

Principle of Physical Metallurgy

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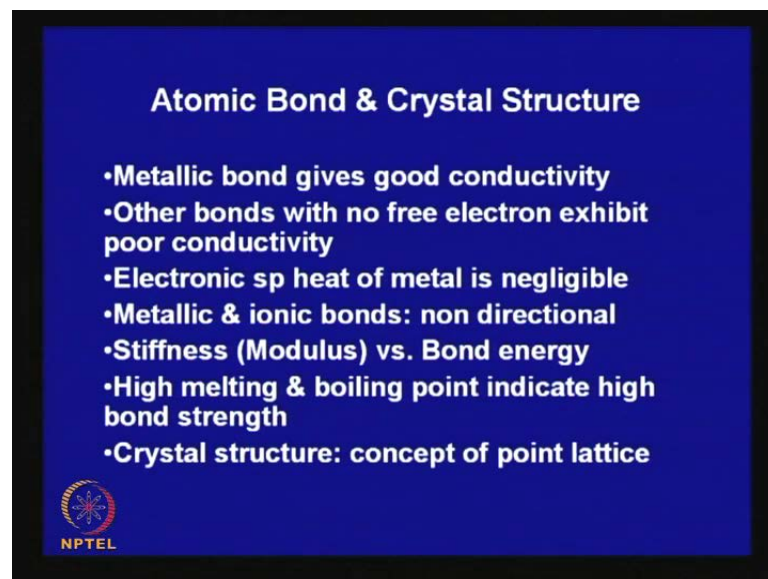
Lecture No. # 03

Atomic Bond and Crystal Structure (contd.)

Good morning. I think, we will continue with lecture on first chapter; that is atomic bond and crystal structure. We have talked so far, about different types of bonds which are there in material. And amongst them, we looked at metallic bond a little more in detail. Metallic bond as has been told, it has free electrons, which are shared by all atoms and that is why it has certain specific properties. And we also looked that how these properties are affected say for example, by temperature or impurities.


Later on, and the last class we talked about the periodic arrangement of atoms in solids. We talked about crystal structures, types of crystals which are there; we talked about seven types of crystals. And among them in metal this crystals structure is much simpler, we talked about to be important crystal structures, that we get in metal.

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Atomic Bond & Crystal Structure

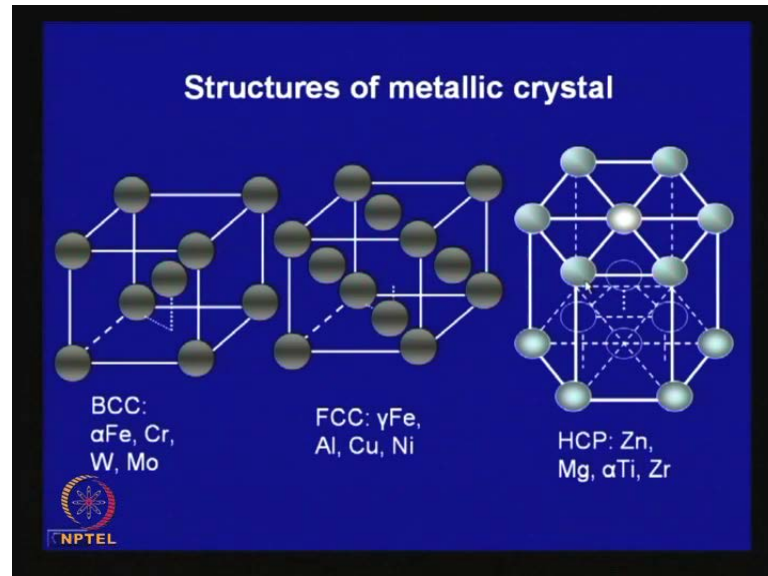
- Metallic bond gives good conductivity
- Other bonds with no free electron exhibit poor conductivity
- Electronic sp heat of metal is negligible
- Metallic & ionic bonds: non directional
- Stiffness (Modulus) vs. Bond energy
- High melting & boiling point indicate high bond strength
- Crystal structure: concept of point lattice

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In short, I think so far, we talked about these points, and I also give you few examples, and few problems to be solved. And I hope you have done that, because as we proceed

further, this will be quite important for you to understand the concepts; that we are going to develop.

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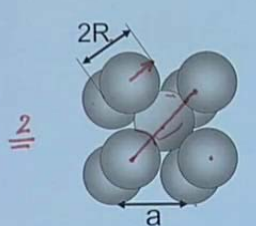
Now just to repeat here, the three types of metallic crystals that are available in metal, primarily one is a body centered cubic; so the position of atoms which are shown here. And normally you get this type of structure, and few common metals which are listed here, iron I named it as alpha iron; that is the form of iron which we normally get at room temperature then chromium, tungsten, molybdenum.

The face centered cubic structure you get in gamma iron, aluminum, copper and nickel. And this gamma iron does not exist at room temperature; you get this at higher temperature. And here you have atoms at the corner of the cube and each of the face centers. And hexagonal closed pack structures you get in metals like zinc, magnesium, alpha titanium; this is the room temperature form of titanium and zirconium, and several others. This list definitely is no means by complete. And here the atoms are arranged like this, in a hexagonal pattern as shown over here, and you have a set of atom down below.

And also you have an intermediate layer, and here you should carefully note that position of this intermediate layer; it is just above this centroid of these three basal planes. Similarly, the next one is just above these three, and the third one is just above this three.

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Packing density



$2R$

a

2

W, Mo, α Fe, Cr

PD = 0.68

Exercise: Find out PD for fcc & hcp structure, are they same?

