Symmetry and Structure in the Solid State
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Lecture – 10
Details of Stereographic Projections

So, in the last class we stopped that what we did with respect to the points in the northern hemisphere.

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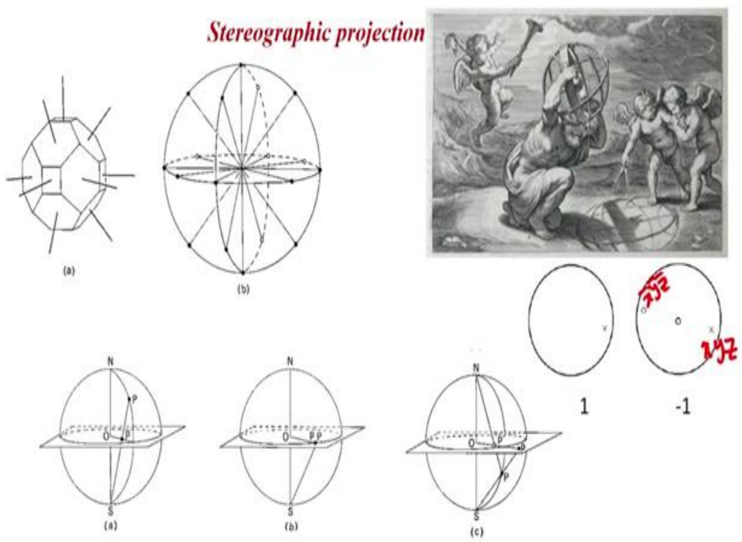

So, you consider these as the points in the northern hemisphere. These are the points which are drawn here in the northern hemisphere on the sphere and we take the South Pole and connect it to the point which intersects the sphere on the northern hemisphere, this point P let us say, we correct we take it here and then we take the equatorial plane. So, it is again an orange. Now, what we do is we take the central part of the orange cut it open halfway through and take this slice out, that will define the equatorial plane. So, this slice is the representation of the equatorial plane.

So, when we do this South Pole to the North Pole points, all the points in the North Pole are joined from the South Pole and their intersection with the equatorial plane is indicated by the point P. So, the little point P here which is a closed circle now represents all these intersections. The intersections of the South Pole region, the southern hemisphere region with respect to the North Pole, now are joined, likewise and that point is indicated by an open circle.

So, when we have a crystal with this kind of symmetry and do this operation then we will now slice open this equatorial plane and take it out, take it out and spread it on the plane. When we spread it out on the plane we will get diagrams of this kind. So, this is now the equatorial plane and depending upon the nature of the crystal and the symmetry that is associated with the crystal, we will get points associated with the intersection with the North Pole which is indicated by x and the intersection from the South Pole indicated by open 0 or vice versa, it does not matter. As long as we identify the points with respect to the North Pole and with respect to the South Pole we keep that identity the same.

So, this equatorial plane now represents two possible symmetries you see we can read the symmetry directly because this now represents the 360 projection. So, we have this sphere which is a 360 sphere and we therefore, now represent the 360 degree representation and we see there is only one point. If there is only one radial point which is emanating into the crystal from that point we say that the point group symmetry is 1. So, this is the projection diagram and these are called stereographic projection diagrams of various point groups. For every point group therefore, we can draw these kind of diagrams by taking examples of crystals which belong to different crystal systems and therefore, different point groups.

So, when such studies are made we will see that in case of the $\bar{1}$ system we will have an intersection with respect to the North Pole and the South Pole, the open circle and the x point will now indicate this. It not only indicates this it indicates the relationship between this point and this point. If this point is xyz, this point is xyz, let me tell you that clearly. If this point is taken as xyz, now this point now is on the opposite side, this is northern hemisphere, this is on the southern hemisphere of the sphere. So, therefore, you get -x -y -z. So, when we get a distribution like this we identify the position of the presence of a center of symmetry or an inversion center. So, this therefore, belongs to $\bar{1}$.

So, we have therefore, the stereographic representation of 1 and $\bar{1}$ as we see here. So, the obvious extension is now to take the crystal systems associate them with respect to the stereographic projections of symmetry elements and associate therefore, the point group symmetries to each and every crystal system.

