Principles of Physical Metallurgy

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Lecture No. # 04

Atomic Bond and Crystal Structure (Contd.)

Good morning, we start with the fourth lecture on the subject an physical metallurgy, and we continue with the first chapter that is an atomic bond and crystal structure. And in the last class, we talked about point lattice, which is used to represent crystal structure in an material, we looked at atomic arrangement in a few simple crystal structures that we find in metal namely, face centered cubic, body centered cubic and hexagonal close packed structure. We also looked at the packing density, the relationship between the atomic diameter and the lattice parameter, and also introduce the concept of miller indices to represent planes and directions in a crystal.

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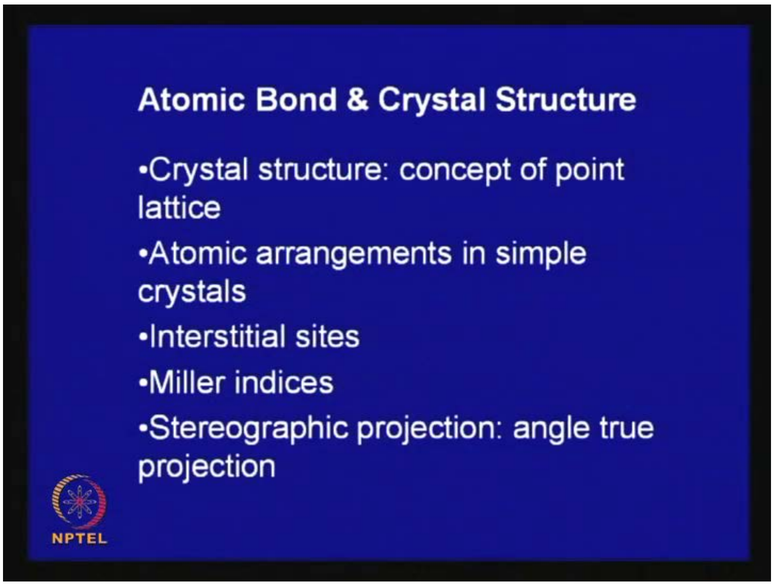

And the end we talked about stereographic projection which is an angle to projection, and this is very frequently used to solve problems and crystal crystallography. Now today, we shall look at particularly stereographic projection in great detail.

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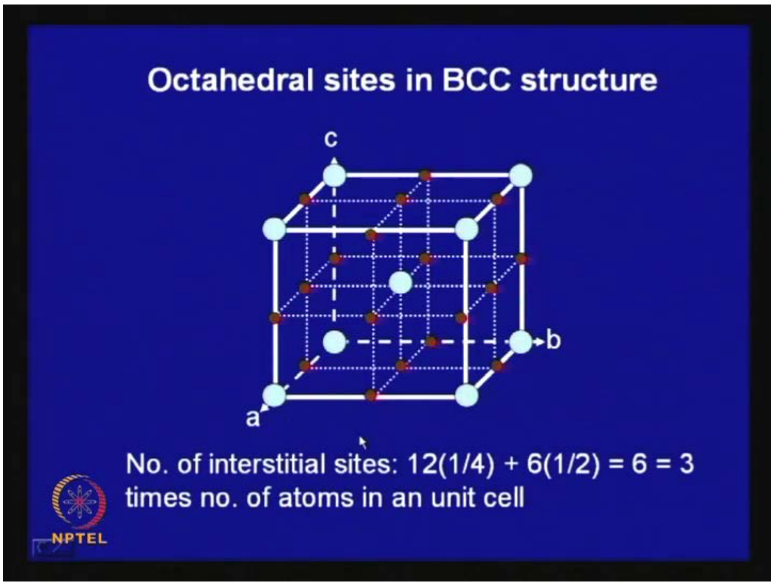

And to recapitulate, look at this octahedral sites we talked about in the last class; this is a body centered cubic structure. The main atoms, they are located at the corner of the cube, and the interstitial sites are the age center and face center. We calculated the number of interstitial site in an unit cell, and here you will clearly see that number of interstitial sites, how to calculate that is given here each of these age center is shared by 4 unit cell, which are placed around this edge.

So, therefore, contribution of edge centered atom will be 12 times one-fourth, and then we also have face centered and this is shared by two neighboring unit's cell, the contribution of each towards the unit cell is half. So, therefore, if you add these up, it comes out to be 6. So that means, there are 6 interstitial sites of octahedral type in a unit cell, and this incidentally happens to be three times the number of atoms in a BCC lattice. Similarly, we looked at tetrahedral sites; tetrahedral sites have made up of four triangular faces; now this each of these triangle is an isosceles triangle, two edges are equal to half the diagonal say like this and this, and the other edge is equal to the edge of the cube that is lattice parameter a. So, this is a, this will be root 3 a over 2.

And here also you can calculate the number of interstitial site, which is given here, here all the four sites in a face, we know they are they will belong to 2 unit cell; one this, one top of this; and there are 6 faces, so total number of site is 4 times 6 that is 24, and each face being shared by 2 unit cell, the net contribution comes out to be 4 into 6 times half.

So, this comes out to be 12. So, therefore, it is 6 times the number of atom in a unit cell. And last time, you also calculated the packing density; so this packing density, you know it is the gaps are divided in to octahedral and tetrahedral sites. So, here you have more number of sites so obviously, this is going to be smaller than octahedral sites.