$PD = \frac{Vol.occupied}{Unit\ cell\ vol.}$

$= \frac{2 \left(\frac{4\pi}{3} R^3 \right)}{a^3} = \frac{8\pi}{3} \left(\frac{R}{a} \right)^3$

$R = \frac{\sqrt{3}}{4} a$

$4R = \sqrt{3} a$

$\left(\frac{R}{a} \right)^3 = \frac{3\sqrt{3}}{64}$

It will be worth wide to look at this atomic packing in little more detail. **When we** let us say, suppose we try to find out what is the packing density; we call as you can see here, if we assumed in atoms to be made up of hard ball, and these hard ball in case of a BCC structure, the touch each other along the diagonal of the cube.

And with this assumption that they are made up of hard ball, we can meet few calculations. Some of these calculations like, what is the gap between interstitial that makes between two nearest atom, it is not fully packed; first let us try and find out what is the packing density, and we will see that most of this lattice a substantial amount of space lies vacant. And what is the size of this vacant space, and where are these vacant places located, because this will be the key to the development of materials, where you mix up two elements to get different types of properties.

We will look at some of these calculations, and let us first try to do it for BCC structure. And which is listed here; so, how do you define packing density? You define the packing density as the volume which is occupied by atom, assuming them to be made up of hard sphere over the unit cell volume. So, like here in BCC, the distance between the two atoms center of this and center of this is equal to a . And let us assume that R is the radius of this atom, and then it is possible to find out a relationship between R and the lattice parameter, because the atoms touch each other along the diagonal directions. So, in the

diagonal directions from this point to other corner at the back, you have part of this atom, whole of this and a part of the other atom.

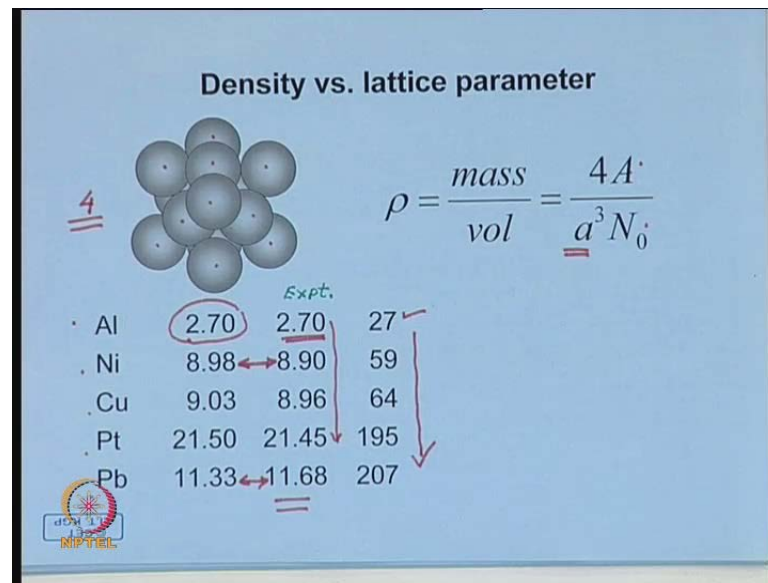
So, therefore, what you have? This diagonal is a $\sqrt{3}a$ actually equal to $4R$ and $4R$ that is $4R$ is equal to the diagonal. So, diagonal is equal to $\sqrt{3}a$. So, therefore, R is equal to $\frac{\sqrt{3}a}{4}$. So, this is the relationship between the radius of the atom, and the lattice parameter. Then we can calculate what the volume which is occupied is; volume occupied is the volume of one sphere, this is $\frac{4}{3}\pi R^3$, this is the volume. And as I have shown last time that in a BCC lattice; number of atom per unit cell is equal to 2.

So, therefore, in each unit cell you have two atoms, the total volume occupied is twice this over the volume of the unit cell; you solve it. And you get in this relationships substitute this over here, then you get what is the part of say, suppose this you raise to the power cube, and then I would try and find out substitute it here. And find out what is the value of the packing density. If you go through this calculation, you will find that packing density for BCC is 0.68. So, which means, a substantial part about 32 volume percent of the lattice is vacant. And depending on the dimension of a second atom I mean, it has a capacity to accommodate very small second atom in this interstitials faces.

So, if the crystal structure changes the nature of this interstitial and the nature of the packing density will change. And you can try and find out the packing density in case of face centered cubic and hexagonal close pack structure. And in the last class, we talked about some layer types of arrangement; if you try and recollect you may find out there is a similarity between face centered cubic and hexagonal close pack structure. So, therefore, possibly when you find out this, you will find this is seen for both at least go through this calculation yourself.

Now having looked at that packing density; let us try and find out the relationship between the densities of a particular say suppose density of R_m , is it related to its lattice parameter. If you want to find out density of any material, what you do? You find out its mass and volume and the ratio is to density. Now assuming that one unit cell is made up of specified number of hard sphere, and they are arranged in a definite crystallographic pattern.

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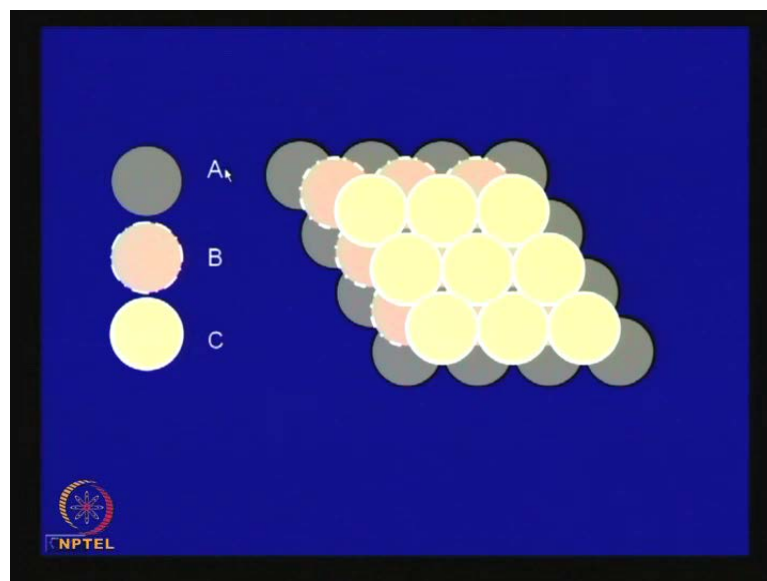
For example, let us consider in this case a face centered cubic structure, which is shown here, where you have atoms at the corner of the cube, and also you have atoms at the center of each of the six faces. So, in this case, we know we have calculated last time; that in an unit cell, you have four atoms in an unit cell. And mass of a particular atom can be calculated, if you know it is atomic weight and avogadro number. So, atomic weight over avogadro number will give you mass of 1 atom.

