Texture in Materials

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Module – 02
Basic Crystallography
Lecture – 04
Crystal Structure and Stereographic Projections

Good day everyone and today is the class of Texture in Materials and today we will start module 2 which is Basic Crystallography. In this lecture, we will understand Crystal Structure and Stereographic Projections.

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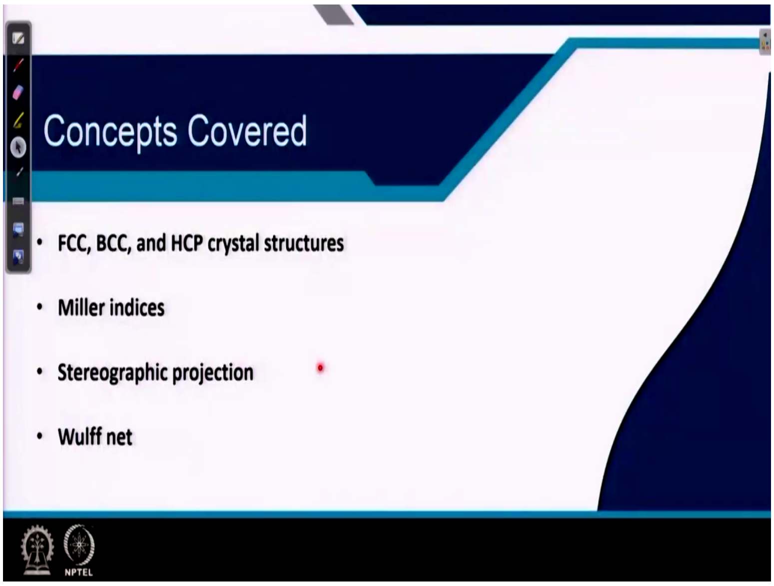

So, the concepts that will be covered in this course in this lecture are Face centered cubic materials, body-centered cubic material, hexagonal close-packed materials, crystal structure, their Miller indices, Stereographic projection, and Wulff net.

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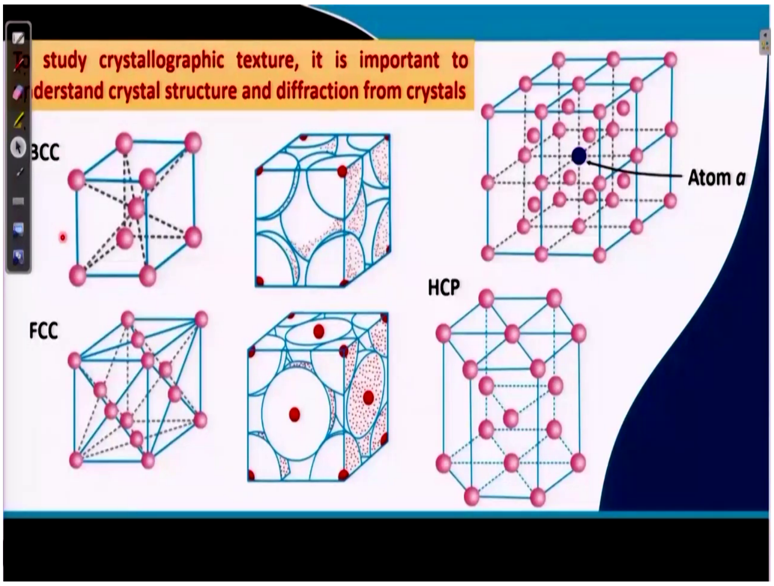

In order to study and understand the crystallographic texture, it is very important to have the knowledge of crystal structure and therefore the knowledge of diffraction that can be obtained from the crystal structures are important.

Here we mostly deal with metals and alloys and of course with materials such as semiconductors and minerals and ceramics etcetera. But most of the time when we deal with metallurgy is with metallic materials and these are usually body-centered cubic, face-centered cubic, or hexagonal close-packed materials. Body-centered cubic materials are basically iron, ferritic iron or you can say all the steels more ferritic steels. On the other hand, face-centered cubic materials say aluminium austenitic stainless steel brass copper etcetera.

The face-centered cubic materials are also divided in terms of their stacking fault energy. Yes, of course, the stacking fault energy is also present in the body-centered cubic materials. But face-centered cubic, for example, aluminium alloy they have a high stacking fault energy, copper they have a medium stacking fault energy, brass has a low stacking fault energy and therefore their behavior differs significantly. Now, coming to the basics body-centered cubic material contains atoms at the corner or you can say basis at the corners which are made up of atoms, and on the other hand, there is always one atom at the center and this consists of a unit cell. In real life scenario, the body-centered cubic materials unit cell may look exactly like see that it consists of 8 atoms at the corner of the body-centered cubic unit cell and each of these 8 atoms are they are shared between 8 different unit cell. So, these

8 atoms at the corner of the body-centered cubic material are actually contributing to a 1 atom per unit cell. On the other hand, the center atom of the unit cell also contributes to 1 atom to a unit cell making it 2 atoms per unit cell in a BCC material.

