Symmetry and Structure in the Solid State
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Lecture – 02
Two Fold Axis Representation with the Help of Esher Diagrams

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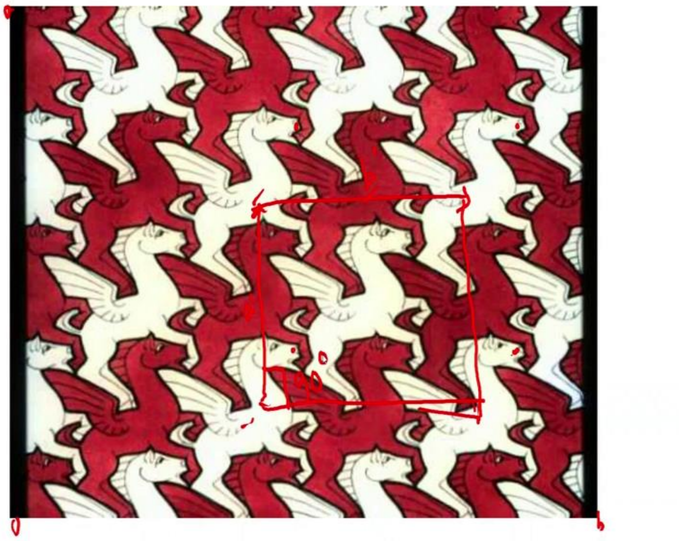

So, therefore we go back to this particular diagram, if this is the simplest of the diagrams where we show only the translation periodicity. So that means, to say that the types of 2-dimensional lattices we can have depends upon the nature of what kind of symmetry elements we can associate with these objects. So, if there is a translation periodicity, there is 2-dimensional lattice. There is a 2-dimensional lattice which has a 2-fold symmetry, there is a 2-dimensional lattice which has a 3-fold symmetry and so on.

So, how can we go further and in what way we relate one object to the other in terms of the symmetry. See we are talking about only translation symmetry; that means; that the object can be 360 degree rotated that is a 1-fold symmetry. We have talked about the 2-fold symmetry presence of 2-fold symmetry, we were talked about 3-fold symmetry, we also talked about the 6-fold symmetry. And, similarly we can talk about the so called 4-fold symmetry. One of the conditions which we have always been telling very quietly is that these diagrams which are drawn by Escher have if, have a close packing and if we have a 5-fold symmetry object and want to do a close packing; we will show later on that it is not going to be possible.

Because, we will have some holes left in this 5-fold symmetry packaging and because of the fact that 5-fold symmetry packaging will have holes; it will not satisfy the conditions that we need for defining a 2-dimensional lattice. And therefore, the number of rotation axis get restricted to 1, 2, 3, 4 and 6. We will mathematically prove in a later class that it is only possible to have 1, 2, 3, 4 and 6 and this restriction comes because, of the presence of the translational periodicity which is in the solid state. So, the presence of the symmetry to 1, 2, 3, 4 and 6 is only there in case of solid materials and particularly in case of crystalline solids.

So, that way the amount of effort we have to spend in understanding the symmetry of objects get reduced because, of the presence of the translational periodicity. Since, there is translation periodicity we do not get 5-fold symmetry operations for example, similarly 7 8 9 and so on are also not possible. We are going to prove it mathematically in the next coming class may be in the next class or so. But, for our current understanding we need the fact that we need to note the fact that once we require close packing, once we have translation periodicity and we have the presence of the symmetry elements; we can now appreciate the Escher's diagram in terms of all these presence of symmetry elements.

And, replace these imaginary of you know abstract object by molecules then we can have these molecules also following the same symmetry operations. So, we can have molecules packing them also in a 2-fold symmetry situation, we can also have the molecules packing together in a 3-fold symmetry situation and so on. One of things we also have to notice is in this particular case is the definition of what we called as a prime and b prime; see here we called this as a prime and b prime. And, we define this so called block and we called it as a unit cell; if you recollect that part which we did in the previous class half an hour class.

So, the angle between these two is 90 degrees. Now this therefore, is a type of a lattice where the lattice points are located in these positions and we have a 90 degree angle between these two. It is not necessary that a prime should be equal to b prime. Say if a prime is equal to b prime you will get a square, if a prime is equal to is not equal to b prime, you will get a rectangle. So, the presence of a square and a rectangle can sort of generate this particular motive depending upon whether a prime is equal to b prime or a prime is not equal to b prime. Now, these two units which we have defined in a this red blocking are referred to as lattices and these are refer to as a plane lattices. So, we have a square lattice and we also have a rectangular lattice.