So, in this particular case since there are 4 atoms mass will be 4 times atomic weight over N_A , divide this by the volume of the unit cell. And repeat this calculation for several elements like which has face centered cubic structure, which is listed here so, aluminum, nickel, copper, platinum, lead. Now each of these cases we go through this calculation, and the results which are shown here. For aluminum it is atomic weight is 27, and the densities you find by this you find there is an x value is 2.7; and experimentally determined density is written here. There is a fair degree of correlation between the two.

Similarly, for nickel also; if you do the same calculation, the theoretically calculated density matches very well with experimental result. But you go down here you find here a there is a large difference, also you see thus as the atomic weight increases down this atomic weight increases; this density goes on increasing, but suddenly here in this case it decreases.

Now, why is it so; try and find out and one of the thing that you can do, you can question the assumptions that we made. We made an assumption that this atoms they are hard sphere there's dimension cannot change. Second when you were doing the packing means by doing the packing, it is dimension does not change. And secondly, we also make an assumption that all the sites or occupied by atom. So, some of these assumptions you try and find out, and you will get an answer why in case of lead there is a such a large difference. (No audio from 14:47 to 14:55)

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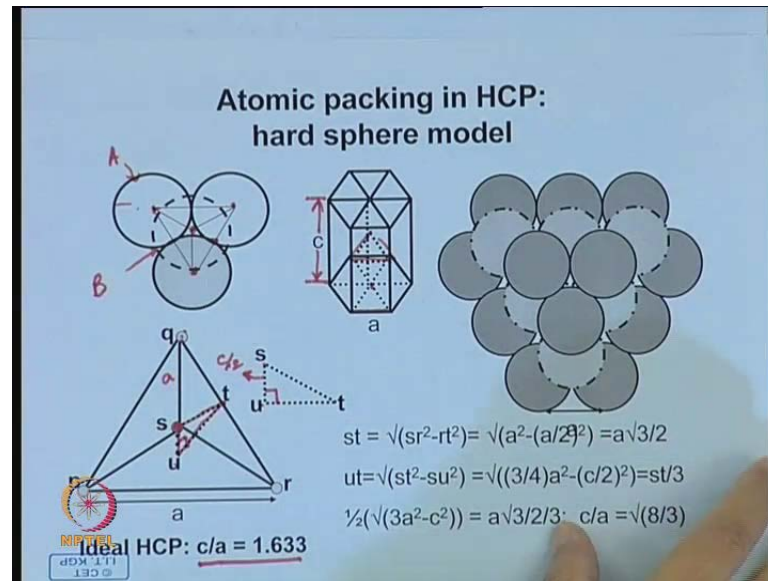


Now, quickly I think, we will look at we will look at the atomic arrangement in a particular plane, and this we I am repeating it this was shown last time. And when you at arrange this hardball like this; you automatically get an hexagonal pattern. And I said that here in the plane you have each atom as 6 nearest neighbor; and next layer of atom if you can put which would also have exactly same arrangement. Now, we can occupy only these values.

Now, if you put an atom here of the same size, it actually block spot of this site. So, either the next layer can occupy this or that, which is shown here. So, this has occupies a first one we call it a, second one as occupied the b side, and then what happens, when you bring in the third? Third it can go to either a side or another side, which has been blocked by this atom.

So, in this particular case we call this site as c. Now in a face centered cubic structure if you look in detail, see this is at the, if you joint this, this, this, this. These are the 4 corner atoms of the cube, and this is the face centered atom; if you look from this side I in case of hexagonal structure, what you have the third layer the c does not exist so, the third layer is again a. So, in hexagonal close pack structure arrangement is A B **A B** like that.

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And it will be interesting to look at atomic packing in hexagonal close pack structure; using this hard sphere model. And here let us see suppose you have one layer of atom and that you put another close pack layer. So obviously, the distance between the two layers will have a direct relationship with atomic diameter. Therefore, hexagonal closed packed arrangement will put and restriction on these two dimensions. So, dimensions along in the plane between two atoms; and the dimension between this layer and the top layer, and which it will be worthwhile to look at what is the magnitude of this. Now, here you have this is the layer a; now let us see this is the layer b, now if you join this center of each of these spheres, what you get is a regular tetrahedron, and this side is a.