Here we have demonstrated that how an atom a which is basically the same atom as the other atom but is shown in a different color is shared between 8 of its unit cell and thereby one-eighth of this atom is shared by a single unit cell can be observed. On the other hand, the face-centered cubic material as one can observe has atoms at the corner of their unit cells. On the other hand, it has atoms at the face-centered of each of its faces. So, that 8 atoms at the corner of the unit cell it is shared each of them are shared by 8 unit cell and thereby they contribute to 1 by 8th of for a single unit cell. Therefore, 8 atoms each contributing 1 by 8 is equal to 1 atom contributing to a unit cell.

On the other hand, the atoms which are at the faces of this unit cell they are shared between 2 unit cell, therefore each atom contributes half towards the unit cell. there are 1 2 3 4 5 and 6 faces in the cubic unit cell, which makes that there are 3 atoms per unit cell in the faces plus 1 atom in the corner of the unit cell. Which in real-life scenarios some look something like this and therefore there are 4 atoms in a face-centered cubic unit cell making it a very closest packed structure. On the other hand, hexagonal close-packed material is certainly different from the cubic materials which are BCC and FCC. Hexagonal close-packed materials are the atoms are at 60 degrees to each other and therefore the crystal structure basically looks like this.

Few important elements structural elements and biomedical elements and other elements are hexagonal close-packed structures, these are titanium and see these hexagonal close-packed structures. they have 1 2 3 4 5 6 atoms at each corner an atom at the face-centered of the this is basal plane and 3 atoms inside. So, each of these 6 atoms is contributing one-sixth for each unit cell, and therefore the contribution from this 6 atom is 1 from the 6 atoms below is also 1 from the face-centered atom is both the atoms together contribute to 1. So, 1 plus 1 that is 2 and then 1 3 and then 4 5 6. So, in a hexagonal close-packed unit cell there are 6 atoms in a unit cell and one can see that both Face centered cubic and the hexagonal unit cells are having the closest packed structure.

So, it is important to understand these positions of the atoms in the unit cell and how the crystal structure basically looks like for FCC, BCC, and HCP at least Miller indices.

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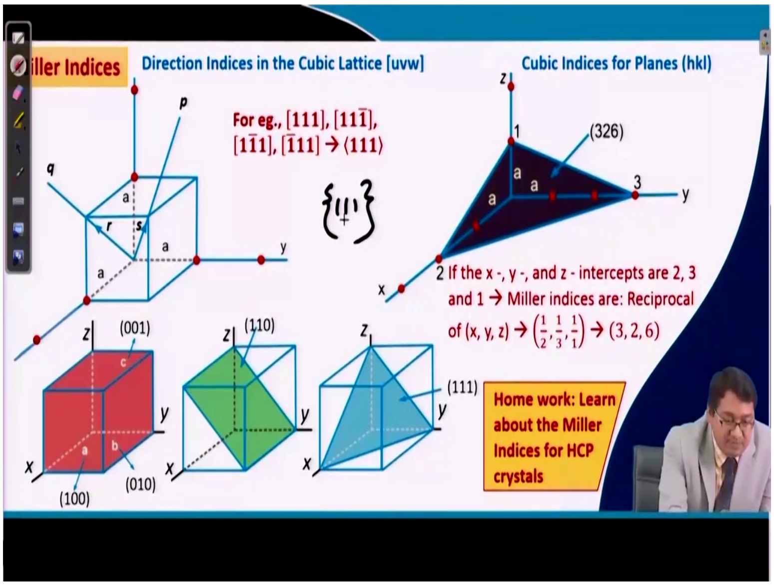

So, when we understand the atomic positions of the cubic and the hexagonal unit cell. Let us start with understanding the Miller indices of these unit cells. Let us start with the cubic structure and we will only show the cubic structure and I hope that you will go home and learn the Miller indices of the hexagonal close-packed crystal and I hope that most of the students who are doing this course may have already know the what is Miller indices and how it is found out.

Now, here is the first image of a unit cell and this image of a unit cell shows a cuboid basically a cube with edges of length a and here is the x-axis look at the pointer and the y axis is shown here, the z-axis is above and that if we say that this is a unified direction. So, a is the unit director, and therefore if we look at this atom at the corner of that unit cell, then and if you say that ok from this origin the burgers vector is coming out towards this atom then this unit is basically a. On the other hand in the y and z direction, this direction this x-direction is not coinciding. So, that the Miller indices for this direction become a 0 0 which is a is a unit so it becomes 1 0 0. On the other hand the Miller indices for the y-direction where it coincides with the y; but it is away from the x and z both and therefore it is not coinciding anywhere in the x and z and therefore it becomes 0 1 0. On the other hand, the z-direction becomes 0 0 1.

Now if we look at a direction which is q and it is unit direction is the r vector and therefore, that it goes straight and it coincides with the corner of the unit cell here. And this corner of the unit cell basically represents that it is at a distance a from in the x-direction and at a distance an in the z-direction. So, the vector r is basically equivalent to a 0, because it does not coincide with the y. So, it coincides with the y at the 0. So, it becomes a 0 a which is again this direction q is basically 1 0 1 direction.

If we look at the vector p which is coming out from the origin to this corner of the unit cell making it as a body diagonal, then you can see that this is this unit vector coincides with the x-direction at 1 in the y-direction at 1 and in the z-direction at 1 and by through this path only we can reach this point. The corner of the unit cell and therefore the vector p basically relates to the direction 1 1 1 and 1 can see that if this direction is 1 1 1 then we must know that this direction is basically perpendicular to the plane 1 1 1 and that we will show this one right.