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32-point groups

- **Triclinic**: $1, \bar{1}$
- **Monoclinic**: $2, \bar{2}=m, 2/m$
- **Orthorhombic**: $222, 2mm, 2/m2/m2/m\ (=mmm)$
- **Tetragonal**: $4, \bar{4}, 4/m, \bar{4}2m, 422\ 4mm\ 4/m2/m2/m$
- **Trigonal**: $3, 3m, 32, \bar{3}, \bar{3}2/m$
- **Hexagonal**: $6, \bar{6}, 6/m, \bar{6}m2, 622, 6mm, 6/m2/m2/m$
- **Cubic**: $23, 2/m\bar{3}, 432, \bar{4}3m, 4/m\bar{3}2/m$

As we saw in the discussion before, this can be done in this particular table. This is have the final result which I will show, but we will discuss each and every point separately with respect to the points which we are going to do, with respect to the diagrams which we are going to do.

So, what we will do is we will do this stereographic projection on the crystalline systems and then from the crystalline systems, we can take individually the presence of the symmetry elements with respect to the projections we got from the North Pole, the projections we got from the South Pole. Conglomerate these results and see what kind of a symmetry this distribution of open circle and the x points indicate and based on that we can decide on the symmetry that is associated with the crystal system.

So, we have now brought in the crystal. The crystal is now 3-dimensional. We have drawn radial lines with respect to the crystals, so that they can be represented as a stereographic projection inscribed inside a sphere. So, effectively the crystal is taken and put inside this sphere and we have taken the intersection points in the northern hemisphere of points are joined to the south a South Pole and those are indicated by open circle and the ones which joined the North Pole from the southern hemisphere are indicated by x points and based on that we can generate and identify the equatorial plane projection which is the stereographic projection and based on the stereographic projection we can identify therefore, the point group symmetry that is associated with crystal.

This is the way in which ancient crystallographers used to do people who study crystals will look at the crystals and do these experiments and now eventually we will develop a methodology which will tell us how to get these symmetry information on a direct basis. So, this now tells us the systems to which we can go into. So, this is a general listing triclinic system. The triclinic system can have 1 and $\bar{1}$, a monoclinic system 2, $\bar{2}$ and 2/m and so on.

So, we will see how each one of them develops with respect to the stereographic projection as we go further.

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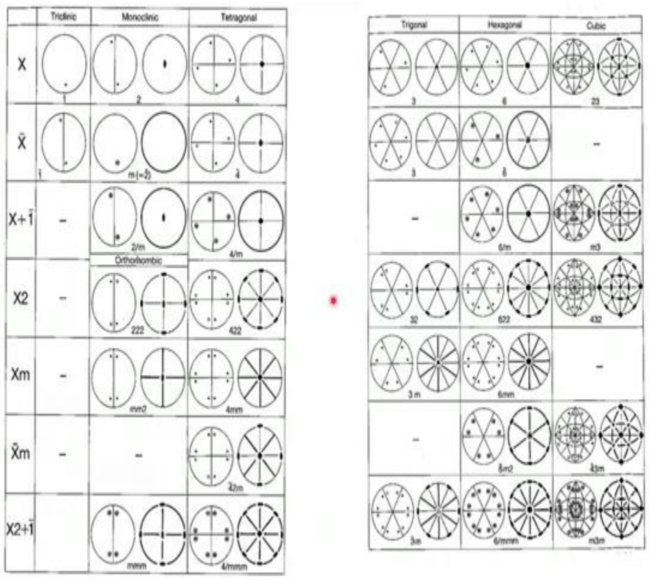

Here is a diagram which shows you the stereographic projections of all types of crystals belonging to these systems. So, here are the crystal systems triclinic monoclinic tetragonal, trigonal, hexagonal cubic and this is the axis of rotation. So, the axis of rotation can take values 1, and then it can take the value of 2, it can take the value of 3, it can take the value of 3, it can take the value of 4, they are grouped together and the way in which we are organized is triclinic, monoclinic, tetragonal, trigonal, hexagonal, cubic. These are the these five in fact, trigonal, monoclinic, tetragonal, trigonal, hexagonal these five systems have single axis symmetries as well as in case of tetragonal, trigonal and hexagonal you can have more than one axis that is present which is indicated here by individual stereographic projections.

So, our job now is to study each one of them. We have to study each one of them and understand how the equivalent points are generated. So, we will make an attempt today to generate to study a few of them and in the next class we will take up a few more of them and then in general we take a few examples from the more complicated looking ones on the right hand side.