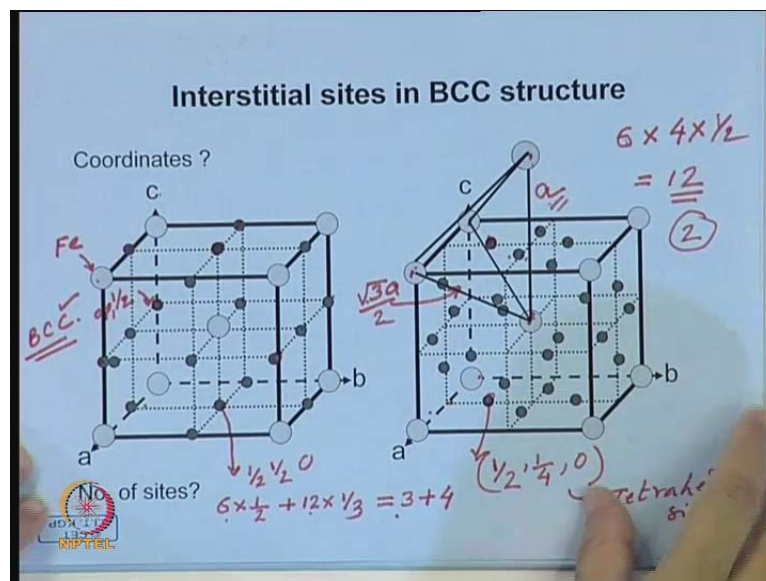
So, this side is also a, this is a, this also is a; q s is also a. Now, what is the distance between this atom on the second layer, and the base plane. And how can you find this out, for this what you can do you can drop it a perpendicular from this vertex to the base plane, join this to the midpoint of this, because mid point is here and joint this. So, in that case this becomes s u t becomes a right angle triangle, then mind your this angle is the

right angle, angle u and which you shown over here. Now, here this distance what is this distance; now we say that hexagonal close pack we say that hexagonal structure that c axis is different from a parameter a . This is a and hexagonal close pack structure this height of this unit cell is called c ; so this $s u$. So, this represents distance between these planes to the central plane. So, therefore, this is c over 2.

And then if you can simply go through these steps of calculation. It will be possible to show that there is a basic relationship, because c is not independent; because the magnitude of c is determined by the diameter of the atom. So, it is not independent of a . And this relationship **it** I mean, if you go through this steps of calculation you will find out that ratio c over a equal to 1.633. The steps are shown here, but I think you try it yourself, but; so, what does this number represent. This number represents c by a ratio in an ideally exact ideal hexagonal close pack structure.

If you look at the lattice parameter of the some of the elements, which I some of the elements which I said have hexagonal close pack structure, like zinc, magnesium, titanium you may find some of these. They have a particular c by a ratio, but none of them are exactly satisfy this; possibly the nearest that comes is magnesium. But you look up the table and see it for yourself

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Now, let us look at this crystal structures a little more carefully, and look at the interstitial sites that are present in a lattice; which can accommodate a second element or

second atom. And this will be quiet of rate in importance and subsequent lecture, particularly to understand structure of that you get in steel; as I said iron steel is an alloy of iron carbon. So, that carbon atom goes into the lattice, and dimension of the carbon atom is so, small in comparison to iron atom. That it can be accommodated at the interstitial sites. So, when a carbon dissolves in iron where it does go.

And to understand that, let us look at the interstitial sites which are there in a body centered cubic structure. Now, here this diagram it is shows the projection of iron atom let us say, and this filled in small circles, they represent the one kind of interstitial sites. Now, we will this type of interstitial site is known as octahedral site; and if you look at this coordinate say look at this atom, and what is the coordinate.

Now in this case this axis a b c a orthogonal, because this is the structure we are talking about is body centered cubic. So, cubic that means, the axis a b c they are all at right angle, and you can find out the coordinates of each of these points. So, particularly this particular point is half, half, 0. We also have so, each of this phase center you can say that these are half, half, 0. And how many phases are there; a cube contains six phases.

Now one of each of these phase center point will be shared by another neighboring unit cell. So, the contribution of this six is 6 times half; in addition we also have sites at these points. Although in this particular case, this if you look at this coordinate it will say half 0, 0, half; this is at big way in the c axis. Similarly, you have each of these edges one particular point. Now there are twelve edges in the cube, and each edge is common to four adjacent unit cells.

So, apart from this there is three other neighbors. So, this contribution of this is twelve times $\frac{1}{3}$. So, therefore, this comes out to be this is 3.

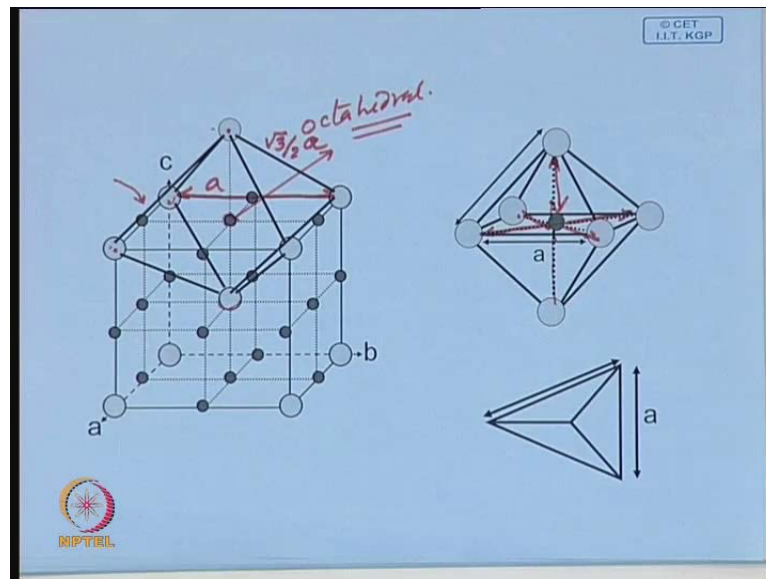
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I again check up this calculation. I think you do it little more carefully; and find out how many numbers of such sites are there in a lattice. Now there is another alternative location, which can accommodate an atom, interstitial atom; which is shown over here. Say this one, so look at this atom; which is a location is a half; along b at is one-fourth, 0. This site is called tetrahedral site. Now tetrahedral site, why it is called tetrahedral site? Look at this; if you join this, this, this and this so, you get a tetrahedron. In this

tetrahedron this two are separated by a distance a whereas, these are separated by a distance, which is half of this diagonal; that is this is $\frac{\sqrt{3}a}{2}$.