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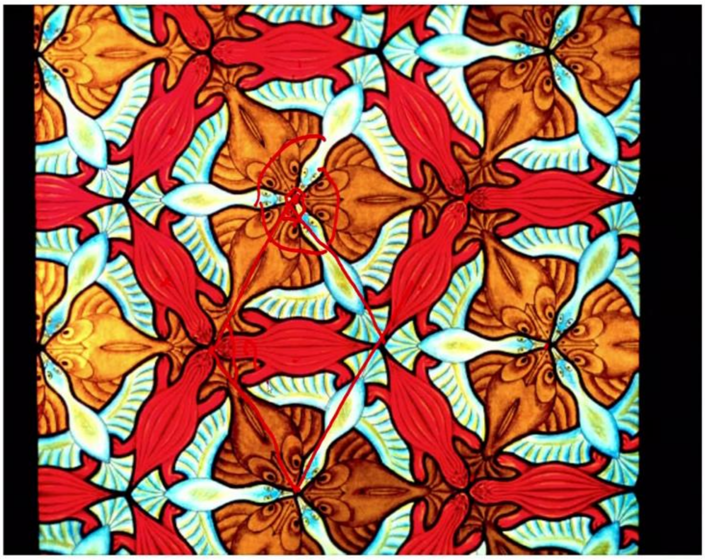

If we got to the next diagram where we had this 3-fold symmetry, you see that this if you take this 3-fold point and join in to that 3-fold point and join this two to this 3-fold point. And, join it to the next 3-fold point something like this, you see now that you get a unit which is now having a different than 90 degree angle.

So, this will now define a different kind of a plain lattice ok. So, we will see as we go along how many plane lattices are possible. What is very interesting is to note the facts that in solids because, of the translation periodicity restriction come to this in terms of the shape of this so, called the unit cell which we are going to define. So, we can define two types unit cells now; three types unit cells. When a is equal to b and alpha is equal to 90 degrees a not equal to b alpha is 90 degrees. And, here you can find out what should be this angle; I want you to think about what could be this angle.

If this angle is 60 degrees or 120 degrees both are possible for this particular unit and therefore, you will get a 3-fold as well as 6-fold rotation that can be describing this particular lattice. So, we will come back to this translation periodicity again and in this particular case as we have already notice, there is close packing and also there is translation periodicity. So, this comes because of a fact that we this object will repeat, this object will repeat itself at that part of object and that object will repeat itself in this object and so on.

So, we also defining the some kind of a unit cell, we will expand on that little more before we go and understand the symbols that we are going to use. Because, the symbols that we are going to use which that will become a very critical issue.

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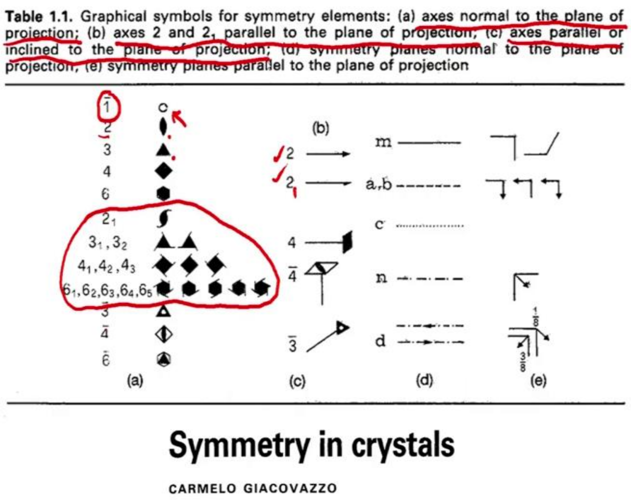

The types of symbols which we are going to use are listed here. The reason why I have given this particular slide for which to about which I will refer again later on is to tell you the representation of symmetry. For example, if you have symmetry like 1 bar you represent it by closed circle. So, if there is a 2-dimensional lattice and there is a 1 bar symmetry in that one that is, the inversion symmetry, then you represent the point at which the inversion is occurring by showing a small little open circle to represent where exactly is this particular inversion center located. So, if you now consider the 2-dimensional object which has an inversion center then that particular 2-dimensional object will have largest inversion center indicated, it will also have translation periodicity.

So, if it has translation periodicity it will have a plain lattice, if it as a plain lattice then it will have either no fold symmetry or a 360 degree rotation 1-fold or 2-fold or 3-fold or 4-fold or 6-fold. It would not be having any other symmetry elements which will coming. We are going to mathematically do that in the next class, but at this particular point we will see what are the symbols which are universally used in literature. Because, this is what will be used in crystallography and we are going to use it repeatedly as we go through the course. These are the symbols for example, for the 2-fold we have this representation and for the 3-fold we represent it that way. This is as long as the axis or normal to the plane of projection.

