, the symmetry which it has is now P m m 2, or it is generally written as P 2 m m this is how generally it would be written.

Student: (Refer Time: 24:16) last one.

Last one. Here if you look at it, this is a motif around the lattice point, I put a mirror along the y-direction then all these points get reflected here. Now, I look around each of these can be considered as a motif which is getting repeated itself.

Student: (Refer Time: 24:43).

Now, I look around each of the lattice point, what is the symmetry which is available. This P gets 2-fold rotation, it will come here around the z-axis, and this one will get 2-fold rotation, which is going to be there. Then along these, if I put a mirror, now what I have is that there is a mirror, which is there, mirror symmetry in this direction also there is a mirror symmetry is there. So, along x-direction now we have a mirror y-direction there is a mirror, z-direction there is a 2-fold. So, the symmetry which we have is that P m m 2 we write it primitive m m 2 p.

Student: (Refer Time: 25:26) Primitive (Refer Time: 25:27).

The lattice when its gets repeated the number of lattice points per unit cell, if you look at it there is only 1. Because any lattice point if we consider it corresponds to one as well as the other. If I take a lattice as I mentioned adjacent two adjacent lattice points, this point will correspond to this side and on this side, this lattice point also on this side and this side two into half. So, the number turns to be one, so it is primitive. And generally one should remember at this stage that small p is used to represent primitive in 1-dimension and 2-dimension; and capital P is used always in 3-dimension. Is it clear?

Student: Yes.

Let us proceed. So, so far we have considered all the operations are called as point group operations correct. It is only around a point we have looked at what are the types of symmetry elements. So, these are all the type of five point group symmetries are possible even in 1-dimension.

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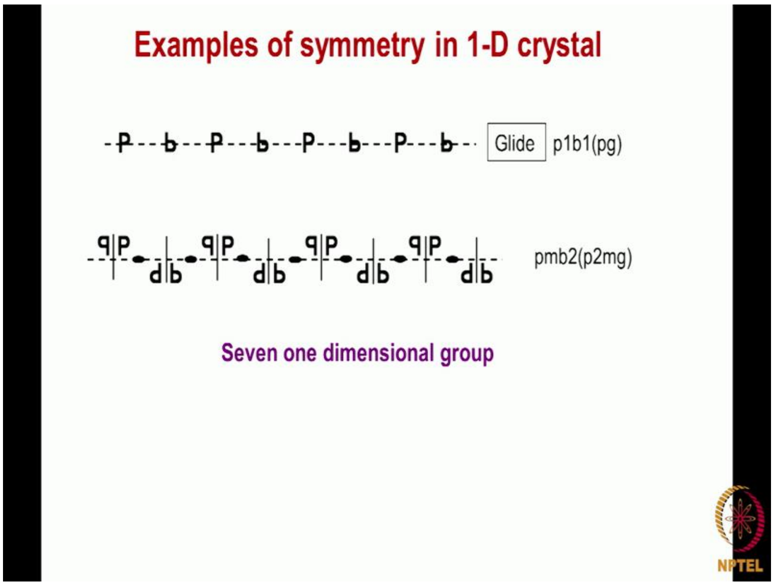

Now, let us look can we have any other type of a symmetry which is possible other than these for the crystal. Here, what I have done essentially is taken that lattice which essentially this particular lattice. If I shift the bottom portion by a by 2, then all the atom positions will be coming at in between right bottom portion, top portion remains that same that is what exactly which has been done. And what is the direction in which it has been done, it has been done along the y-axis right or I can show that this is around this axis, a shift has been given and around this axis, a mirror image also has been created. It is equivalent to I shift this P from here to a by 2, and then take a mirror, then this will be created. Again shift it by a by 2, then take a mirror operation, it will come; and from this point to this point is where the periodicity is occurring.

This type of symmetry operation we can see it only in lattices not around points. So, this is called as a light symmetry. Light symmetry is one, where we have done an operation of a mirror and the translation. In the other case, what we have done is most of the cases where we consider it is we are doing a symmetry operation of a mirror, which is consistence with translation, so that the structure looks identical. Whereas, here there is a translation which is involved there is a combination where rotation and reflection which is consistence with translation, here what we have shown is where we have a mirror plus the translation, this is the subtle difference between these two.

Similarly, the other option which we have is that which does not work in 1-dimension is that we can have a rotation and also a translation that will become a screw axis. This we will see it only in 3-dimensional structures, not in any other structure that we will come to later when we talk about 3-dimensional structures, we will mention about that. Here what we have done it is again as you remember the one which has got that P m m 2, this is one part of the motif. The other part of the motif was here. Now, we have shifted it when we shift that motif by a by 2, then it occupies a position where it is nothing, but a glide again is going to be there.

Now, we have a mirror in the x-direction right and a y-direction there is a glide and then we have in between these points we have a 2-fold rotation is also there. So, this symmetry is pmb2 is written. What is b means at this point m denotes mirror if there is a glide along a-axis it is generally denoted by a letter a, and b-axis it is written by a symbol b, so that is way the p m b 2, 2 represents the 2-fold rotation. And this is generally represented p 2 m g, g is for glide that is a symbol which is being used. But here what we are done we have the detail of glide is along which direction then we have to mention that it is a glide or a b glide or a c glide. So, this is details of all the symmetry elements which are there, this is a general notation. This we followed in 2D as well as 3D, it is equivalent to 3-dimension we called as space group. So, here we have seven one-dimensional space groups we can say that point groups are five, and space groups are seven.