So, some of this edges of this tetrahedron have dimension a , and some have dimension $\frac{\sqrt{3}a}{2}$. And you have each of these phases, you have four such sites. So, a cube has a six phases a cube has six phases; so, which six phases, each of these six phases you have four points. But each phases shared by so, therefore, this comes out to be 12. So, you have twelve tetrahedral sites in a lattice whereas, atom number of a dam atom in this lattice, and number of atom in a BCC lattice is 2. So, number of interstitial sites per unit cell is much more.

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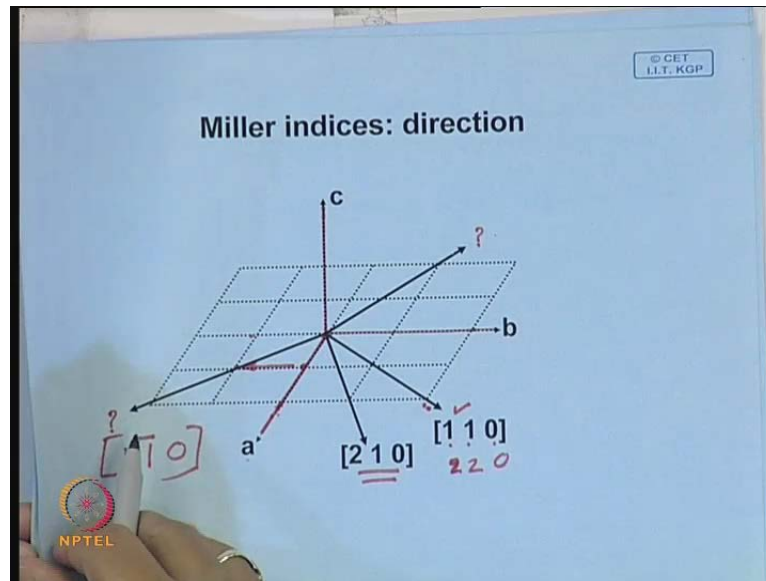


Now, if you look at this diagram a little more carefully. The other side where you have this interstitial site is present at the center of the phase, and the center of the edges. If you join these atoms with this; similarly, one at this center of the cube you get an octahedron. So, this site is therefore, known as each of these sites they are known as octahedral sites. So, octahedral it is surrounded by identical so, equal as identical as similar phases eight phases this. So, these phases they not necessarily, see this dimension between this is a whereas, this dimension is $\frac{\sqrt{3}a}{2}$; this is half of the diagonal. And which is this diagram is shown over here.

So, it will be a worthwhile for you to try and calculate, what is the dimension of these interstitial sites; and try and find out what is the dimension along this and along this. Is it

same in all directions; it is a dimension along the face diagonal, and the dimension of the gap, along the edge try and find out what are their values are the same. And similar thing you can repeat for tetrahedral site as well. Now with this we have now your fairly good idea, about the crystal structures of simple metals; and how the atoms are arranged, and what are they are in a gaps, where can very small atom can be accommodated.

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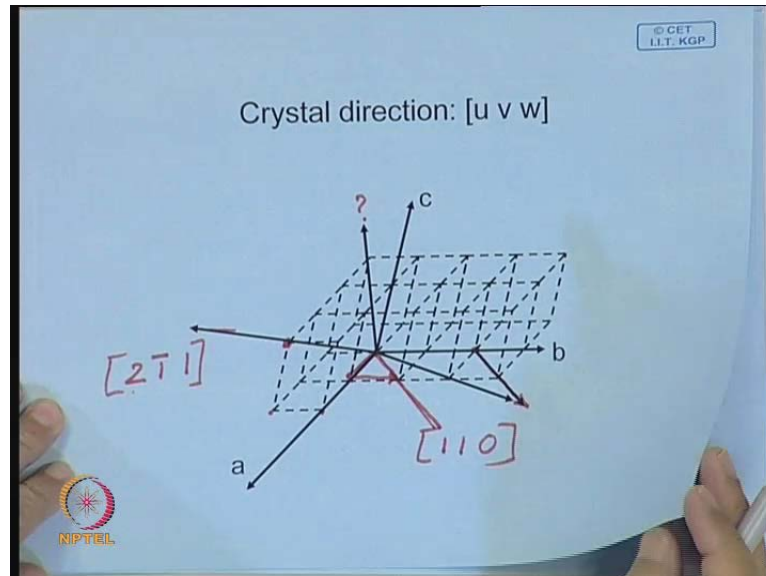


Now, let us look at, how different directions and planes in a crystal are represented? Here we use a system call miller indices; we use this to represent directions and the lattice, direction and the crystal as well as planes of a crystal. Now direction is rather simple which is shown here in this diagram, and you use basically the crystal axis as the reference. a, b, c these are the crystal axis. Now here intentionally you have shown one plane, that is the base plane; plane passing through a, b. And the grid lines had drawn, and to represent a directions say for example, this direction how will you represent, you move two steps, two units. Let us say along a direction two units along b direction.

So, therefore, you represent this direction by this indices 1, 1, 0 although it is 2, 2, 0 and 2 is common. So, you can see that this direction is 1, 1, and 0. Similarly, in this case you go to step along a 1 along b therefore, this is 2, 1, 0. What happens if it goes and the negative direction; like in this case. Here you go along a the positive direction of a one unit. And then you go another unit in the negative direction of b. So, in this case, you will write this is 01 that negative along b, and it is customer it to represent the site as a

bar 1, 1 bar, 0. Similarly, you try and find out what will be the indices of these particular directions.

