Symmetry and Structure in the Solid State
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Lecture - 09
Bravais Lattices

So, we have been discussing the 5 plane lattices in the last class.

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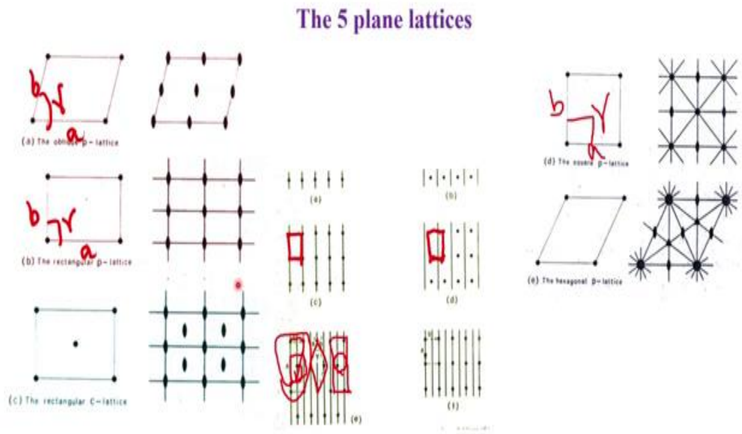

And we discussed the oblique p lattice, we also discuss the; we discuss the oblique p lattice, we also discuss the rectangular p lattice. And we found that there are two ways in which we can represent this rectangular p lattice. One is to show the points along the line of symmetry and show the points half way between the lines of symmetry and both these will now give rise to the rectangular p lattice. So, if you consider this point, these four points now we will define our unit cell, these four points will define our unit cell and this is a primitive lattice. And the two fold rotation axis will appear here, here, here, here because any plane lattice will have a twofold symmetry.

And therefore, the plane lattices will always have a twofold symmetry at the origin and that one unit translation. So, that is already represented along with that we have the lines of symmetry. So, the lines of symmetry will repeat at these positions and as we discussed, whatever is the symmetry at the origin and one unit translation will automatically appear at halfway point because of the heat translation periodicity. So, the similar thing happens here. Even though these points are in the middle of these lines of symmetry, the unit cell is still having one point which is which is now again a primitive rectangular lattice.

So, we can also have another type of a lattice where we have the overlap of the lines of symmetry the way in which these are repeated. So, we take this unit, the one dimensional unit, overlap this one dimensional unit with this one dimensional unit and that is represented here. So, we have this line of symmetry, this is the repeat distance a and this is the repeat distance b; here the points are with respect to this dimension. So, we have this point, this point, this point and this point and between them we inter leave this one now. Because of the fact that we inter leave this fellow, this one has come in between and that also has a line of symmetry by definition which we have given here.

And therefore now, we see that there are lattice points are these four points and also a lattice point in middle and this now defines a different kind of a rectangular lattice which we call as the rectangular c lattice. So, the rectangular lattices there are two types; primitive as well as the central lattice and this is represented by this picture here. So, what happens is because of the fact that we have a centred position here, the property of this repeats at the centre and therefore, the property of whatever is happening here will also repeat at the centre.

And so, we get additional two fold symmetries now placed at one fourth between one and half the additional symmetries are placed at one fourth, but there displaced by another one fourth. So, at one fourth, one fourth, we get a twofold axis and therefore, this now defines a new type of a plane lattice which is a rectangular c lattice. On the other hand, if we just have these alternate ones, but no occupancy of the middle, this is similar to the one above here and therefore, we will get a rectangular p lattice.

So, f represent a rectangular p lattice corresponding to b; on the other hand, the e represents a rectangular c lattice where we have a centre. I think I should describe this again for the convenience of people who have a difficulty in understanding this. We have in a rectangular system, a equals b a not equal to b, but gamma is 90 degrees. The fact that gamma is 90 degrees will ensure that these two fold symmetries which came here without the presence of gamma being 90 will always represent at these positions. So, the moment we have a plane lattice, the two fold symmetry is will appear at the origin one translation along a, one translation along b and they will also appear along the half distances.