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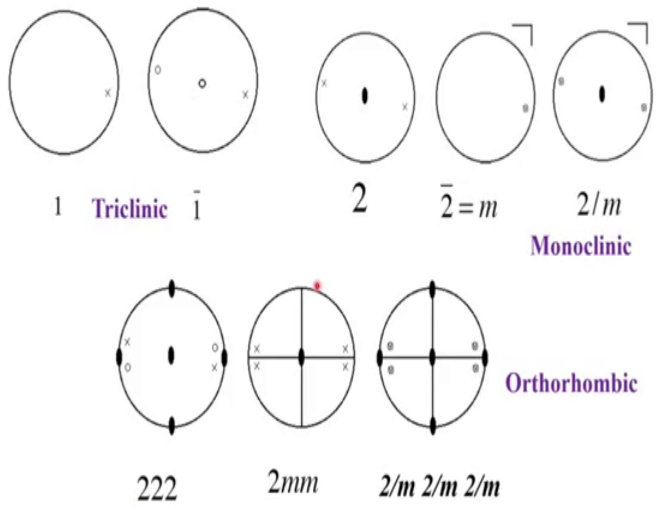

And, then we will go into a representation of each one of them separately as we saw here and as we discussed in the case of stereographic projection and then distribute them to the various crystal systems.

So, this looks very complicated, but one once we do it and one once we revise what we have done we will see that it can all be fitted into one single understanding of these point group symmetry, the crystal system and then the distribution of these systems with respect to generation of equivalent points. We have already discussed the generation of equivalent points in case of 1 bar symmetry for a given xyz there is an $\bar{x}$ $\bar{y}$ $\bar{z}$ bar and that is in fact, illustrated here you have an xyz and an $\bar{x}$ $\bar{y}$ $\bar{z}$.

Since this line now represents the line of demarcation and the location of the centre of symmetry is here and because the location of the centre of symmetry is here and this is the projection which has been done we see both of them as open circles you might be asking why if this is one is open and one should be closed, right because if there is a center symmetry and that projection is 90 degree oriented with respect to this projection. In this projection we are considering the axis of rotation to be 1 and then the axis of rotation $\bar{1}$. So, the axis of rotation is the one which is now shown along this direction.

And, therefore, you see this is xyz, this is $\bar{x}\ \bar{y}\ \bar{z}$ or vice versa because of the fact that the central symmetry sits here it does not matter whether you have the xyz or $\bar{x}\ \bar{y}\ \bar{z}$. So, that therefore, tells you the two point group symmetries that can be associated with the triclinic system. So, a triclinic system therefore, has two equivalent points in case we have presence of a center of symmetry or more appropriately an inversion center and that inversion center is present at this point where the pointer is shown.

Then we go to the monoclinic system and in the monoclinic system we see that we generate again these two. Remember, now this is a projection which is showing in a perpendicular direction two of the angles are 90 degrees with respect to each other we can also show this as a two-fold rotation here. Now, you might be wondering what is going on here because this is shown nothing here and this is shown as a picture where we have one below the other and in this case one away from the other.

So, what is shown here are the two diagrams; it is not necessary to show two diagrams in triclinic because there is no their axis of rotation. The moment you have an axis of rotation we show these are the equivalent point positions and this is the symmetry position. So, for every point group therefore, we show two diagrams and therefore, these are the two diagrams which will be shown for each crystal system.

So, then we will go further into the presence of the twofold symmetry as I mentioned that two diagrams now I have to be given for each one of these and this is now showing the equivalent points, this is showing the symmetry position. So, this is the mirror operation and you see that in the mirror operation I do not know whether you see it very thoroughly here, this has to be a bold circle. This circle is lighter than this circle so; that means, the mirror is now flat with respect to the diagram we are showing.

So, if you see the original textbook you will see it better this is from the textbook of (Refer Time: 11:45). In fact, there is a proposal from my side that we will give you the handouts and we will discuss with the NPTEL authorities and see we give a set of handouts for each and every lecture to follow and that is something which will be very useful for this symmetry class because symmetry and structure is very fundamental for all areas of science and engineering and therefore, I want you to get a clear hang of these symmetries. So, a handout will be accompanying the lecture series.