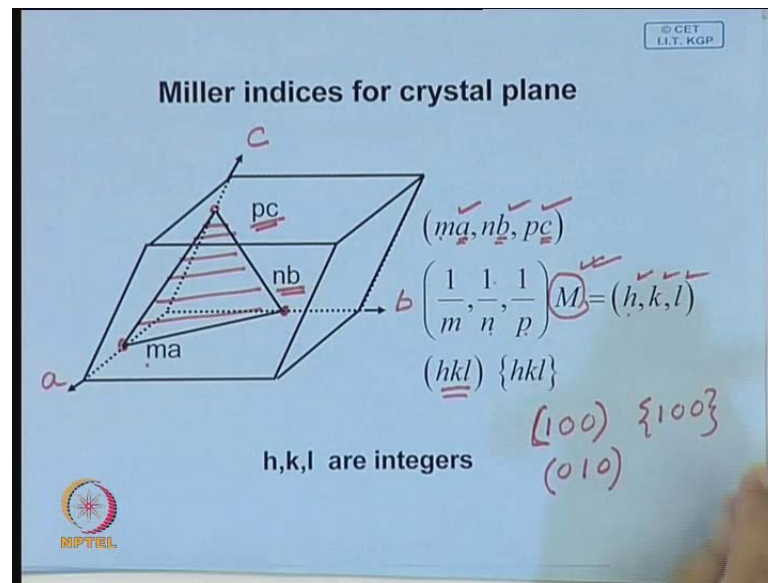
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But in crystal you will have arrangements and in 3 dimensions, which is shown and the next figure. Here it takes one particular case; say what is this particular direction we have join this point, but this point. So, you calculate, find out you go 1, 2, 2 step along a so, you in the positive direction, then one step along b in the negative direction 2, 1 bar, and 1 along c directions. So, this is called 2, 1 bar, 1.

In certain cases, the direction may be you are interested to know, what is the indices of this? In that case, it is not passing through the origin. What one has to do, is draw in line parallel to this passing through the origin which is shown here. And now, you find this is you go one direction here unit direction along a, unit direction along b. So, you call this 1, 1, 0; you try to find out the indices of particular say this direction.

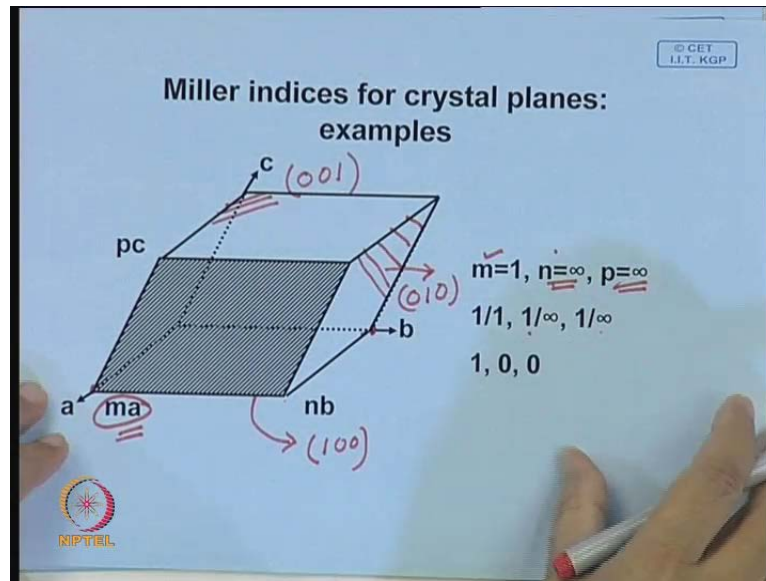
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Now, let us look at the indices of a plane. Now in the case of a plane when you look at this, this is say one crystal; and say these are the axis a, b, c. Now suppose we want to represent find out what is the indices of this plane, how will you represent this plane. So, this intersects will look at that square does it intersect is three crystallographic axis. Now this intersects certain a point, which is m times a. Now m is any magnitude, **I am in not** I am in it can be less than 1, it can be more than 1. So, if it **is** m is not necessarily an integer, it is m times a, here intersect is n times b, and c; the intersect is b c.

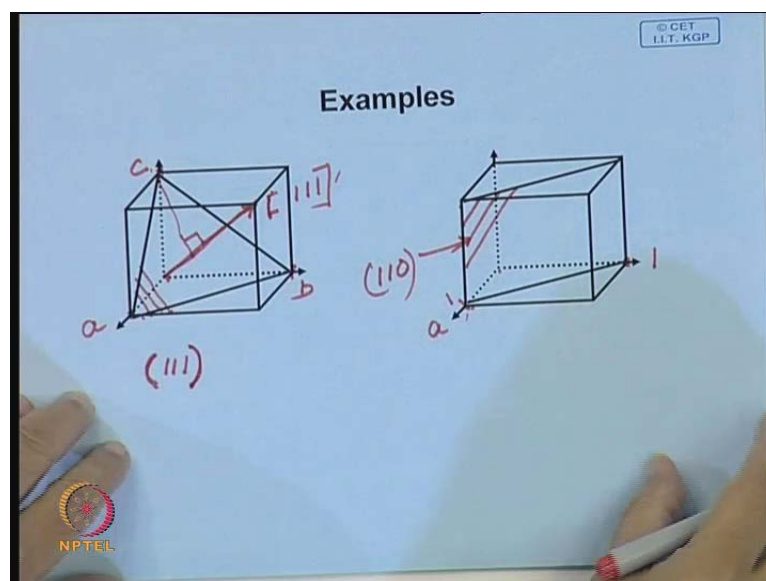
So, look at, write down this indices a these intersects, now what we do in normalize it with respect to the lattice parameters a, b, c. And in that case, and then what we do we took so, in that case it will be m, n, p. Now take the reciprocal of that 1 over m, 1 over n, 1 over p. And think about a multiplier M, now you choose this multiplier in such a way that this reduces to integer number h, k, l. So, h, k, l are integer, and this is called the miller indices of this particular plane. And in a crystal you may have similar types, a set of similar planes, when you have a set of similar plane you call it, you represented as h, k, l. Suppose, when a cubic structure, what do you mean by this similar plane; say suppose it make cube structure you look at a cube plane which you will represent as 1, 0, 0; you can also have another cube plane 0, 1, 0. So, they are all similar. So, we say that cube plane will be represented by 1, 0, 0; and this will be x clear and that is possible in this next one.