Apart from that, the fact that a is equal to b and gamma is 90 degrees introduces a line of symmetry and this line of symmetry can be now represented in this one dimensional lattice by these points. The same one dimensional lattice now can move the lines of symmetries halfway and the points of representation could be halfway between the lines of symmetry. Both of them represent the one dimensional lattice and the corresponding 2 d lattices are shown in c and d.

Both c and d now represent a rectangular lattice, but this now is a primitive lattice because the total number of points add up to 1. So, the number of lattice points is 1 and therefore, we have a p lattice. We can always interview inter leave this a and b together and therefore, we can have alternate layers of this line of symmetry and that line of symmetry existing parallel to each other as I will just shown in the diagram e.

Here we show that the a type is existing in these alternate lines and the other alternate lines are represented by this b type. And then this happens you see that this defines the unit cell with a equals b and gamma is 90 degrees which is a rectangular representation; however, we get a point at the centre. In fact, if you look at the most primitive cell that can be generated in this unit cell, this could be here. I will show by marking with the pen what I mean by this.

So, if you see this, this, this and this: this refines a rhombus and in this case a dash and b dash are the two distances and gamma dash is the angle and this represents a primitive rhombus. The problem with the definition of a primitive rhombus a is that we do not have a value for gamma prime. Gamma prime is not any value. It has to take this value corresponding to the rhombus and what is the value associated with the rhombus? The value associated with the rhombus gamma can be calculated as a prime plus b prime divided by 2, etc, etc. And therefore, this is not a uniquely defined gamma prime.

So, even though there is a possibility of a rhombus being defined here, the most convenient way of representing because all the symmetry elements associated with this will represent the presence of the rectangular lattice. So, the rectangular c lattice if centred will define now this unit cell. This will now involve the possibility of including this particular centre as well. So, we have therefore, here a and this is a this is b and this will now represent our unit cell with an atom with a lattice point of this centre. So, the total number of lattice point 1, 2, 3, 4 will define one and this will add additional lattice point. And therefore, the number of lattice points is two and therefore this becomes rectangular c lattice.

So, the occurrence of the rectangular c lattice is because of the presence of an additional lattice points. Since we have two lattice points here this can be represented as a centred rectangular lattice and so, we have two types of plane lattices in a rectangular system. So, what is the implication of this? The implication of this is that effectively there are only four plane lattices, but then among the four plane lattices which you can call which we can could have called as two dimensional crystal systems.

There is an additional lattice that is possible which is the so called c centred rectangular lattice. So, it now makes it possible to have therefore, 5 lattices. The fourth one is a equals b, here it is a and this is b and here a equals b because it is a square lattice in square the gamma is the angle here which is 90 degrees. And therefore, we get a definition of a square lattice which is something like this.

Now, what is very interesting is to see how these fellows all developing. How the symmetry elements develop in a situation like this? If you look at this particular point this represents now because it is a square lattice it represents a fourfold symmetry. So, as a presents of the fourfold symmetry of here is repeated at unit cell lines. Notice, that in the case of the oblique lattice and also in the case of the rectangular lattice the same symmetry element repeated.

Here, the fourfold symmetry now is not repeated because of the fact that these two now which are diagonals they intersect at the centre and there we get the definition of the presence of a fourfold symmetry which implies that we get additional two fold symmetries at these half points. Now, why is that it is because of the fact that if we take now assume that this is also fourfold symmetry, then this fourfold this fourfold together will not generate the central fourfold.

If we want to generate the central fourfold, these have to be only two fold. Think about it, if we have to generate the central fourfold and also they are the fourfold symmetries at this are ledgers, this has to be two fold it cannot be any other value. If this is also fourfold, then we will not be able to repeat the four fold here. The redundancy comes from the fact that these diagonals will now represent the central point and these diagonals now automatically carry the two fold information and since these diagonals now carry the two fold information.

This central now becomes the four fold symmetry, and as a consequence these directions will have now at the midpoint two fold symmetries. The same argument goes for the hexagonal p lattice where a is equal to b and gamma is 120 degrees and you see that the sic fold symmetry goes up in the edges and three fold symmetry is develop in these positions where we have shown and the central between the six and the six is always a twofold.