So, we have this is the 2-dimensional projection and we are looking at the normal to the projection; that means, we are looking down to this screen. And, when we do that these are the representations of the inversion symmetry. If there is no symmetry, there is no representation which is 1 of course; the 360 rotation there is no need to represent a 360 degree rotation. So, we do not have any representation. It essentially tells you that the object is on to itself. So, the object is on to itself in 1 bar, it is on to itself into 2-fold, it is on to itself in 3-fold and so on. There is also additional symbols which we will describe in more detail as we go long and these symbols represent the so, called screw motion.

If you go back to the previous class you will see that we talk about the objects of direct coregents. The objects of direct coregents can have these kinds of symmetry elements. These sort of symmetry elements which are refer to as 2_1 3_1 3_2 4_1 4_2 etc. These are called this screw axes. What 2_1 represent is interesting; it represents the presence of a 2-fold symmetry. And, it is not just presence of a 2-fold symmetry, but there is a translation associated with a 2-fold symmetry of one half the unit cell.

Let me explain again that when you say 2_1 axes you have the presence of a 2-folds symmetry and then there is a translation the 2-fold symmetry alone is not finishing the operation. So, the object now will see the 2-fold and it will also see the half translation along the unit cell. It is something like you know you driving a screw through the wall, then you your screw send through the wall, what you do is a rotation which you give on the screw driver. So, there is a screw fit fitting into the wall you give a rotation in this direction. When you do this rotation the forward point of the screw will go inwards.

If you do the opposite rotation the forward point of the screw will come back and it design in such a way these 2_1 screw means, that when we rotate it by 180 degrees; the advance that is made is equivalent of half the unit cell in that particular direction and that is therefore, it is effectively 1 divided by 2. So, this is referred to as this screw. We will be seeing examples in more detailed for this kind of operations. Similarly, we have the 3 bar, 4 bar and 6 bar. These are 3-fold rotation with inversion centers, 4-fold rotation with inversion center and so on.

The representation of axes which are 2_1 2_1 parallel to the plane of projection ; that means, a 2-fold or a 2_1 screw axes which are parallel to the plane of projection. So, this is parallel to this plane than we represent them like this. This is the 2-fold representation, this is the 2_1 representation, there is a 2_1 representation. So therefore, all the possible symmetry elements which occur in 2-dimensions under eventually the 3-dimensional issue will come up in these representations. So, these representations for example, of a mirror is essentially telling us that the axes parallel to or inclined to the plane of projection. So that means, that there is a mirror plane which is like this passing through this plane; there is a mirror plane which goes through like this.

If it is perpendicular that it is shown in the right side. So, if you study this table carefully this are the various symbols which will appear in the description of this crystals structure and also this so, called paint groups and space groups which will describe in a coming class. You will see the symmetry elements displayed on the side or on the object itself. These are known as symmetry diagrams and when we talk about symmetry diagrams, we will read this into more detail. At this movement I showed essentially to tell you that we will be using some of this symbols for the next part of some of our understanding, of how to locate the symmetry elements on a 2-dimensional object and that is why I have given this table.

This table will repeat again during the course where, we will go individually and explain the performance each of these rotation operations with respect to a point in our molecule or material or the object in general. As you should always remember that even though we talked about the objects and similarity of objects, the once we refer to the 3-dimensional space and associate the symmetry with that 3-dimensional space; it is always the fact that 3-dimensional space will have that symmetry. Suppose there is a 2-fold rotation associated with the object which we have described like the flying cat in our previous example, then the entire space has 2-fold symmetry whether there is a cat or not the entire space has 2-fold symmetry.

And therefore, this space is now itself is gaunt by the presence of the 2-fold symmetry; anything you place in any point in this 2-dimensional space therefore, will follow the 2-fold rotation. So, if you are have an object coming at a particular point that point will now undergo a 180 degree rotation to represent 2-fold. The only important thing is the direction of the axes and that is why this table is shown here. The direction of the axes if it is perpendicular to the plane is represented this way; if it is along the plane, it is represented that way. So, which is perpendicular to the plane it is represented to this way and if it is along the plane it is represented that way. So, these are representations which we will see associated with the so called space group diagrams. And, eventually this will be the one which will be describe the nature of the object inside the unit cell and how these object repeat themselves using the symmetry concept. So, that is what we will study towards the next few classes, we will get an understanding of how these all happens.