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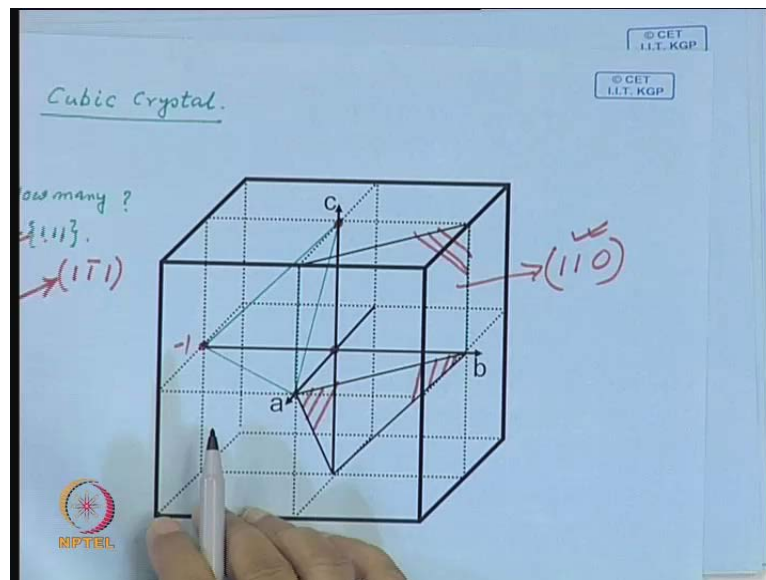
Look at this crystal, and let us try and find out the miller indices of this phase, which intersects only the x axis at a point m, a. Now write down this numbers m, n, p; since, it is parallel to b, it intersects b at an infinite distance n is infinite. Similarly, it intersects c at infinity so, p is infinity; so, reciprocal of that is this; so, this is 1, 0, 0. Now in this case this is not a cubic crystal so, here 1, 0, 0; and this particular plane is not the same as this plane. So, we say that this indices is miller indices is 1, 0, 0. Similarly, this intersects only b so, we say that this is 0, 1, 0 this plane intersects only c this is 0, 0, 1.

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Now let us look at it this particular crystal, and try an index this. We say that this axis is a, this unit is a, this is b lattice parameter; this is c. Now, it is intersecting at these corners of this units cell at a b c. So, in this case therefore, the index will be 1, 1, 1; whereas, in this case this particular plane, it intersects x is a at unit distance it axis, b at unit distance and it is parallel to c intersects c, at infinity. So, in this case this index will be 1, 1, and 0. Whereas, if you look at this direction 1 this will be 1, 1, 1 direction. And as per convention we represent dimensions a deduction with this box bracket; whereas, the planes with the first bracket. And in a cubic or orthogonal crystals; a particular in cubic crystal, this direction will be perpendicular to this plane. So, this will be normal to this plane.

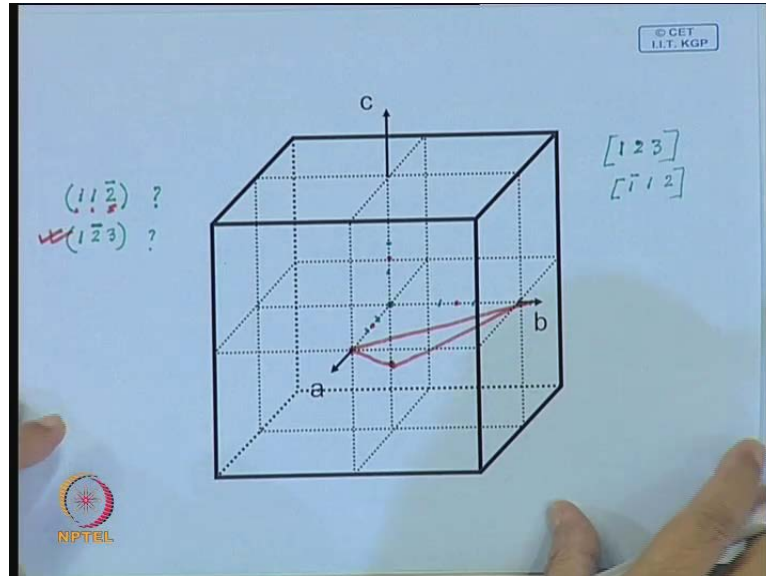
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Now, this planes can intersect and the negative direction as well. For example, here we have put this origin over here this center look at this plane here, it intersects c at let us unit distance a, at unit distance and b at minus 1. So, in this case this will be indices of this plane is 1, 1 bar, 1. Now this 1, 1, 1 plane in a face centered cubic structure is of considerable importance, look at the atomic arrangement in plane 1, 1, 1. And try to correlated with diagram which I should where you know the hard balls, they are arranged in a plane, and you bring another plane another plane sliding over it. So, what is the indices of that close pack plane? In fact, we will find the close pack plane will come out to be 1, 1, 1; try and find out how many 1, 1, 1 planes are there. And it try and find out