So, this now of course, will eventually as you can anticipate will come as an assignment and you will have to work it out why this now has additional symmetry elements are different points like 1/3 and 2/3. Why the 1/3 and the 2/3 develops could be in the form of an assignment and this therefore, tells us that there are 5 plane lattices what we have learnt in this particular set of discussion is that there are 5 plane lattices, the oblique p lattice the rectangular p lattice, c lattice. So, we have an additional lattice with a centring which is associated with the rectangular lattice. We also have this square lattice and the hexagonal lattice.

Remember, the rotation axis that can be associated with this are the two fold axis of here, two fold axis of their, four fold axis here and the six fold axis there. You also see that the presence of the three fold axis is automatically invoked in the hexagonal p lattice. So, there is no trigonal p lattice, the trigonal p lattice plane because it is already there. Suppose, you consider this as the origin then you can define three fold symmetry primitive lattice associated with the plane lattice. So, it is redundant. So, the six fold is the one which now dominates in this particular occupation.

Therefore, there are only 5 plane lattices. So, even though there are we talked about seven crystal systems, here there are only five, four crystal systems and 5 lattices. So, in among the plane lattices, there are four crystal systems and in two dimensions and 5 lattices. Now, we will see now what happens to the seven plane lattices, seven crystal systems and how many lattices we can generate with the same logic.

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The 5 plane lattices

Lattice type	Point group of lattice	Possible crystal point groups	Shape of conventional unit-mesh
Oblique p	2	1, 2	$a \neq b$; γ general
Rectangular p Rectangular c	$2mm$	$1m$, $2mm$	$a \neq b$; $\gamma = 90°$
Square p	$4mm$	4, $4mm$	$a = b$; $\gamma = 90°$
Hexagonal p	$6mm$	6, $6mm$ 3, $3m$	$a = b$; $\gamma = 120°$

Before we go further we will examine in detail the definitions of the 5 plane lattices. This is something which is very important and crucial you see that indicates of an oblique lattice, the lattice type is p, the point group associated with the lattices 2. This is the maximum point group symmetry that can be associated with the lattice. But, when you come to the case of a crystal it depends upon what kind of an object is sitting inside this oblique axis. If there is a material which is now containing an object let say molecules that molecule has no two fold symmetry, it can still go into an oblique p lattice with a value of 1.

So, the possible crystal point groups are 1 and 2, both 1 and 2 are possible in an oblique p situation where a is not equal to b and gamma is a general value other then 90 degrees. Having understood that we have the remaining p and c, we point group symmetry the maximum symmetry is 2 mm and then depending upon the type of object we are going to put in the crystal it could be 1m or 2mm. So, in logic appears to the square symmetry as well as the hexagonal symmetry, you see that in the case of the square lattice we get a 4 and a 4mm, 4 mm is a possibility because we remember you remember that we have the Elures theorem and one once you have the proper, improper, improper that combination is allowed and therefore, we will have 4 mm.

So, in general the point group symmetry of this lattice a is a proper, improper, improper axis combination in the value is a equal b gamma 90 degrees and when the value of gamma becomes 120 degrees you have the hexagonal symmetry. The hexagonal symmetry as you see can also have the threefold symmetry as we saw from the previous diagram of here it is also got the presents of the threefold symmetry; one third removed from the six fold symmetry, two third removed from the six fold symmetry, we have the presents of the three fold symmetries and this surroundings of this suppose, we have we call this as 0 0 0 at this particular origin there is a six fold symmetry, then the three fold symmetry is removed by one third. We can always move the origin to the three fold symmetry position.

Then, we will invoke a six fold symmetry because of the presence of the two fold at the centre of these unit cell and therefore, we have these both the possibilities, it is coming up here the presence of six fold as well as the three fold. So, we can therefore, have objects which belong to the hexagonal symmetry, we can have objects belong into the trigonal symmetry, both going into a hexagonal small p. The small p and the small p the tell us that these belong to now two dimensional lattices; p represents a total lattice point of 1; c represents a total lattice point of 2. So, the number of lattice points in rectangular c is 2. The point symmetry is different from the number of lattice points in the in the lattice. So, the lattice now decides how many combinations of symmetries it can have because of the presence of either p or a c.