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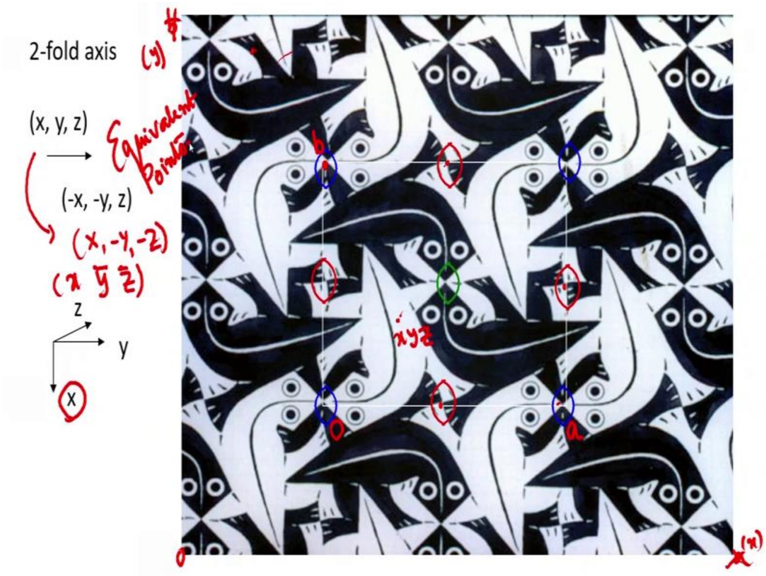

Now, let us go further. Here is an example of a presence of a 2-fold rotation axis which is now perpendicular to the plane. So, in the plane this is the Escher's diagram again you see some results here, white and black results. This is very beautiful representation even though Escher himself was not a crystallographer; all of crystallographer is there in a

Escher's diagram. So, this is very beautiful if you look at these diagrams and try to understand the concepts. And, that is why I bring in this issue of Escher's pictures. For example, here if you take this white lizard and take this white lizard, these two white lizards are related to each other with respect to this particular point where the noses are interesting for example, and they have I have marked a 2-fold symmetry at this particular position. That means, any point in this object will have an equivalent point in that object, please note the word equivalent.

So, these if you take a point x y z here, if you take a point x y z which now represent the 2-fold axis. See this entire 2-dimensional space now is filled with 2-fold axis. And, I have given a representation of a unit cell. This unit cell now can is like a frame, I can move this unit cell this is attempt this is showing this is let us say a. The distance at which this translation periodicity repeats itself; that means, these two motives repeat again in these two motives and black ones; for example, and the white one again repeats here. So, this is the so called unit cell which now repeats itself in both directions to generate the 2-dimensional lattice. Now, we have identified the position of the 2-folds screw axes here, the 2-fold axes here not screw sorry 2-fold axis here; this is a 2-dimensional object.

And, then we also see that in addition one once we have identified 2-fold symmetry here automatically there is a 2-fold symmetry comes up there which is due to the unit translation. And, the 2-folds symmetry comes here due to unit translation, 2-fold symmetry comes here due to unit translation. So, if you take any point in space x y z that in the 2-dimensional space it could be here, here, here, here, here, here, anywhere. It will take the object that particular point x y z will use the rotation axis; now the rotation axis is perpendicular. So, every where you can think of 2-fold rotations coming in this space so, any point here will now undergo the 2-fold rotation. So, mathematically x y z now will go to minus of x, minus of y z in this particular case we are looking at the x y projection; that means, this is now 0 and this is a and that is b let us say.

Or in fact, we should write here x and this is y and the unit cell vector in this direction I am using the word vector, I am assuming that there is a basic knowledge of vector analysis which all of you have a undergone in your mathematics classes around standard 12. So, I am assuming that you to have an idea of what a vector is just to recollect or recount your idea of a vector. A vector is one which we represent not only the magnitude, but it will also have a direction. So, if we take this point as 0 and then, we move in this particular direction like that and reach this point which is now again, the end of the unit cell. And, I will call this as a and this is along the x direction and along the y direction I will call this as b. So, this representation we will not call this a here, we will not call that a here we will not call that b here because, a and b now represent the dimensions of the unit cell and this x and y represent directions.

So, you see that the any points in space something like this point which is let us say x y z. Now, we will see the 2-fold symmetry, it will see the 2-fold symmetry let us say at this point. This is at 0 0 0 of our unit cell, than if you see this 2-fold symmetry x y z will now generate a minus x minus y z where, do you think it will come. It will now undergo this 2-fold rotation. So, it will go like that and come some where there ok. So, there is we a 2-fold rotation about that particular point. What is very interesting about this lattice is that, one once we have the lattice which is generated with respect to a and b as unit cell dimensions 2-fold symmetry is exits at every one of this point in every point in the 2-dimension space and, certainly at these points where you have the 2-fold rotation in this particular example.