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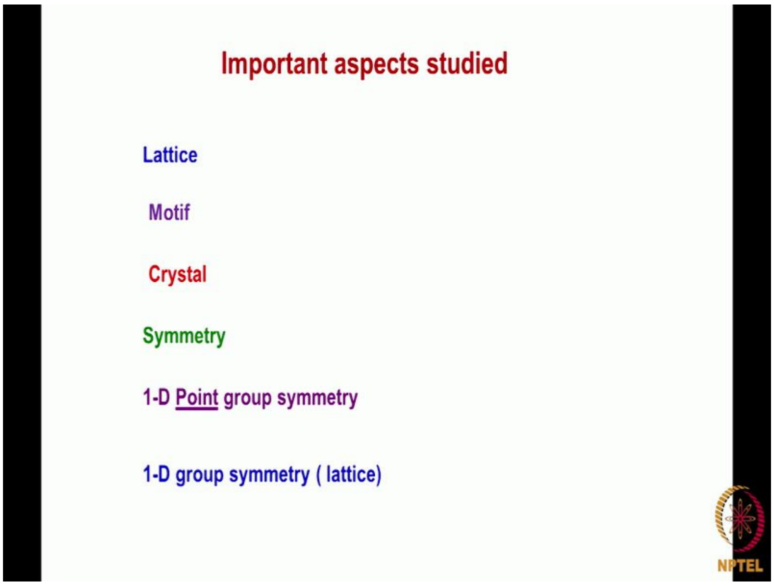

So, what all important things which we have studied so far that is even looking at a simple 1-dimensional lattice and a 1-dimensional crystal we have got information about the lattice about the motif, some idea of what motif some definitions we have looked at it. What is a crystal that we have looked at, then symmetry what is symmetry. And then we have seen that around lattice also we have a symmetry, there are some symmetries which we can see associated with motif, because only motifs with these symmetries are consistent with the 1-dimensional periodicity. Then we have seen point group symmetry because point groups what are the symmetry operations, which we have 1-fold, 2-fold and mirror.

Generally, point group symmetry is nothing but a combination of these operations 1 and m is just nothing but mirror; 2 and m is what it turns on to be 2 m m then a 2-fold then mirror along can be there, so that is how when we look at it we have all these five point group symmetries. Then when the glide operation comes into it similar to space group symmetry we have in 1-dimension seven 1-dimensional symmetry is there, 1-dimensional group whether to call it as a because space group you cannot use it because

1-dimension you call it as a space or not. If you call it as a space we can say 1-dimensional space group.

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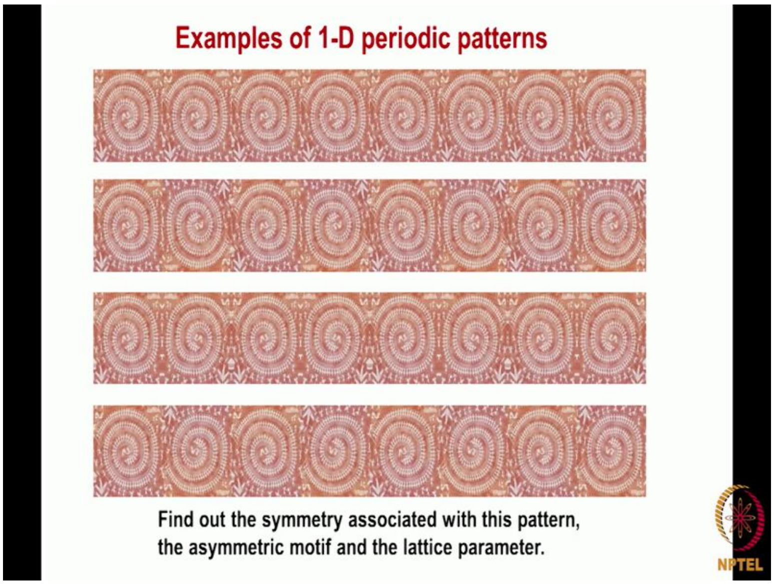

Here, I had given some examples of few patterns. What I want you people to work out is what is the lattice parameter, what is the 1-dimensional lattice which is present on this, what is the symmetry which is associated with this designs, the symmetry of the lattice and the symmetry of these various types of designs. With this, we will stop discussion on 1-dimensional lattice. In fact, in 1-dimensional lattice, we can have many other patterns like we have taken an asymmetric pattern as a (Refer Time: 33:48) of P, which is a dark written in dark, we can write it in red then.

If you put them together then there the many types of patterns which can be generated where this patterns become important not only in cryptography, if you look at the tilling of the floor, architecture, everywhere symmetry is a concept which is very important. Symmetry actually though words that the higher the symmetry the lower or the stabler in which stable situation in which the system remains.

Now, in the next class, we will talk about 2-D lattice.