In addition, we have his presence of symmetry elements and therefore, the objects now which find themselves inside these unit cells will have to look at both the point group symmetry as well as the lattice symmetry. So, the presents of the lattices symmetry in conjunction with a point groups symmetry and of course, the nature of the material which goes into this lattice; all these combinations will decide what kind of a symmetry one has to take in this particular case.

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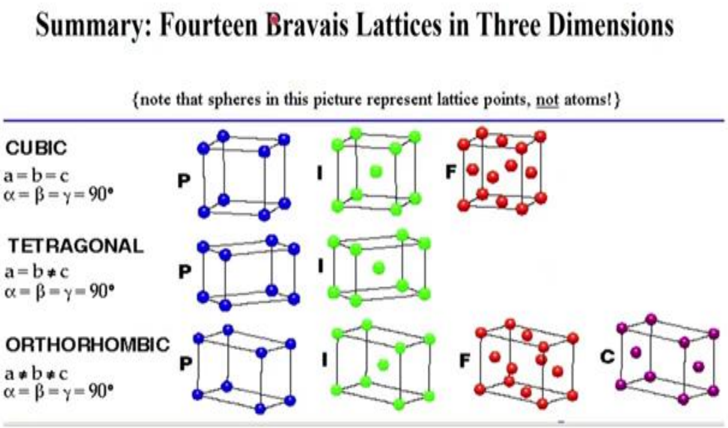

Extending the same logic of finding these symmetry elements and we saw that there are 5 plane lattices. Since there are seven crystal systems, the seven crystal systems now will generate 14 lattices just like the 4 crystal systems in plane lattices generated 5 lattices, here the 7 crystal systems will generate 14 of them and these are referred to as the Bravais lattice this after the name of the person who discovered this. And this there for now represents the three third dimensions, the three dimensions and then we see here the cubic system in the case of the cubic system we therefore, have these points these are the lattice points please note that.

These are lattice points are not atoms is always a confusion. So, we should remember that we have not brought in any realistic atom or molecules in the in our discussion so far. So, the points which are appearing here are the lattice points. So, the lattice points therefore, now represent the presence of a primitive lattice because here now which is three dimensions. So, each point will now represent one eight. So, the total number of this will be 1, 2, 3, 4, 5, 6, 7, 8 multiplied by one eight. So, that will make it 1. So, the primitive lattice always has one lattice point we can have the centre of the cube centre of the cube located in such a way that we will have what is known as a I-centred the body centred lattice.

So, the cube is appear which represents one lattice point, this 1 represents the second lattice point. So, the number of lattice points saying a body centred cubic system is 2. If we can have also the each and every face centred, we will have four possible positions in which we can have the occupancies defined and therefore, we have the lattice points at the corners during one lattice point, in addition the faces give half lattice point. So, since there are three faces; half, half, half will add up to 3. So, 3 plus 1 therefore, there are four lattice points associated with the f lattice. Now, other possibilities exist in case of a cubic system which is the highest symmetry system.

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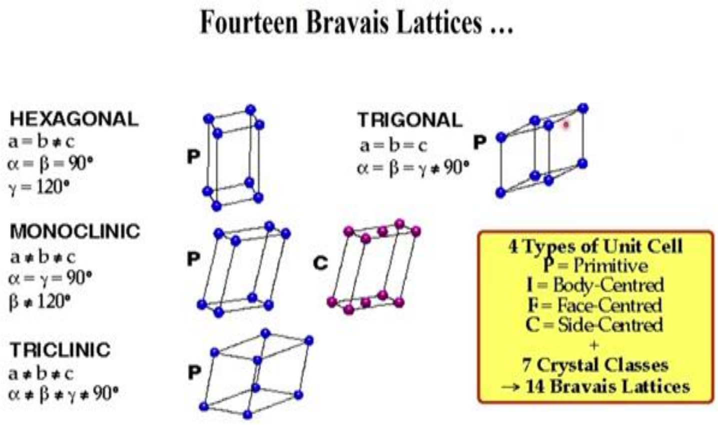