If we, if we look at the below, figure we have shown that with respect to the x-axis which we showed has a direction 1 0 0, the plane a which is basically this plane has the Miller indices of 1 0 0. Why because it is perpendicular to the direction 1 0 0. So, the plane with Miller indices 1 0 0 has the direction 1 0 0 perpendicular to it. On the other hand, if we look here the y axis is perpendicular to the b plane and the y axis has a directional vector 0 1 0. Therefore the b plane has the Miller indices 0 1 0. On the other hand, similarly, the c plane which is perpendicular to the z-axis 0 0 1 has a 0 0 1 Miller indices. So as for example, we have seen the vector q which has a Miller index of 1 0 1 right and if we look into the plane this plane and this plane has basically a Miller index of 1 1 0 and how it comes to 1 1 0 one can say that if we look into this direction from the origin like I am pointing it towards this corner.

This direction is basically perpendicular to the direction of this plane and this direction is basically 1 1 0 direction, therefore the plane which is perpendicular to this direction has also the 1 1 0 Miller indices. If we find out Miller indices of the directions and the planes like this it looks very simple. But that let's go to the directions of the Miller indices directions and let's show that how many say for example like I have shown that this p vector has a Miller index of 1 1 1 right.

Like that there could be other vectors which are body diagonal right this one, for example, this one for another example this one. So, like that one can obtain body diagonal directions for the unit cell and it could be 1 1 1 which represent the vector as 1 1 bar 1 1. And then the opposite of this could also be obtained like 1 bar 1 bar 1 bar 1 bar 1 bar 1 1 bar 1 1 bar 1 1 bar 1 bar and these all 8 directions of body diagonal basically represents the family of 1 1 1 directions. On the other hand though from the family of directions and perpendicular to it in the case of the cubic unit cell we can find out Miller indices of the plane, that it is better to find the Miller indices of the planes by using this method which is shown here.

For example, we have the x y and z directions with atoms present at an equal distance in both x y and z and say we are talking about a plane which consists of something like this and so it is meeting the second atom in the x-direction the third atom in the y-direction and the first atom in the z-direction. So, if the x y z intercepts are 2 3 and 1 this is of this plane should be basically the reciprocal of this x y and z that is reciprocal of 2 3 and 1, and therefore the Miller indices of this plane are basically 3 2 6. So, this is basically the way in which the Miller indices of each plane are being determined. So, if we look into this plane which we said is the 1 1 0 plane, and see if we look into this plane it crosses the y axis at 1 the z-axis also at 1, but it does not cross the x-axis anywhere right. So, it crosses the x-axis at infinity. So, the Miller indices of this plane will be 1 divided by infinity comma 1 divided by 1 comma 1 divided by 1. So, the Miller indices of this plane are not 1 1 0 it is 0 1 1.

On the other hand, if we look into another plane as I said here which is basically the plane perpendicular to this s vector that is the x y z plane, then that this plane is crossing the x-axis at 1 the y axis at 1, and the z-axis at 1. And therefore, 1 divided by the x-axis 1, 1 divided by the y axis 1, 1 divided by the z-axis 1 makes it 1 1 1 plane, and therefore we can simply understand that how Miller indices of directions and planes are determined. To let that the Miller indices of directions are shown by square brackets, whereas the Miller indices of the plane are shown by circular brackets. On the other hand, the Miller indices of the family of direction are shown by this symbol and on the other hand, the Miller indices of family of the plane are shown in terms of curly brackets something like this ok. So, 1 1 1 type of family of planes let us go to the next slide.

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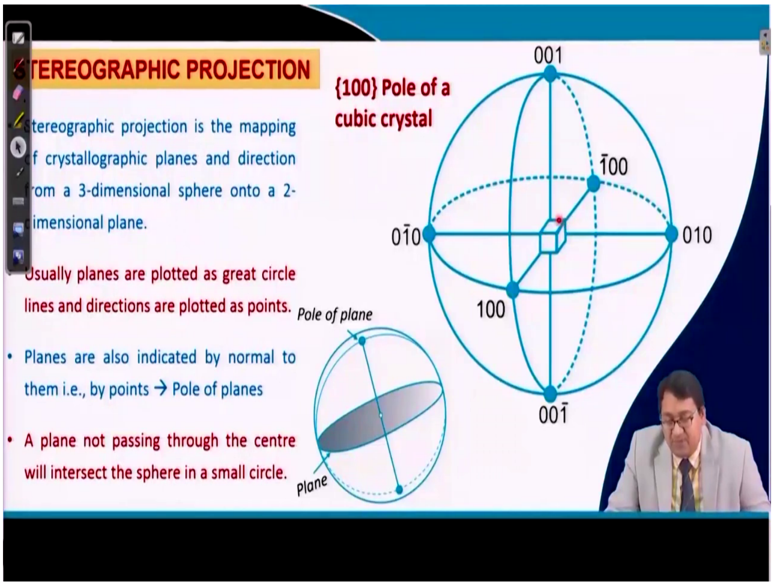

So, here we come as we understood the crystal structure here we come to the stereographic projection. stereographic projection is a mapping of these crystallographic planes and direction from a 3-dimensional sphere to a 2-dimensional stereographic projection or you can say that from a 3-dimensional stereogram to a 2-dimensional stereographic projection right. So, how it is done is that a unit cell for example is kept at the origin of the sphere and it is kept in such a way that the origin of the unit cell is exactly at the center of the sphere as shown in this figure. And that the important direction of these unit cells are the x-direction the y-direction and the z-directions.