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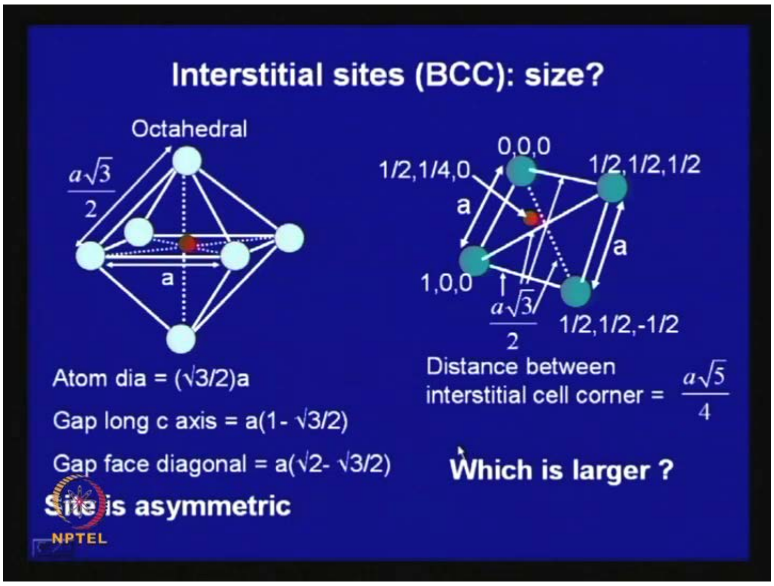

And here is a method, which is illustrated in to calculate the gap or dimension of the interstitial site; octahedral site is much easier to visualize. These are the 4 corner atom on the face; and this is the face centre, which is an octahedral site in a BCC structure, and you have it isosceles triangles basically. So, this is dimension a, and this dimension is half of the diagonal. So, you have eight faces surrounding this interstitial site. And the atomic diameter we estimated last time, this is equal to root 3 a by 2. So, once you know this, then it is possible to calculate the this gap.

Now this distance between this atom and this atom is equal to a and therefore, the gap along C axis will be this distance a minus this atomic diameter, because half of this atom and half of this atom had to get that one atom. So, one atomic diameter, you subtract, you get the gap along C axis. But in this if you calculate the gap along the diagonal in the same way, the diagonal is this is a, this is a, so the diagonal is a root two; so if the gap in the face diagonal therefore, will be a times root 2 minus 3 by root 3 by 2 and obviously, this is larger than this.

So, therefore, what it says that this site is asymmetric, if you try to put an atom, it will get these two will get this place more than these two. In the same way, it is possible to calculate the interstitial sites dimension in case of tetrahedral site, which is shown here. It is possible to find out the coordinates of each of the corner atoms basically, you have one corner atom here, one corner atom, and this distance is a similarly, you have one face centered atom, another face center atom. So, this coordinate if you say 0 0 0 this coordinate is half half half, and these diagonal, this is half the face diagonal, which is equal to a root 3 over 2.

So, therefore, the distance between any of this any of this corner point with this interstitial site, it is possible to find out from geometrical relationship say if. So, this is the coordinate half 1 4 0 is the coordinate of the this site, and if you try to find out distance between this coordinate and this, it will clearly come out to be a root 5 over 4.

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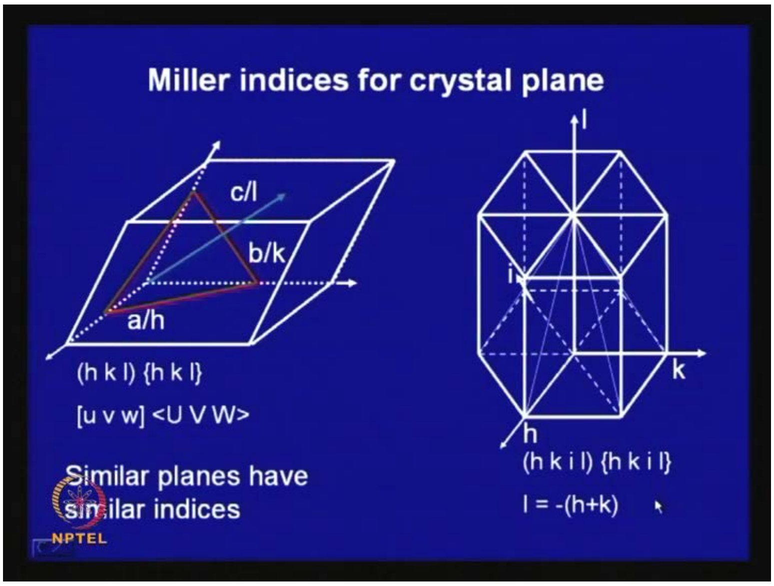

We also looked at miller indices of for crystal plane, say these are the crystal axis a b c, and if you represent an atom in terms of this fractional indices or intercepts, like this is the plane which intercepts a axis at 1 over edge, b axis one over k, c axis at one over l, then indices of this plane we call it, we defined it as h k l, which is the reciprocal of these intercepts. And we represent this particular plane as h k l, but in the crystal because of symmetric, there will be several planes, which may have, may be similar having h k l indices the atomic arrangement to similar, and this set of search planes are represented by this curl bracket. And the same way it is possible to represent the directions directions, a particularly this is a crystallographic direction which we represent simply by these coordinates in terms of this crystallographic axis. So, you move if this coordinate is u v w that means, you move u distance along a axis, v distance along b axis, and w distance along c axis.

And here also similar directions if you want to represent, we represent it in terms of this angular brackets. And always in a crystallography type of system that we use all similar planes have similar indices. Now in case of a hexagonal crystal, these are the crystal axis h k l; and here also you can apply this same concept, but here last time it was shown that say this particular plane, this is a prism plane.

Now, this prism plane its indices 1 0 0 miller indices, where as if we take this particular plane, this is also exactly similar plane, this also should have same indices and this in fact, it is as 0 1 0. But if you look at this particular plane, say this particular plane, which intersects h at 1, k at minus 1, so this is actually 1 minus 1 0. So, this and this although they are same indices are different that is why in the case we make k 3 is a slight difference, we say that we use four indices, this is call indices h k i l, i is actually redundant, and that this i is equal to minus h plus k. And a system of plane is represented like this.