In fact, I should have shown you the other way around, this 14 Bravais lattices; I purposely so the cubic one to show the complexity of the situation. Now, we will look at it in a simple way. The simple ways is that we have a primitive lattice which is represented by P , we can have the C side centres lattice which is the case with a monoclinic system. Because, the monoclinic system here now can have since the angle is 90 degrees, the alpha and gamma are 90 degrees because of that fact we will have this as a possible C centred primitive lattice.

So, since it is a central primitive lattice, it could be alone say C or A or B. But in this particular example, we have a C centred lattice; that means, there are two lattice points associated with the monoclinic symmetry. So, triclinic symmetry always has only one lattice point, monoclinic symmetry depending upon the case whether it is primitive or centred will have one and two; hexagonal system always has only one lattice point, a trigonal system always has only one lattice point.

The most common one is the orthorhombic system where we have four possibilities; one is the lattice centring of course, in this particular case a, b and c are not equal to each other. So, when we have a C centred lattice, we will not have the A and B centred and therefore, we can have a single face centred lattice which is represented as C. We can have also face centred as well which is referred to as F. We have the body centred lattice which is I in the orthorhombic primitive is also possible. So, if we count the total number of all these which now we will account to 14 lattices. So, we have seven crystal systems classified into 14 Bravais lattice.

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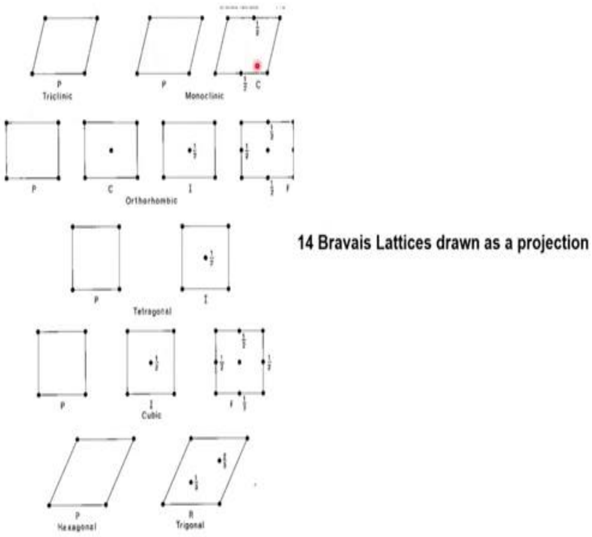

I how got a another illustration which is much more simple and straightforward and this is drawn in projection. So, I have drawn the 14 Bravais lattices in projection and this draw drawing will clearly tell us how we can arrive at the 14 Bravais lattices in to you know we always want two dimensional representations. So, here you see that in case of the triclinic system, we have only a primitive lattice. In case of the monoclinic system, we have the primitive lattice. Now, why did I show like this because I am now showing the angle beta this is a c diagram. In fact, this is to show that the c centring can be done in this particular projection.

So, this is P, the primitive lattice. This is the in this case it is a here and c there and this angle is beta in this case, this is c here and the a there and that angle is beta. The c direction is centred with respect to the lattice centring. Therefore, we have two plane lattices associated with monoclinic P and C and therefore, we have P and C lattices coming in three dimensions as well. So, triclinic as one one Bravais lattice, monoclinic as two Bravais lattices, orthorhombic will have four Bravais lattices represented in two dimensions here, tetragonal has two, trigonal has three, tetragonal has three sorry, orthorhombic the tetragonal has two cubic has three, hexagonal has one.

And this is a very special case as I mentioned when a equals b equals c, alpha beta gamma are same value then we have what is known a trigonal system. This is in, this diagram is in conjunction with the diagram we saw just a few minutes ago in the respect to this one, you see that there is a one third and the two third, three fold rotation and that is what is depicted here in three dimensions as well. So, there is a one third and a two third, three fold rotation that is present in a rhombohedral system.