These directions are basically 1 0 0, 0 1 0, 0 0 1 and it protrudes out to the circumference of the sphere and we get poles and these poles are basically 1 0 0 poles and this pole is the 0 1 0 pole this is the 0 0 1 pole and imagine that this is the sphere where we are projecting. So, this is the front of the sphere this is the back of the sphere this is the back of the sphere and this is the front of the sphere. And therefore, that in the front of the sphere when we are projecting 1 0 0 in the back of the sphere automatically the 1 bar 0 0 is being projected. At the circumference on the other hand if on the right of the sphere we are projecting 0 1 0 on the left of the sphere 0 1 bar 0 is already projected on the circumference like that on the top 0 0 1 then below it is 0 0 1 bar. So, this 3 D stereogram obtained the information of some direction of the unit cell like this we can obtain information of each and every plane and direction of this cubic unit cell in this 3 D stereogram. So, a stereographic projection is basically the projection or mapping of this information in this 3 D stereogram on a 2 D 2-dimensional plane right. So, in this case, you will also notice that when we are plotting this direction along the x-axis we are saying that it is the 1 0 0 direction and it is shown by a spot and therefore it is called a pole. On the other hand, if we look exactly perpendicular to this 1 0 0 direction you will get the 1 0 0 planes and this 1 0 0 plane is basically if we take this 1 0 0 plane and let us take the plane which is in the backside from where the origin of the crystal is matching with the center of the sphere. And that if we expand this plane, if we take this plane and if we expand this plane and it expands and it reaches to the circumference of this sphere and it will cut the circumference of a sphere and through this circumference right.

On the other hand, if we take another plane which plane the plane which is perpendicular to the 0 0 1 and this plane is also going through the center of the sphere and if we expand this one 0 1 0 plane then it expands to the stereographic 3 D stereographic sphere and it will cut down the sphere in the circumference like this right. On the other hand, if we take the 0 0 1 plane the 0 plane which is perpendicular to this 0 0 1 direction then this plane, then this plane also will cut down the sphere and form right and these things which are forming on this 3-dimensional sphere are basically known as great circles or great circle lines. Usually in stereographic projection the directions are plotted as points or poles, whereas the planes are plotted as great circles. So, planes are also sometimes indicated by the normal to them that is they are also represented by the perpendicular direction which is perpendicular to the right.

Sometimes they are also represented by points or poles and they are called poles of the plane right. So, here I have shown a small figure and you can see that if there is a plane which has a great circle like this and if it is perpendicular direction is protruding like that on the circumference of the sphere. Then this spot or pole is basically not only representing the direction that is perpendicular to the plane, but also the pole of the plane right. On the other hand, if any plane is not passing through the center of the sphere, then for example a plane which is the stop plane right the one which is having this plane is basically 0 0 1 which is producing this great circle and is perpendicular to this direction 0 0 1. But if of another plane which is just above it and say this stop plane which is also a 0 zero plane 0 0 1 plane, but it is not passing through the center of the sphere then it if you protrude this sphere if we expand this sphere and it will match and it will cut the circumference of this 3 D stereogram somewhere here right and then making it a smaller circle, so it is called a small circle.

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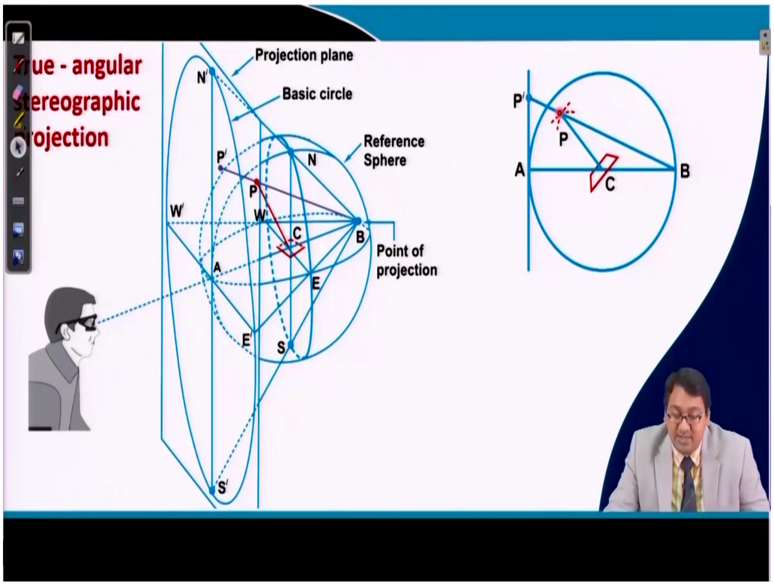

So, a stereographic projection is basically a true angular projection and this true angular projection is based upon the principles of the ray of light, it shows that if a crystal is kept at the center of a sphere and a torch is lit at this point. Say, for example, this point is known as the point of projection then from this point whatever shadow appears on the screen of a 2 two dimensional paper will make a two-dimensional stereographic projection ok. Let us go a little deeper and show how it is done. Say, for example, we have a 3 D stereogram which is like this I hope that this is visible and we have tried to make it as clear as possible by drawing it again. And that if we have a unit cell here a similar unit cell and that we have to define certain points in this 3 D stereographic projection or a 3 D stereogram and these points are say that B is the point of projection A is the point where the plane of projection lies and so here is the projector screen and A is the center of this projector screen.