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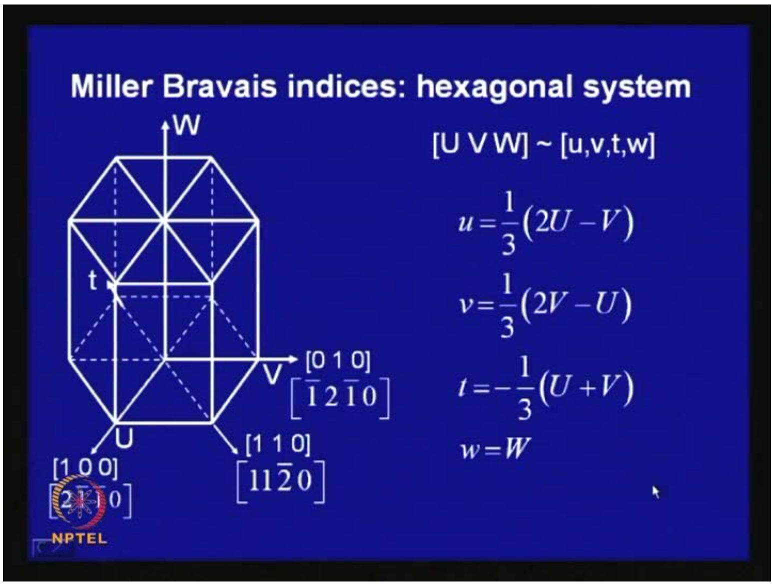

Same thing, you can extend it to direction as well. Now here it is little quickly; so, which is shown over here, because all these directions say suppose if you followed that earlier convention, then this direction should have been this direction should have been 1 1 0, but crystalographically this direction and this direction they are same. So, here also, we use four indices system u v t w, the t is as such redundant, this is equal to minus one-third of u plus v; this capital u v w is the normal miller indices, and smaller u v w is the Miller Bravais system.

So, with this set of conversion, it is possible to show that all these equivalent directions will have identical or similar indices. A later on, we will see that this type of representation allows us to do lot of matrix calculations or vector calculation or if this will help you to geometrically to represent crystal planes and directions in a projection. Now then we looked at the concept of stereographic projection; say normal engineering projection the distance the relationship between the distances are maintained. If you take a projection as an engineering projection of a 3D object, the distance between two point even if it is scale down, it maintains a definite relationship even on the projection; whereas in case of a stereographic projection, it is no longer a distance to projection, it is an angle to projection.

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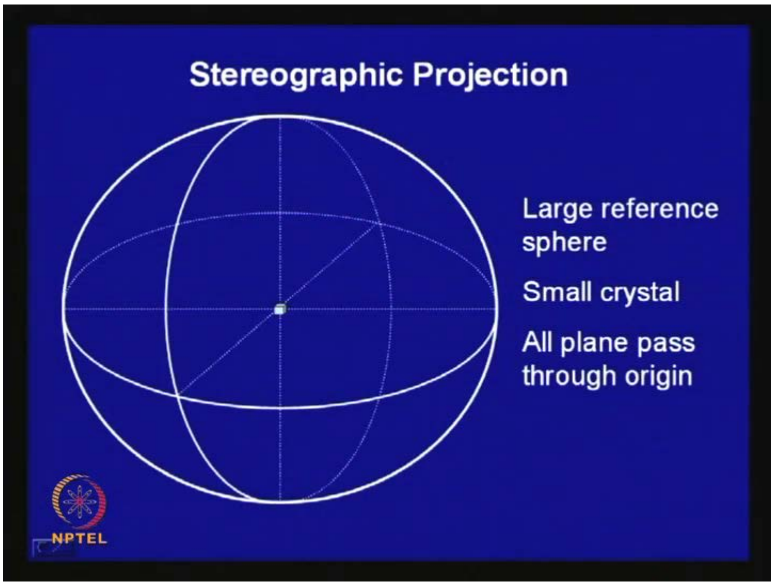

And the concept of this projection is illustrated here, you imagine the crystal to be very small, and it is place in a three in in a in at the centre of a hemisphere like this, and the size of the crystal is so small in comparison to this sphere. That is any plane that you draw here, even on the top surface or bottom surface, they all will coincide, they will pass through the centre of this sphere, and this will intersect the reference sphere along these great circles. So, this is one plane, this is another vertical plane, so we call, so therefore, the list of assumptions is here, the reference sphere dimension is very large, crystal is very small. So, that all plane pass through the origin.

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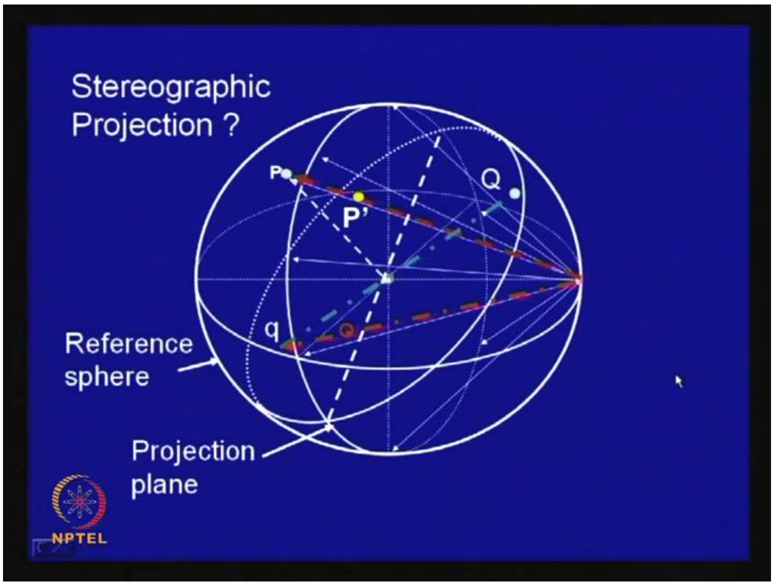

Now, what is the stereographic projection? We try to illustrate this here, say suppose here we have placed this crystal; now imagine and here this is the reference sphere. Now drawn a plane and the crystal extend it to meet the reference sphere, it meets the reference sphere along this great circle. So, radius of this circle and the radius of the reference sphere, they are seen. Now, there a perpendicular to this; it an extend it, to meet the reference sphere, it meets that point P.