So, there is a threefold axis which goes along the diagonal. So, if you take a rhombohedral system and put it along the diagonal and rotate that one, in such a way that we can rotate it in such a way that the angle becomes 90 degrees we will have a cubic system a equals b equals c, alpha beta gamma are 90 degrees. So, this therefore, now defines the 14 Bravais lattices. So, we have 32 point groups, seven crystal systems and 14 Bravais lattices. So obviously, the next step is very clear.

We have to take these symmetries into account we have to take the translational periodicity into account, we have to take the crystal system into account, we have to take the 14 Bravais lattices into account and then distribute the 32 point groups among all these crystal systems. When we do that, the prime groups now will alien with respect to these 14 Bravais lattice and generate what is known as the 3 dimensional space groups. That is because now in space, these symmetries get redistributed how in space the symmetry is get redistributed we will see as we go along.

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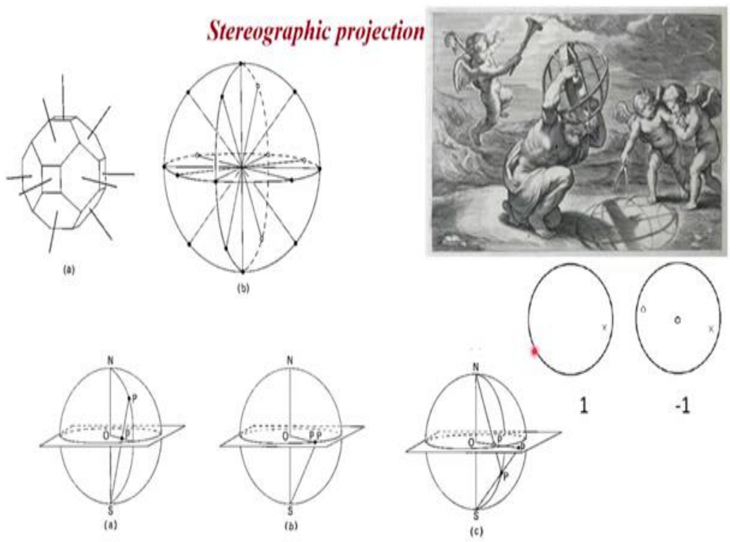

And now, before we go further, you remember that we decided to see everything in two dimensions, but it is not always possible to see everything in two dimensions. Because we saw the meiosis diagram, we understood the concept of periodicity from meiosis diagram and we have those objects repeating themselves generating the periodicity, generating the symmetry elements and so on. And, then we have to look into the aspect that how one can really look into three dimensions and this is in real situations. In real situations, we will have a crystal the crystal have different kinds of faces. So, these different kinds of faces in the crystal have to now be inscribed into a highly symmetric spherical system. So, sphere is the most symmetric object.

So, we take this sphere which is the most symmetric object. Take the crystal and insert in in it inside a sphere in other wards you describe a sphere passing through these points which I will stated here and you will get this sphere. Now, we take the centre of the crystal and draw directions have to various planes about which the crystallize has this is a very beautiful ground crystal, not always the crystals are so good but in this example, you see that we are drawn from the centre here perpendicular radial direction.

So, the radial symmetry of the crystal you gets have represented here. Why do we represent the radial symmetry because the radial symmetry is the one which is most common with respect to spherical objects. For example, if you put a centre here all the symmetry elements now associated with this particular sphere can be along the radial directions.

So, if the crystal has a certain symmetry, the external morphology has a certain symmetry that symmetry can be fitted inside the stereographic projection. I will just diagnostic little bit at this particular point because we have to see why stereographic projection is very crucial in looking at crystals. And this is in fact, the way in which crystallographer practiced and identified all the symmetry elements associated with the crystals. Nobody did x-ray diffraction in those days because extra diffraction was discovered much much later.

All these concepts of point group symmetries and the space groups and so on were kept and derived way back in the 18 century the in 18 century 1735 to be exact. In that particular year, it was already shown that there are 32 point groups and because of the fact that we have now crystalline objects which will not displace these point group symmetries in the lattices, the combination of the lattices and the point group symmetries will give rise to 230 space groups.