So, this now will be the darker one. So, it shows that the presence of this. In the case of the orthorhombic system now we show the presence of 2/m this is the presence of a two-fold followed by one bar rotation. The twofold followed by one bar rotation generates two possibilities; one is the presence of these equivalent points now you see the mirror is in the middle and therefore, this is a presence of a two-fold and now this is a darker circle. So, the twofold axis is coming towards us the darker circle is the perpendicular to the twofold axis. So, it is a 2/m symmetry and $\bar{2}$ which is mirror and 2/ m symmetry now represent all the possible point groups associated with a monoclinic system. So, triclinic has two point groups monoclinic has three point groups.

We go further now into orthorhombic symmetry in case of the orthorhombic symmetry we can have three twofold axis mutually perpendicular to each other that is because we have an a axis, an b axis and the c axis. The angle between a and b, b and c and c and a are all 90 degrees with respect to each other. Because we have these 90 degree angles we will have their two-fold axis along a, two-fold axis along b, two-fold axis along c. This generates the equivalent diagram of this kind where you have a open circle and a closed circle open circle and a closed circle. So, the number of equivalent points you generate in a 222 point groups will be xyz then you first operate the twofold symmetry operation in one direction. Let us say along the x direction, then you will have x $\bar{y}\,\bar{z}$, then you operate the twofold along the y direction which will be $\bar{x}$ y $\bar{z}$ and then you operate the twofold along the z direction which will be $\bar{x}$ $\bar{y}$ z. So, which means that, it generates four equivalent positions.

In case of the triclinic system, for example, you will generate two equivalent positions; xyz, $\bar{x}\,\bar{y}\,\bar{z}$. Please note that this picture I do not know how clear is there up there this is a close circle and this is a open circle you do you do see that? No. So, this diagram is not that very good I will be showing it more detailed in the next set of diagrams.

So, the presence of the three intersecting twofold axis now generate the symmetry disposition. These are the symmetry disposition diagram where you see there is a twofold along this circle, the two-fold along the direction along x and direction along y. So, all three directions have twofold symmetries. So, this represents 222.

Now, the combinations of 222 can be 2mm because we can have a proper axis and improper axis and followed by another improper axis. No other combination is possible which we have discussed much earlier with several classes ago. So, this can be 2mm or 2mm is same as mm2 and m2m because a b and c in an orthorhombic system are interchangeable. We can always call a as b, b as c and c as a because the only condition we put in orthorhombic systems is the condition on alpha beta gamma being 90 degrees. So, we can interchange a, b and c.

So, this represents a common representation where we have a and b directions associated with the mirror planes and the c direction associated with a two-fold. So, the symmetry diagram is up here it tells now these are darker as you can clearly see that represents the mirrors. So, one mirror here, another mirror there and the c direction which is coming towards you has a two-fold symmetry.

So, the equivalent point diagram again is shown here. This should have therefore, how many do you expect as the number of equivalent points? In this particular case of 222 we are expected four equivalent points, in case of mm2 we expect again four equivalent points. On the other hand when we have a symmetry which is mmm; mmm actually represents 2/ m 2/m 2/ m and therefore, you will have number of equivalent points as 8; four up and four down in this diagram, four up and four down that is totally 8 and this now becomes all dark in the sense that there are three mirrors perpendicular to each other.

The presence of the mirror and the angle 90 degrees will invoke automatically the twofold axis around all three directions. So, there are perpendicular two-fold axis coming towards us then the mirror planes which are intersecting in all three directions and that represents the highest symmetry that is possible in case of an orthorhombic system.

So, today we have covered the triclinic, the monoclinic and the orthorhombic systems we have shown how the equivalent points developed. The next thing is we will have to see how the tetragonal system develops. In case of the tetragonal system we now look at the possible symmetry positions which are coming with respect to the operation. So, as we go back here x represents the rotation axis.

So, there is a fourfold rotation. There is a four-fold rotation with a mirror combination that is with a inversions combination which is $\bar{4}$ symmetry and we also have a four-fold rotation which accompanies a mirror symmetry. These are single point operations; that means, these are single symmetry operations the moment you have a four-fold symmetry, you will have also the presence of an inversion center associated with it just like the monoclinic system we had a twofold symmetry, you had a $\bar{2}$ symmetry. So, with 4 , we will have a $\bar{4}$ and we also have a 2/ m therefore, with for symmetry we have a 4/ m symmetry.