Now, let us try to project this point P on to this projection plane, projection plane is this circle is the projection plane by placing a light source here. Imagine that this pole is marked by a dark color say, black this is a transparence sphere, this is a black dot over here, and put a flash bulb over here. And try and find out the line joining this and this; where does it intersect the projection plane? This is the projection plane, and this is the line joining this and this particular point, and this is where it intersects the projection plane, we call this the stereographic projection of point P.

And this plane also intersects the projection plane at these two points; and later on, we will see that trace of this line, this great circle will also be projected on the projection plane as a great circle. Now the problem comes that if we take a projection like this, we can project all the point in the part of the hemisphere, which is away from the source of light, what happens to the points up to the poles, which appear in the hemisphere, which contains the light source? Suppose, this example is taken here, how do you represent the point Q. What we do? We draw a line join this point Q with the centre extend it to meet the other half of the reference sphere. So, this is the diametrically opposite point of this; and we say thus this is small Q. And project this on to the projection plane, and represent it by an open circle, not a filed in circle. So, which signifies this is a point on the semi sphere.

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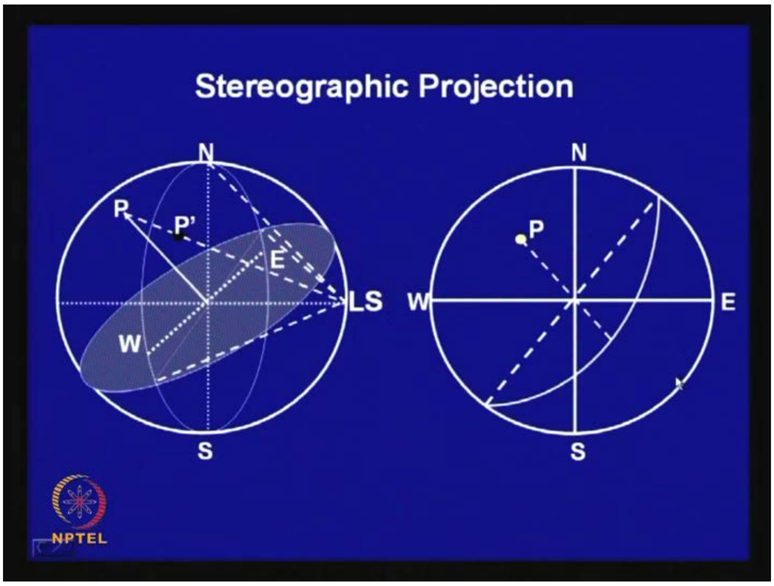

Now, we look at the same thing say, so far our try to explain you with respect to other three dimensional object. Now what happens if we do the same thing on a 2D or represent in a two dimension, this is the projection plane. Now here, this is the plane, which was drawn, this is the perpendicular and this is the projection here. So, this is still now here also this is the three dimension representation, we convert it into two dimension, then it will look like this. This is point east, this is point west; so this is getting projected and east and west, these are the two points this point P it comes here; that means, this pole is represented by its projection in a 2D like this. And this great circle, this great circle is represented here as a plane; and we will see later the distance the angular, this is an angle to projection and P is normal to this plane; so this angular relationship must be maintained. So here, we will see that the distance angular distance between this and discrete circle this will be 90 degree.

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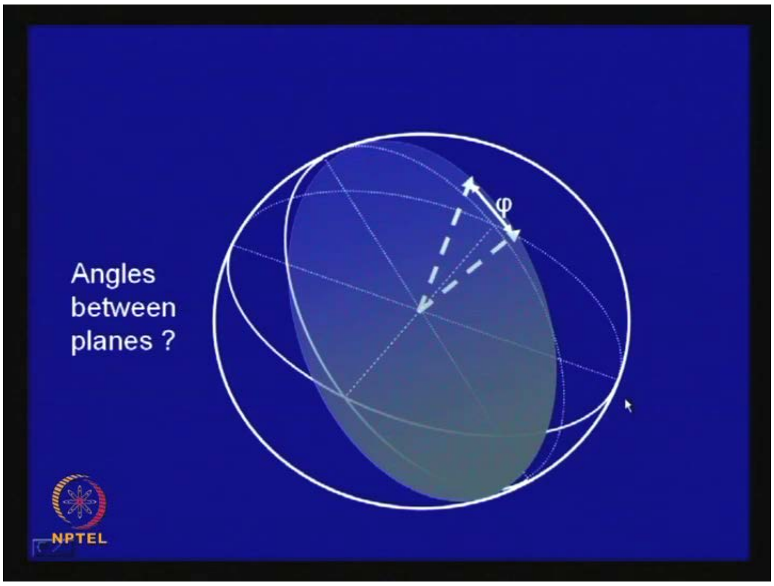

Now, let us see how you represent angles between planes? This is illustrated here; and here also we use the reference sphere so that means, in this drawing, I am trying to still represent it in terms of a 3D diagram. So, take this is a plane draw a normal to the plane, which intersects the reference sphere at this point. Draw another plane this is the other plane, draw the perpendicular to this plane passing through the origin. So, this is the other plane; and this two plane the intersect along this line, which is shown here. Now to measure this angle, how do you measure this angle? You have to visualize a plane passing through these two lines, which is shown here. And then on that plane therefore, you can put a protector and measure the angle.