If we have one great circle, say for example we have one great circle which is North N E which is East South and West and this great circle may form an important crystallographic plane. Say, for example, it forms from a certain important crystallographic plane say 1 0 0 or any HKL and therefore these this whole circle of the great circle can be projected if it is torched from here and each point of this great circle is projected can be projected in the 3 from this three-dimensional inner sphere to a two-dimensional circle like this. So, N becomes N dash and the great circle goes like this, and the E which is east becomes E dash and it goes like this and the S becomes S dash and then it goes and that west which is W become W dash and it goes like this. So, the great circle is projected on this two-dimensional screen which is known as the stereographic projection shows N dash E dash S dash W dash with respect to the N E S and W of a great circle from the 3 D stereogram.

On the other hand, there is another great circle right the great circle which consists of B E A, and W and it goes to B again. So, if this great circle is projected on the 2 D stereogram it becomes it seems that it becomes a line right. So, it lines where it projects the W to W dash E to E dash and the B and A at the same point here at A. So, the projection plane is basically a tangential surface over point A which is the A point an important point of a 3 D stereogram from this one can observe that there are great circles that could be projected either as a curve or as a line. Another example if I give is this great circle the great circle consisting of N A and it goes like this to say S and then it goes to B and then it goes again to N and this great circle not drawn fully could be projected as a vertical line on the 2 D stereographic projection making it the N becomes N dash A and B becomes B and the S becomes S dash and that it the great circle becomes a line. So that the poles and the great circles in the 3 D stereogram which is obtained from the unit cell which is kept at the origin at the center of this 3 D stereogram can be converted into a 2 D image which is basically known as an equiangular stereographic projection. This equiangular stereographic projection has all the information of the crystallographic planes and directions and angular relationships between them because they are true angular.

Now, if we keep a plane at a certain angle inside this 3 D stereogram and this is shown by this red inner plane and this plane basically I am talking about a crystallographic plane HKL plane being kept inside this 3 D stereogram. And if that a normal to the plane is protruding at the circumference of this 3 D stereogram somewhere at P and if B is the point of projection and then the ray of light comes and spots the P and its shadows at the position P dash on this 2 D stereographic projection. Therefore, any plane any pole on the stereographic on the 3 D stereogram can be represented in a 2 D stereographic projection. Here we have shown the same thing in a much simpler 2 D manner from the side; where this is the 2 D stereographic projection and it is shown by the line. Because we are showing it from the side and then that this is the plane we were talking about.

So, the perpendicular to the plane p is coming out from the circumference of the 3 D stereogram which is looking like a circle here, and then B which is the point of projection the light rays fall on this spot and then the shadow of the spot falls on the P dash right. The P dash is shown here in the large figure. So, this is the way a stereographic projection works.

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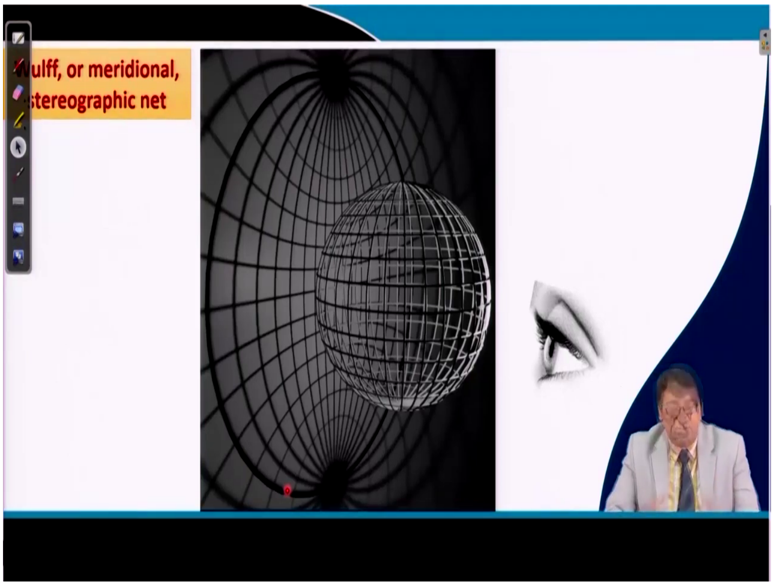

Now, a stereographic projection as I said consists of a 3 D stereogram something like that and I said that there are longitudinal lines and latitudinal lines. And the longitudinal lines in these stereographic projections are basically come from the top to bottom and they are all great circles it is given in a 3 D image. So, maybe it is easier for someone to visualize and difficult for somebody.