Now, these represents again the equivalent points on the left side and the symmetry diagram on the right and this therefore, represents the tetragonal system. The tetragonal system can also have more than one axis. The fact that we have these orthorhombic systems which are more than one axis PPP, PII and so on applies to these systems as well, and therefore, in a tetragonal system we have 422 and 4mm; just like we have 222, mm2 we can have it 4mm because we always represent the z-axis to be associated with the four-fold rotation. The moment the z-axis is associated with fourfold rotation we will have this issue of 4mm and that is unique that has here mm2 could be 2mm m2m and so on.

So, because we have 422 and 4mm and we have just $\bar{4}$ symmetry. 4 bar symmetry will give rise to $\bar{4}$2m and also 4/m 4/m 4/m where we have the combination 4/m sorry 4/m 2/m 2/m which is now representing the overall highest symmetry that is associated with a tetragonal system. So, the tetragonal point groups are 4, $\bar{4}$, 4/m, 422, 4mm, $\bar{4}$2m and 4/mmm. So, 1 2 3 4 5 6 7, so, seven point groups can be associated with a tetragonal system, monoclinic has three, orthorhombic has three and triclinic has two. So, this left hand side of this slide now covers 1 2 3 4 5, 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15. So, we have covered fifteen of the possible 32 space groups by going from triclinic to monoclinic to orthorhombic and lastly to tetragonal system.

Now, we on the right hand side is the remaining crystal systems. The remaining crystal systems you not we already see that hexagonal and trigonal are a little complicated in terms of having both the six-fold as well as the three-fold. So, it depends upon where the origin is and where the threefold and the six-fold are located in these compounds. It is not necessary to have a threefold symmetry and the six-fold symmetry looking one and the same; obviously, it is not as you see from the equivalent point diagram and also from the diagram which we have drawn on the right side. So, this gives rise to the threefold symmetry, a single rotation axis symmetry which will give rise to $\bar{3}$.

Now, as far as the 3 and $\bar{3}$ are concerned these operations now introduces these translation symmetry which is not 1/2 or 1/4. Because the translation symmetry is not half or one fourth, the issue comes up with the point group symmetry because we have to have the definition of a point group; that means, when we start generating the points with respect to these operations they should come back to the original point, that is the definition of a point group. So, if you start from in this example if you start from xyz you got a $\bar{x}$ $\bar{y}$ $\bar{z}$ you have to come back to xyz by operating it again. So, that repetition of operations will occur in case of 3 and $\bar{3}$, but they will not occur if we consider the case of 3 or $\bar{3}$/ m or 3/m.

So, that is because of the fact that the three-fold axis appears at a rotation distance at a uniform distance of 2/3 and 1/3 from the axis. And, the location of the threefold axis in the case of the six-fold axis again there will be three-fold axis which will be rotated at 1/3 and 2/3 and therefore, we will have in this particular case no possibility of extension of 3 and 6 being same and therefore, $\bar{3}$ and $\bar{6}$ are different from each other.

Since $\bar{3}$ and $\bar{6}$ are different from each other we can have a combination of 6 and a mirror perpendicular to. A combination of the three fold and a mirror perpendicular is not allowed. This is something which we probably will give you as an assignment I do not know, but I think it could be a heavy assignment in such situations we will worry about that fact whether we can you will be able to digest that as an assignment as we go along.

But, the fact remains that with the trigonal as well and along with the hexagonal system we should have the more than one axis intersecting at a point. When we bring in that issue we will have these additional point group symmetries 32, 3m and $\bar{3}$m and the equivalent point diagram is on the left and the symmetry diagram is on the right. and, that is illustrated for all these hexagonal systems as well as from the trigonal systems because of the fact that 3 and $\bar{3}$ create problems we do not have a $\bar{3}$m2 here. And, therefore, we have 6 in fact, we have five trigonal point groups and 3 plus 3 6 plus 1, 7 hexagonal point groups.

Cubic system is quite complicated as we saw in the earlier classes also because of the fact that the axis do not coincide with a, b or c. The only axis which coincides with a or b or c is the two-fold axis which is a redundant operation in a cubic system and the issue that the cubic system axis should not appear either along a or along b or along c the minima the symmetry that is required is also very crucial and therefore, we generate very complicated diagrams, stereographic diagrams as is shown here.

We will probably spend a little time on this or not we are not sure as we go along that these can be studied with respect to the tetrahedral and the octahedral distribution we discussed in several classes ago. We did talk about the way in which the distribution occurs when we discuss individual rotation axis and then brought in the issue of the location of these retention axis and with respect to that therefore, we now have a total of 32 point groups. And, this I think is more or less the stage at which I would like to end here.