So, all these were worked out much much before. So, we have to find out how they would our did out, not that we are going to do this way, we are going to actually use x-ray diffraction techniques which is a experimentally reliable and develops technique in recent years. In fact, x ray is well discovered only in 1900 by Rontgen. So, only after that time, but before that all the space groups and all the presence of point groups space groups etcetera you are already established.

So, how was it done? It was done by looking at crystals and people got all the very large crystals or size crystals so that they can hold it in their hand and then examine the perpendicular faces the perpendiculars to the faces, make an impression of that on to sphere and on that sphere, we can mark the intersection point. So, if this is the point find which is they appear we mark the intersection point by a open circle.

Now, I will define what is this open circle and close circle in a minute. Before that, as I mentioned we will digress a little bit. We have a similar situation in case of earth we have a three dimensional object; earth is a three dimensional sphere and when you want to study the geography associated with the earth, we do a different kind of a projection that is not a stereographic projection. We do what is known as the Mercator projection.

In that projection, what we do if we take they were earth the surface of the earth hold on to it is diameter and then press the earth. It is like taking an orange and press it of course, though did because it will push and spread and your dress, but essentially you take this orange diameter and press it like this and when you press it like this, it flatulence out and flat and out is your map.

So, then you take out the reasons of what you would like to inspect in this flat and out map. If this is on this side, we will exam in those ones we both northern hemisphere and southern hemisphere units will be represented and also the northern hemisphere or southern hemisphere units will be represented on the other side. Essentially, we have to then open it and spread it, this is the diagram we will see in all atlases. So, you press it, open it and spread it around and therefore, you see the Americas on the left side and the rest of the world on this side, Americas are always separate. So, that is what we will see and now we want to determine in the distance between Mumbai and Bangalore as we discussed earlier in with respect to this diagram.

So, this diagram is telling as is it clear this diagram. So, this diagram is telling as that the story of Atlas. This is a Greek mythology the Atlas is carrying his the earth and you shoulder and these two angels want to measure just like as the distance between Bangalore and Mumbai. So, there holding this divider and then this angel, the third one is helping them out why shining light on this so that we get a projected image of the surface of the earth and this is on the ground and therefore, it is two dimensional and they now measure this distance and have a scale factor which will work out to the corresponding distance between Bangalore and Mumbai.

Now, there is a flow in this particular type of projection because it depends upon on what point on the surface of the earth we have done this projection. So, that way this projection is not a very convenient way of looking at actual systems. In other words, suppose instead of taking this equator and pressing it suppose I take let us say in fact, time when I visited New Zealand, this is what I we saw you take New Zealand as this part and compress the rest of the earth and top of New Zealand.

New Zealand as you all know is the size of our state Karnataka but when you do this kind of an operations New Zealand will appear very very huge. With respect to New Zealand, India will appear very very small it may be a little bit of a short length. And of course, U K will appear as a point that is not true, but this is what happens in this kind of projections. So, we need to find out a proper way of generating the projection diagram and that is where the stereographic projection comes in handy. So, what we therefore do is, we draw all these radial lines with respect to the centre passing through the plane of various plane so that the crystal is made up of various plane. This is let us say diamond, many of you where diamond many of the students wear diamonds and the diamonds has got very nice lustrous planes.

So, from the centre you draw this normals, the normal to the plane is the one which is now collected on the surface of the sphere. So, we are not now compressing or pressing this sphere which is remaining as such and then we do this projection. So, when we do this particular projection, what happens is that we will have points with respect to the northern part of this crystal, we also have points corresponding to the southern part of the crystal.

So, if now we see the northern part of crystal as we shown here, if there is a point P on northern hemisphere, we take the south pole and connect it to the north to the point p and represent this little p in the equatorial plane as a point as a close the circle a little close circle as you see here. This is the point p which is now the representation of the projection of this particular point on to the south pole. A similar construction is done with respect to the north pole.

And I think we will stop here.