So, I will go through few slides regarding this and you will see that there are actually longitudinal lines and these lines are basically great circles 3 D stereogram. And if we are keeping the point of projection somewhere here then the ray of light will allow you to shadow these great circles and the spots on a screen and which will look something like this and so this is basically the 2-dimensional stereographic projection that we obtain.

So, in this figure what we have done is that we have given a great circle we have shown the great circle in terms of the longitudinal lines. Whereas, the latitudinal lines are being shown as small circles except for the one which is exactly at the center and if you have done a little bit of geometry during your schooling.

Then the equatorial line is the north pole and the south pole and the east and the west and therefore we can relate it to the geometrical stereographic projection that we have done to map the world on a sphere right. But just to let you remember that stereographic projections to map the world are basically equi-aerial stereographic projections and therefore, they are not equiangular. So, if you put equiangular then it will not remain equi-aerial and thereby depending upon it is position means a position of a country on the sphere and the point from where we are projecting it a country may look bigger or smaller and which may not mean it will not look equivalent to the area of the country. Maybe a large country with a larger area may look smaller and a country with a smaller area may look larger. So it is very the stereographic projection equi-aerial stereographic projection that we usually do in geography is quite difficult to understand sometimes. But the equiangular stereographic projection actually occurs means actually the calculation is done using the ray of light which is quite simple. So, this stereographic projection that we are going we are doing here is quite simple and it follows the ray of light. Now, that the latitudinal lines except the equatorial line this equatorial line see I have started showing it on the 2 D stereographic projection because it is much easier to observe it on the 2 D instead of the 3 D which is here this equatorial line is basically the great circle all the other latitudinal lines shows the small circles right.

On the other hand, all the longitudinal lines show the great circle. And this kind of projection of longitudinal lines and latitudinal lines is basically known as Wulff net or meridional stereographic net and these are used to understand or calculate angular relationships in the stereographic projection.

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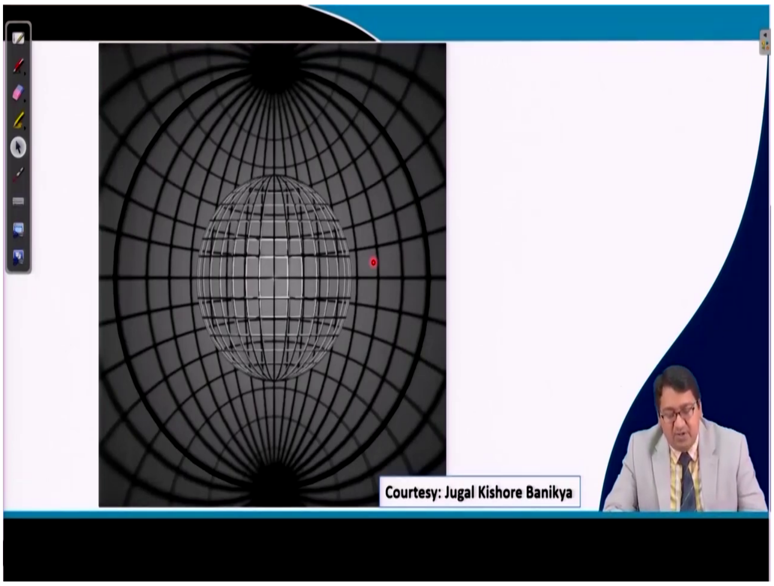

Here is another view of the stereographic projection from the direction of the point of projection and one can see that this stereographic projection how nicely divides the angular areas from the top to bottom into longitudinal and latitudinal lines. So, this is from this is drawn by my student Jugal Kishore Banikya.

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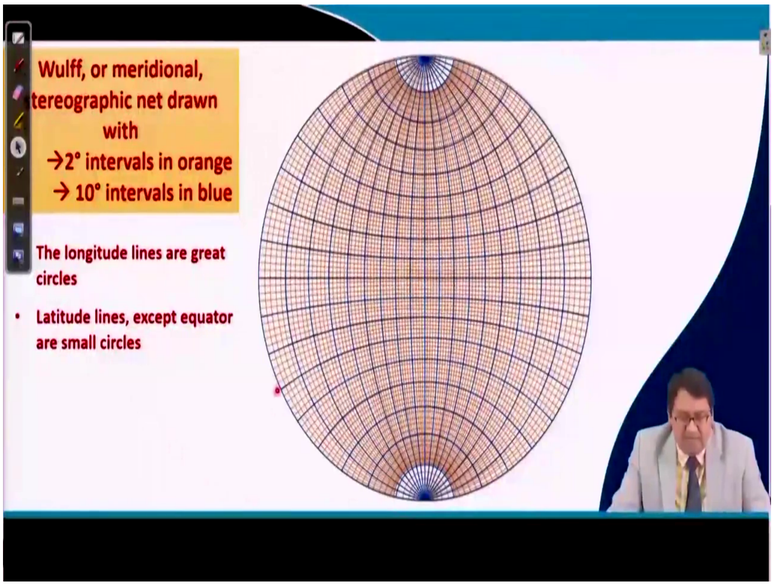

So basically a Wulff net which is basically cooler to observe and quantify the stereographic projection is shown the orange-colored Wulff net has basically degree graduation of 2 degrees and the blue colored Wulff net has a graduation of 10 degrees.