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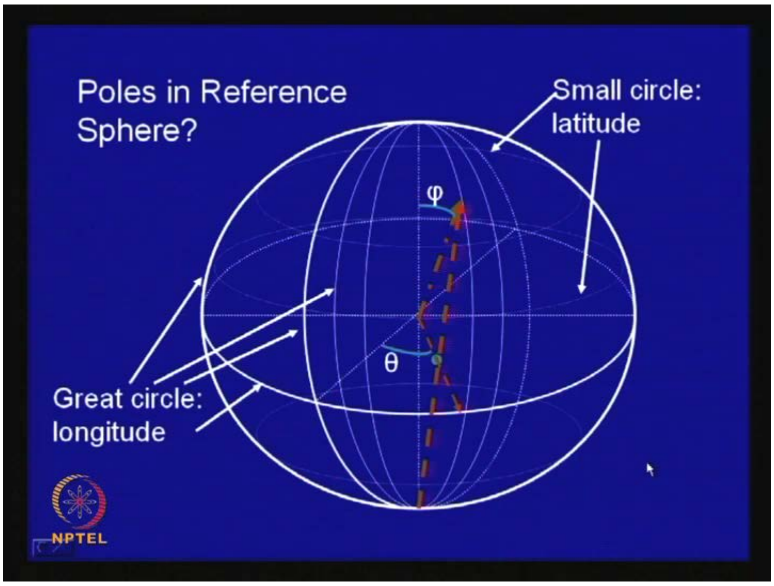

So, this is the basic principle of measuring angle in a on a three dimension reference here. Now, poles in a reference sphere; now in this reference sphere, we draw certain reference lines or planes. So now, this particular plane, this is the great circles, we also use a set of small circles, which are drawn like this; so they are called latitudes and these are great circles. And we can draw similar great circles at regular interval; these are all great circles. Now we represent any angle or any angular position of any pole on this sphere, in terms of this angular coordinates. Suppose we want to represent this point here, we will represent it by two angles; say one angle say joining this pole other this perpendicular line that angle it sustains with this reference lines. So, this angle is 5, which is measured along this great circle; another angle is theta say, we take say this is the line here, this great circle it meets here; and we say this angle is theta. So, by these two coordinates, theta and phi, we represent a point on the glow. So, this is very much similar to geographical glow, where we have a set of lines say, longitudes they are great circles and the latitudes are the small circles.

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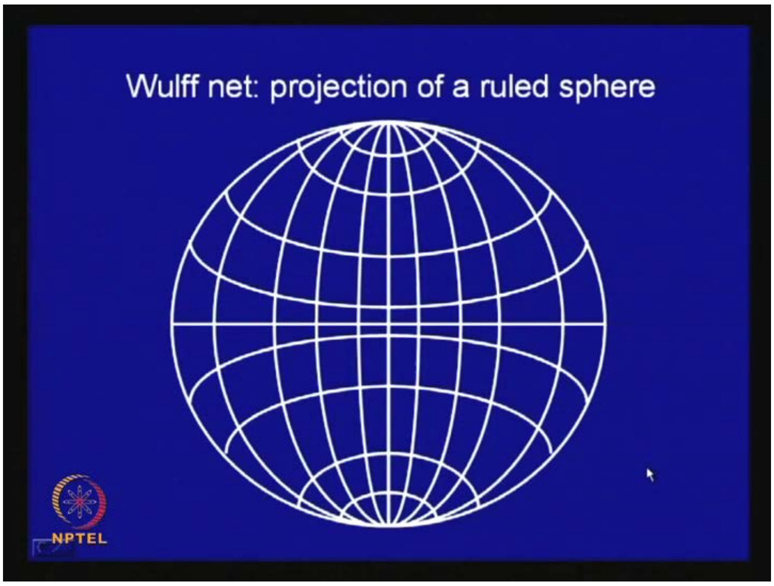

If it takes a projection of that kind of a ruled glow, we get a net called Wulff net and this helps us to measure angles on the stereographic projections. Now here these great circles, they are the longitudes, and these are the projections of the small circles called latitudes. Now in Wulff net, these lines are drawn at a regular angular interval and usually for most calculation we use Wulff net, where these lines are drawn at an interval of 2 degrees.

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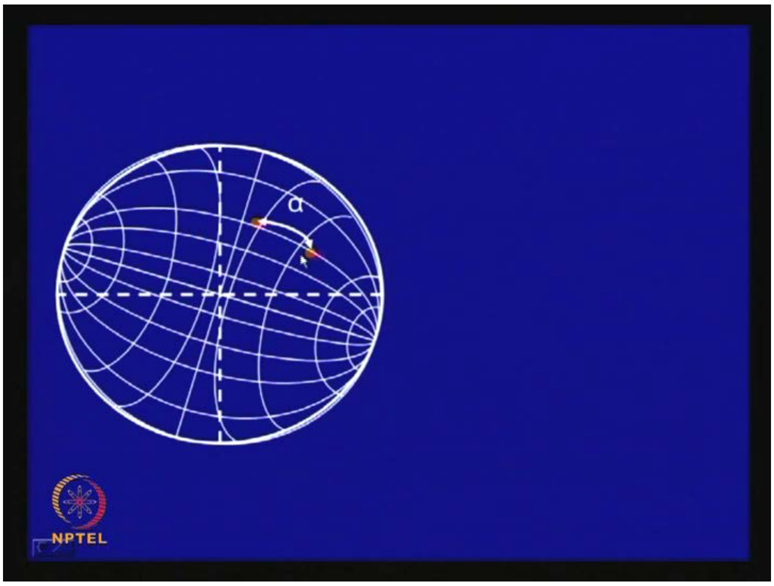

Now, I will try to show you an illustration. So, suppose this is the 2 D projection stereographic projection, now here are two poles, two crystallographic directions how do you measure this angle using Wulff net? Now, place it over the Wulff net, now here to measure an angle both these pole must lie on one plane, and here it is not and here one plane in a Wulff net is represented by this longitude. So, they are not lying on any longitude.