And therefore, you it will also see the presence of 2-fold at this point. These are additional 2-fold symmetries; they come due to the translational periodicity. What you see here is that this centre of symmetry, this 2-fold symmetry is with respect to the presence of the intersection of knows of each one of these lizards. Whereas, here you see that it is at the intersection of the 2 legs of the lizards. So, the object is so oriented that you will have at presence of additional symmetry is which appear. So, whatever symmetry appears here at half the distance along a and half the distance along b an additional symmetry exists. Like for example, you have this point and this is that 0 0 0 this is the 0 0 0 because, we taken this as the origin.

Then at a we get a 2-fold so, this is that 1 unit translation, than again one more unit translation in this direction will give you then next a and so on. In addition to the presence of this 2-fold rotation because, of the fact that we have a 2-fold here and a 2-fold here an additional to 2-fold will represent will develop at this point. So, the objects therefore, which arrange themselves in which the 2-fold symmetry in this particular motive has to sort of remember. For example, this lizard now cannot move its leg away from here. It has to be keep itself the leg in that position in order to get the 2-fold symmetry, otherwise it would not fit into this motive. So, if Escher had made a mistake and shown this leg as different leg then it will not be close pact feeling motive, therefore, the restriction comes now on the objects.

So, the object now therefore, must have the 2 legs intersecting at this particular point, if it has to keep that shape. And, it is very interesting that lizards can do that kind of an operation and therefore, we can set the lizards into the 2-dimensional motive. So, molecules when they fit in they also have remember the fact that apart from the presence of the 2-fold symmetry, they also have the invoking of the 2-fold symmetry at this point. And, again at half this distances along a, half this distance along b and also half of a half of b which is a different 2-fold symmetry, that is why I shown it in different colors. The ones at the ends I have shown by blue, the ones in the middle that half distance is shown by red and the one in the very middle are shown by green.

We will see the significance of these when we actually look into the way in which molecules pack when we discuss this space groups. And, they are presence of additional symmetry which appear because, of the fact that we have lattice and they lattice has to obey certain rules which we are going to formulate as we go along. Right now, we are looking only at the symmetries that are possible with respect to this motif. The presence of additional symmetries is a crucial thing because; the presence of additional symmetry will bring in the issue of defining this 2-fold axis in the same way. That means, if you have an x y z and an minus x minus y minus z this point will now, also see this 2-fold symmetry.

And therefore, this point will now go over there with a 180 degree rotation something like this it will rotate by 180 degrees and go there, and therefore, we will have these equivalents of x bar y bar z bar. So, in this particular 2-dimensions space therefore, we define x bar y bar z bar x bar y bar z rather as the operation which takes the object on to itself using the 2-fold axis; the presence of the 2-fold axis in this motive given there x y z directions. Suppose, that is the 2-fold axis which is in the x direction than we see that the fold axis is associated with the x direction than your x y z will than go if this is the direction x direction. And, we look at now they y z plane than x y z will go over to what, to x y z will now become x y bar z bar.

So, it will go to x minus y minus z and it is the way I pronounce it we always use this x y bar z bar and in crystallographic notation; we will represent that has $x\ \bar{y}\ \bar{z}$. So, will I write a bar over y and z and pronounce it as bar. So, if the axis about we so, suppose x is coming towards out of we plane of this diagram than the x y z will go to x -y and -z. And, that represents the 2-fold symmetry along the x direction; similarly along the y direction we can define the 2-fold symmetry. We will see very interesting observations which come out of the fact that we can have 2-dimensional, 2-fold axis intersecting with each other and so on. Right now, we are discussing only the presence of one 2-fold axis in this diagram and we will restrict ourselves to one 2-fold axis.

So, I think at this stage we come to the end of the second part of the talk; this is the second half hour. So, what have what I will do is I will conclude what we have done so far. What we have done so far is that we have looked at motives and we have looked at the possibility of arrangement in 2-dimensions. And, we have looked at the arrangement in such a way that we identify the presence of symmetry elements. And, we have taken one example of the presence of a 2-fold axis which is now generating the so, called equivalent points.

So, these are refer to as equivalent points. So, in a in a 2-fold symmetry containing objective if there is a 2-fold axis, the equivalent points are x y z, x bar y bar z; if z is the direction of the 2-fold axis. In other words if, z coincides with the 2-fold axis as we have shown in this particular picture; I think that come to the second end of the second half of a the talk. We will now go to further and examine from this stage how we now can look at the other axis which can come up, other symmetry positions which can come up.

So, I think we will stop here for today.

Thank you.