So, one can map the angles between planes and directions and everything with respect to this Wulff net, and as I said earlier in the slide that longitudinal lines that is this these lines are always a great circle. Whereas, latitudinal lines except the equator is always are always small circles.

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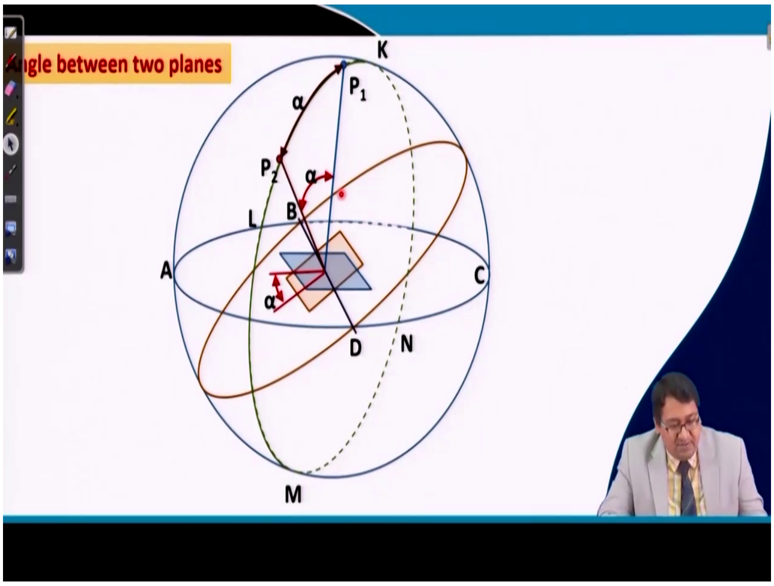

So, for example 2 planes are present in a crystal and we need to measure the angle between these 2 planes. Now if we project this the brown color plane it will project out to the circumference of the 3 D stereogram like this and it will form a great circle. On the other hand, if we take this blue colors plane and it will protrude outside to the circumference and become another great circle and this will happen only if both the planes are passing through the origin and therefore that you if we need to find out the angle between these 2 planes we have to see that both the planes have to pass through the center of the 3 D stereogram. If we draw a perpendicular to the brown-colored plane and it will protrude and come out at P 2 and if we draw another perpendicular direction to the blue-colored plane it will protrude to another direction say P1. So, we obtain P1 and P 2 2 positions on the circumference of the 3 D stereogram.

Now, if both of these planes are passing through the center of the sphere, and then if we connect P 1 and P 2 and we if we expand this the expand this over the circumference of the sphere it will form another great circle. And because it forms another great circle then if we the angle between P 1 and P 2 could be obtained from the angular deviation because this is this 3 D stereogram has an equiangular division right. So, the angle between the 2 planes alpha can be obtained from the 3 D stereogram from the angle between 2 directions P 1 and P 2. But that is the 3 how difficult it becomes to find out the angle between P 1 and P 2. But if we have a 2 D stereographic projection from this 3 D stereogram and if we could superimpose the Wulff net over it like this.

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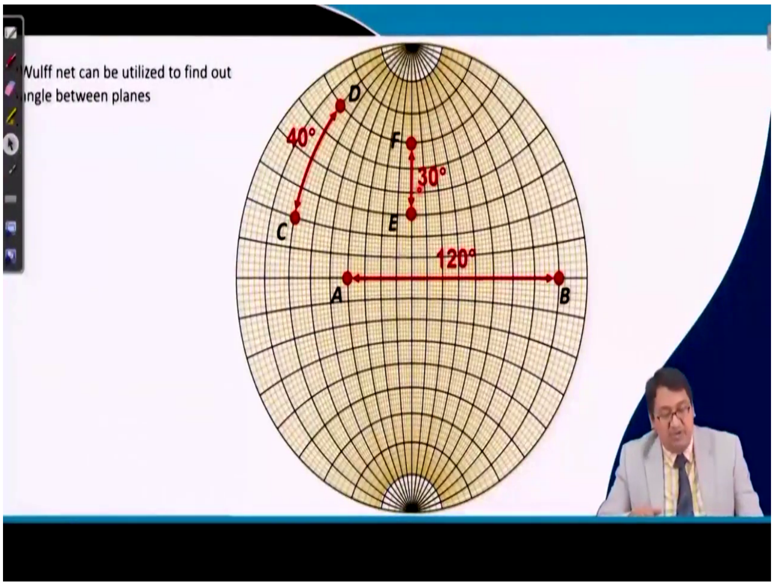

We can utilize this Wulff net to find the angular deviation between the 2 planes right. Say, for example, if you have 2 planes that are something like this then we can find out the angular deviation between the 2 planes which is by calculating as I said that the larger ones have 10-degree graduation. So, 10 20 30 40 50 60 70 80 90 100 110 120. So, the angle between the 2 planes can be obtained from the Wulff net to be 120. But to let this that we can obtain the angle between the 2 planes only, if if you can superimpose their poles over the great circle if the poles are superimposed on the small circle then the angle measurement may not be correct.