So, therefore, you cannot it is difficult to measure this projection, what we do we try and rotate this and by rotating, we try to bring it in a such a position that these two points the lie on one longitude as shown over here. And this longitude is graduated at regular interval look at the coordinates that latitude over here, latitude over here, and read the difference. So, therefore this angular graduation, red along this longitude is the angle between the two pole. Now, we very often use standard projection of certain crystals, we will mostly concentrate on cubic crystal and let as try an understand, how do we construct standard projection of a cubic crystal.

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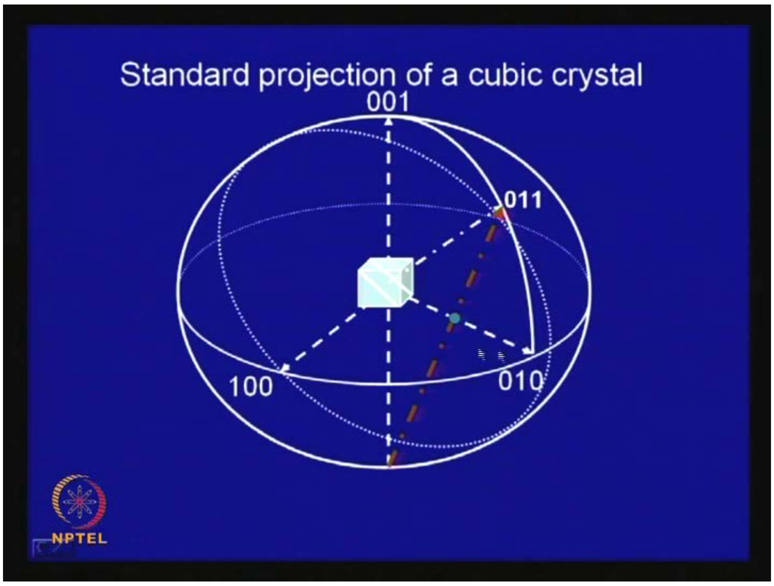

This is illustrated here, imagine say this is a reference sphere, place a crystal at the centre; the crystal is very small with respect to the reference sphere; these are the crystallographic axis, and we will try to construct o o 1 standard projections. Now, if you extend this cube planes, they will intersect this plane here, here, and the other one will intersect this plane great circle at this point. So, these are the three poles. Now, let us try to construct the projection of this particular plane in the crystal. What is the indices of this plane? This plane is joining two opposite ages, so that means and it is it contains the face diagonal. So, therefore the indices of this plane is 011, we extant this plane. So, this is the plane then we construct the normal to this and extend did to intersect the reference sphere it intersect sphere, an also it intersects this is it is half way between this pole and this pole on this great circle, this is 011.

Now, project it we look at it from this particular point just opposite diametrically opposite to 001, to get a 001 standard projection we must look at 001 from its diametrically opposite point. And try to project it on this projection plane, and this is what is done over here then it projects at this particular point which is half way angular distance wise half way between this point and this point.

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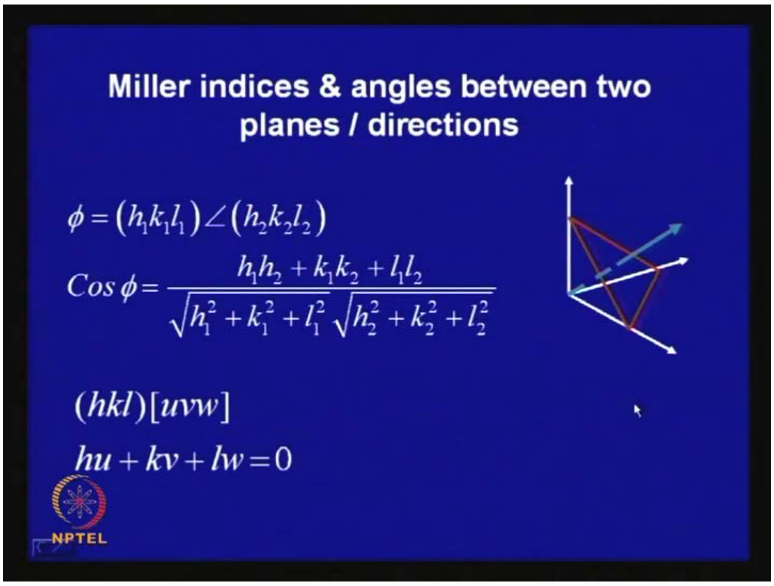

Now to draw this type of projection we often use angular relationship between different crystallographic planes. For example, one plane has an indices h 1 k 1 l 1 - this is the miller indices, and this is the another plane has h 2 k 2 l 2 are geometrically it can be shown that angle between the two is given by this relationship cos phi can be determine, if the indices of the plane unknown. And it is also possible to show that in cubic crystal where this axis there orthogonal. So, any crystal system where the axes are orthogonal, if a plane is like this, if a plane is like this; an indices h k l and normal to this plane is drawn here, normal to this plane is u v w, the angle between this plane h k l and its normal u v w is 90 degree. So, therefore, so in place of h 2 k 2 l 2, if you substitute u v w you get this relationship, if h u plus k v plus l w equal to 0.

So, this relationship will be valid; for example, the plane 111 in a cubic crystal and the pole are perpendicular direction which is represented that also by 111 angle between these two will be 90 degree, and this relationship is very frequently use to construct as standard projection.

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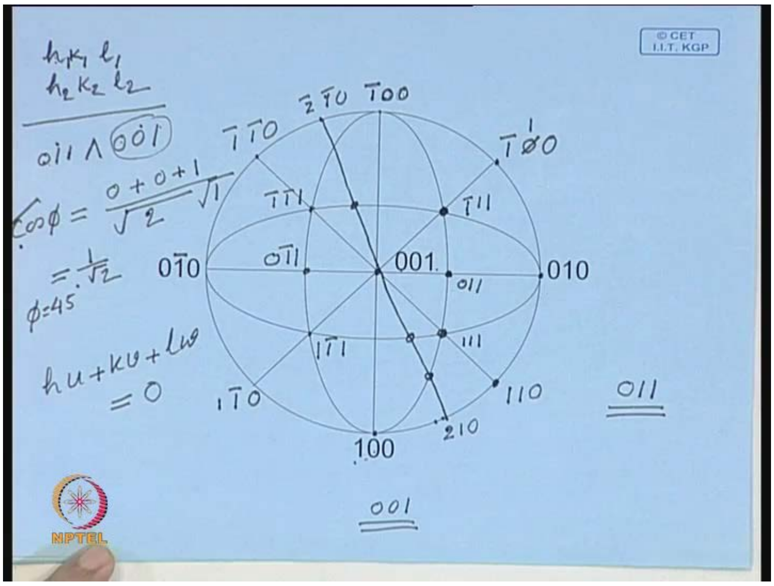

Let us try to construct the standard projection of a cubic crystal on the projection plane 001. Now, obviously projection plane 001. So, centre of this is 001 and on and this is the pole 001 and this is plane 001. And the pole 100, 110 will be located here, and the pole 010 will be located here. And it is best illustrated by let us try to do this exercise on paper, now here this is pole 001 which is represented by this point, this is 100 which is represented by this point, this is 010 is represented by this point. Now, the opposite of this the point diametrically opposite of this is this. So, indices of this will be minus 100 we call it bar 100 like this it will be 0 bar 1 0, and we have shown little while ago on the reference sphere how to locate the pole 011. So, 011 will be located between these 2 pole on this equator, this is 011. Now, here if we recollect the relationship between two planes of indices h 1 k 1 l 1 and h 2 k 2 l 2, we try and find out the angle between 011 an angle 001.

So, this is equal to is given by cos phi equal to the product of 0 times 0. So, this is 0 product this times this that is 0 plus this times this that is one, and then it is root over h1 square plus t 1 square plus l 1 square. So, which is root two and in this case particularly it is root one. So, therefore this equal to one over root two, so that means, phi is 45. So, likewise it is possible to index all these, this is also the angle 45 and its indices is 110 opposite of this is 1 bar 1 bar 0, this point is 1 bar 00.

Now, it is quite simple if we represent recollect this zone relationship, that is h u plus k v plus l w equal to 0, in that case it is possible to show that if you add this and this you get 110. So, that also we lie that indices will lie on this particular plane; it may not give you the exact where, but sum where in between these two. And then we can find out the angle between this, and this which also can be shown in the same way to be 45, so this is here like this. Similarly, what is the index of this is 1 1 bar 0 which is I think this is one bar is a mistake a 1 bar 1 0. So, it is diametrically opposite to this is 1 bar 1 0, this is 1 1 bar 0. Now, what is the index of this how do we find out, now here if we add this and this what do we get? We get one bar 1 1, so that means, 1 bar 1 1 lies on this great circle.

Similarly, if we add this and this we came get 1 bar 1 1, so that means, this lies on discrete circle. So, therefore, the point of intersection is 1 bar 1 1, and the same way you can show that this also you get by adding this and this you get 1 1 1, similarly adding this and this also you get 1 1 1, so index of this is 1 1 1. And then what is this? This is 1 bar 1 bar 1, this is 0 1 bar 1, this is 1 1 bar 1. So, we have index to always.

So, now it is also possible to index the other directions as well. So, for example, you take somewhere in between the two, in between the two you will get a pole, so if we add this and this, you get 2 1 0 - 2 1 0 will be half way somewhere between the two, you can find out the angle using this type of that angular relationship that cos phi. So, it will (( )) some particular angle with this another angle with is similarly opposite of that will be 2 bar 1 bar 0, you join this and this. So, basically you join this line you get this, and then you try and find out what are the indices of this. So, this is how it is possible to construct is standard 0 0 1 projection.

Now, if you want to convert it to any other projection like, let us see we want 0 1 1 projection, then how will you do it you can this can done by rotating this projections; and rotation this projection is possible with the help of Wulff net, and I will leave it to you as an exercise.

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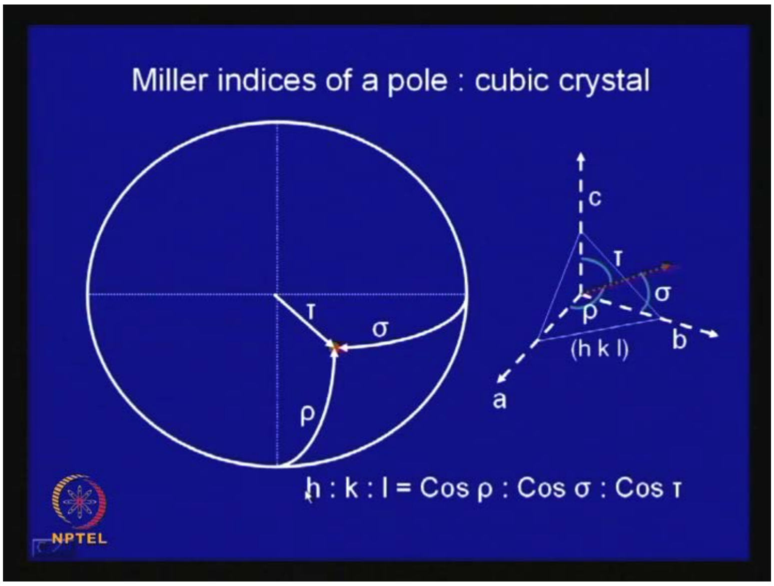

Now often you may have to represent miller indices of a pole in a cubic crystal or a standard projection say suppose this is a standard projection how do you locate a particular pole which substains a set of specific angles. Say suppose, we consider this plane yeah, this plane an indices h k l; the normal to this plane is this. Now we want to represent this pole over here.