Therefore, when we obtain this Wulff net and we showed angles between various planes like for example, planes C and D. And we have always tried to superimpose the poles of these planes on the great on a single great circle so that we can measure the angle correctly. For example, the angle between C and D which is being superimposed on a single great circle this one and is 10 20 30, and 40 the angle between 2 planes E and F or 2 planes whose perpendicular directions R E and F or the poles are E N F is again 10 20 and 30. Here also we have superimposed the 2 planes on the great circle therefore, in order to measure the angle between 2 planes we have to keep the poles of the 2 planes on the great circle of a great circle of the 2 D stereographic projection.

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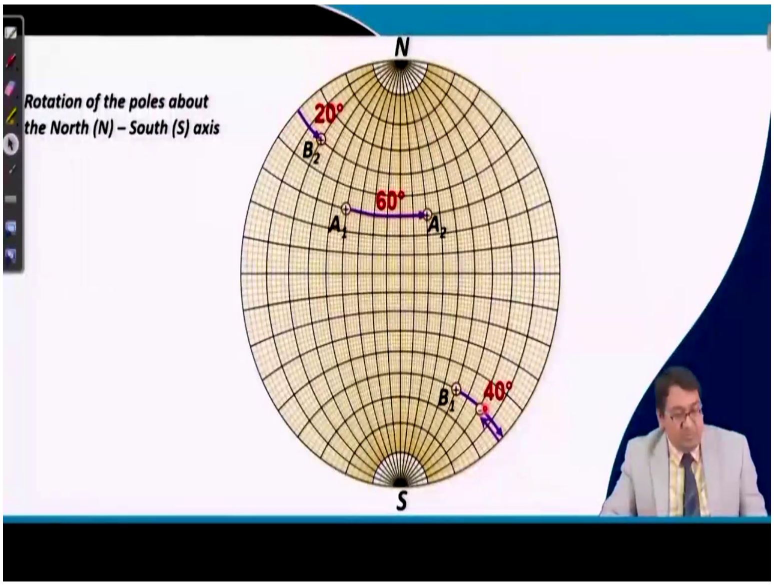

Moreover, we can also observe that how the angle or the positions of the poles of different planes may vary if the stereographic projection is rotated. that lets us rotate the north and the south poles N and the S poles. And we should try to imagine that this is like a circle right sorry like a sphere right projected on a 2 D plane and therefore it becomes a circle right. So, if we rotate this stereographic projection on the North and the South plane thinking that it is a sphere then what will happen if there are 2 planes A1 and B1 and if I am saying that I am rotating these 2 planes along the N S direction by 60 degrees. So, A 1 goes to A 2, and therefore, we have to go 10 20 30 40 50 and 60. So, A 1 goes to A2 and therefore the rotation is 60 degrees.

Now, the B 1 which is with respect to the A 1 is present here and I have shown it by the plus sign because the poles are protruding outside right. Now if that is with respect to A 1 the B 1 is rotated. So, the B 1 will rotate 10 degrees 20 degrees 30 degrees 40 degrees, and then when it will rotate and it will come out here in the opposite direction 50 degrees and 60 degrees. So, the position of B 1 now changed from here to here right, because now we are seeing the opposite direction of the sphere.

On the other hand, if we could protrude the opposite pole of B 2 it will be protruded directly here exactly opposite of it because it will pass through the center of the sphere and will protrude out somewhere here. So, I have shown it by the minus sign.

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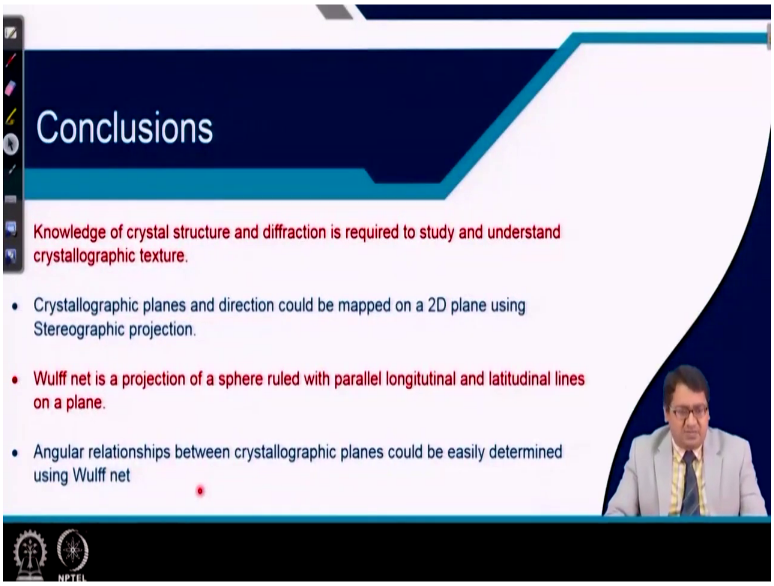

So, in this lecture we found out that the knowledge of crystal structure and diffraction is essential to study and understand the crystallographic texture. The crystallographic planes and directions could be mapped into a 2 D or the two dimensional plane using the method stereographic projection. Wulff net is a projection of the sphere ruled by parallel longitudinal and latitudinal lines on a two dimensional plane. Angular relationship between crystallographic planes and directions actually could be easily determined using stereographic projection and Wulff net.

Thank you.