Now look at are measure the angle, this angle is rho, this angle is sigma, this angle is tau, and now particularly look at this angle tau, this direction h k l sub that pole h k l substains angle tau with respect to this axis c. So that is this axis c is 0 0 1; 0 0 1 is located here. So, along the great circle or long equated here, you can measure this angle top locate this point, and then you locate this angle sigma along this great circle and rho along this great circle, and this can be done by vice versa. So, suppose here is a pole can find out these three angle and you can convert it take cos rho I make it by cos rho cos sigma cos tau will be proportion two h k l.

So, basically if you can magnitude of cos of any angle is a fraction. So, if you can with a suitable multiplier make it in integer, then h k l will be the indices of the plane. So, with is we finish this chapter an atomic bond and crystal structure some of these exercises that I have given, it will be worthwhile for you to pursue that I think the concept of stereographic projection little abstract, and you have to go through some exercises say suppose over here, we try to find out say we have first round is standard 001 projection which was shown here.

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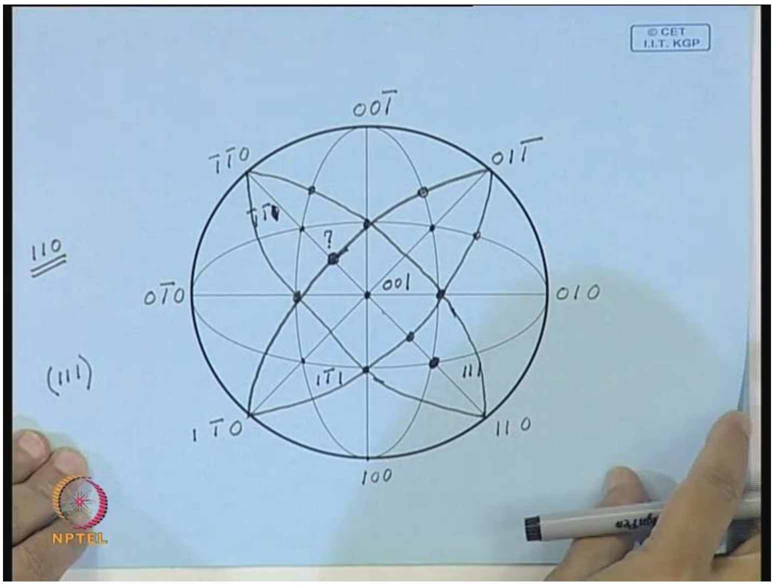

Now, using this say suppose we said that this is 001, this is 100, this is 010, this is 110, this is 1 bar 1 bar 0, this is 0 1 bar 0, this is 001 bar, and this is 011 bar. So, this is 1 1 bar 0, this is bar 1 bar 1 0, this is 1 1 bar 1, this is 111. Now, let us try to find out say suppose the plane 1 1 1. So, reach of these directions say try to find out the directions type of 110 directions, which lie on plane 111 now here this is the pole; pole of 111 an this try and construct the plane 111; plane 111 will be represented by a great circle, and that will be at 90 degree from this.

So, along this diameter using Wulff net try to locate a point which is 90 degree, and try to construct a great circle which passes through this point. And then you try and find out what is the indices of this, same thing can be done with respect to this 1 bar 1 bar 1 pole. So, corresponding to that there will be a plane like this what is the indices of this? Say construct a plane, construct try to find out indices of each of these points of intersections.

So, with is we end this topic on atomic bond and crystal structure, and form time to time we will be subsequently lectures will be referring to these parts in detail, and if you go through this example this will help you to understand subsequent lectures. You sum up we covered that atomic structures how that atomic structures and atomic bond (( )) properties of engineering materials. So, what is the difference between metallic bond and covalent bond, why metallic bond exhibit good conductivity. Now, in metals what type of crystals are, there are three types of crystal primarily face centered cubic, body centered cubic and hexagonal close fact.

We looked at some of the characteristics of this crystal structures, we learnt how to represent different planes and directions in a crystal using concept of miller indices; miller indices in case of hexagonal close packed structure has little problem. If we follow the conventional miller indices, we often do not come across similar indices for similar types of plane. So, therefore, here we had to introduce the concept of Miller Bravise indices using four indices, but you do not need four indices to represent three-dimensional structures. So, one of these is redundant. So, it follows the definite relationship with the other two, and then we looked at standard projections, we looked at 001 standard projections, but it will be worthwhile to construct few other standard projections using Wulff net or using the angular relationship which add given you.

And if you try and do find out what will be standard projection how will the standard projection 011 look like, all a standard projection 111 look like. And this standard projections looking at the standard projection it is also possible to determine the (( )). So, may be if you look at you will find out say in this particular case, say this particular cube axis, you know if you rotate you have one point here, one point here. So that means, if you give way ninety degree rotation it comes to occupies similar projection.

So, this axis is actually if four pole symmetric, similarly try to find out what type of symmetry element is represented by 110; similarly what type of symmetry elements is represented by 111. And try to be convince using standard projections that this exhibits 111 exhibits a three pole symmetry, where as this exhibits the two pole symmetry with this we end this chapter. And we will next chapter we will look at some of the tools and techniques which we use in principle in physical metallurgy to find out structure property correlations, thank you.