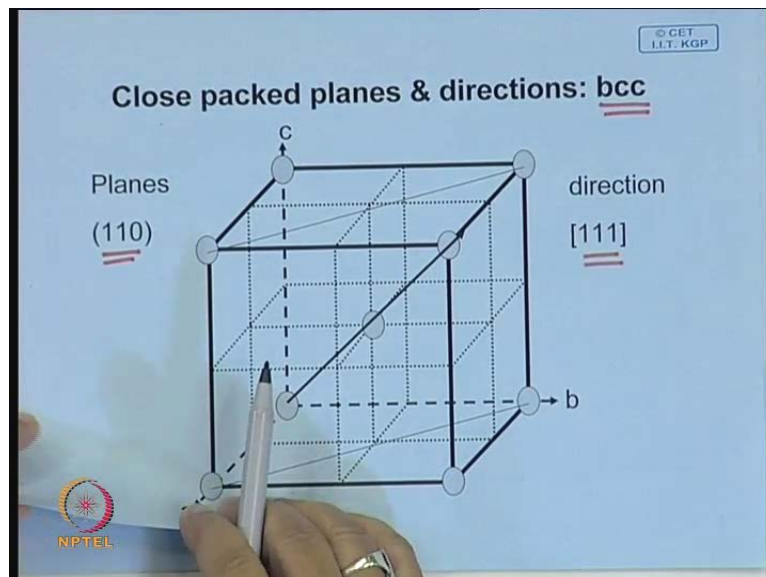
indices of this plane, and this case this is 1, 1, 0; and try, and find out how many such planes are there in a cube.

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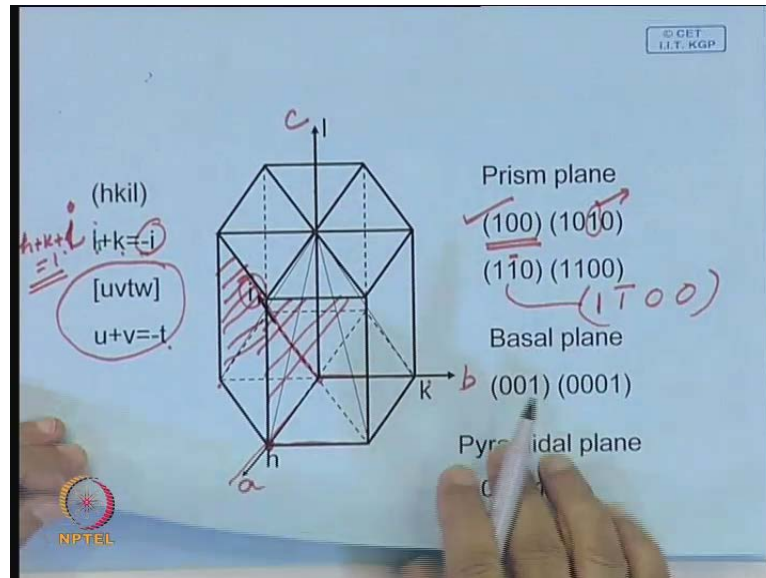
How do you represent, say suppose this indices of a plane is given see this is 1, 1, 2 bar. So, how will you represent this here? So, it intersects a axis at 1, b at 1 so, let us say it intersects a at 1, b at 1, c it is 2 bar so, half along c. So, this is a, b; and c is somewhere along the c axis negative directions. So, this is in the same way you try to locate this plane 1, 2 bar, 3.

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Look at the close packed planes and directions in f c c. And try and find out each of these locate; each of these 1, 1, 1 plane, and each of these directions; how they are arranged. Repeat the same thing, in case of a body centered cubic structure; try to locate all planes of type 1, 1, 0; and all directions of type 1, 1, 1.

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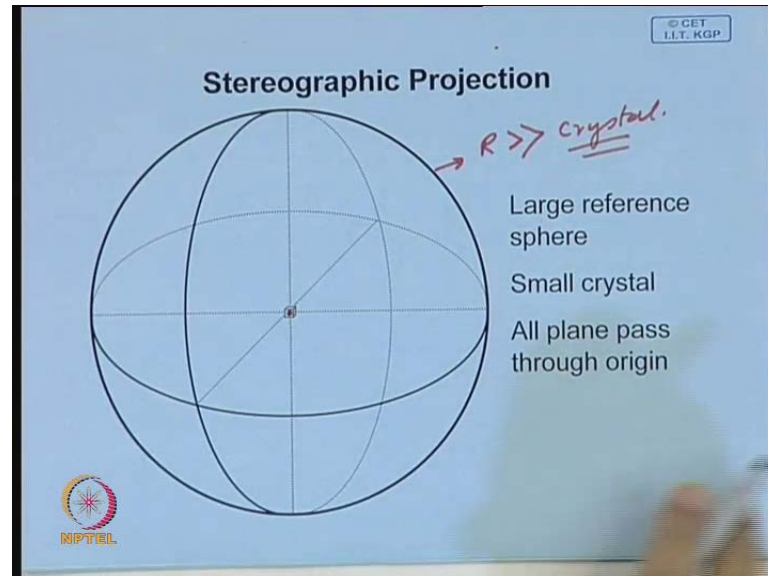


Representation in hexagonal it is little more complex, and particularly this one. But directions; but it is shown over here, in case of a hexagonal lattice this is the direction a, this is b; this is c. Now, suppose you want to find out the indices of a prism plane so, you look at one of the prism plane is like this. It intersects only axis a over here, and it is parallel to both c and d. So, following the rule that we just saw it is 1, 0, 0. But look at another prism plane say suppose this they are identical crystal plane, it intersects a at 1, b at minus 1. So, its index is this, but looking at the indices although they are seen **they are** they look different in the indices.

So, therefore, it will try to represent this by adding another crystal direction. So, this we called at another axis like this, but this axis it is redundant, and usually this relationship will be followed we call this axis I, and this indices in its index i will be sum of h plus k with a negative sign. So, essentially h k plus l is 1; **h k** sorry i is 1. In that case they become similar all prism planes will have similar indices. So, it will be this will be 1, 1 bar, 0; it will be 1, 1 bar, 0, 0.

So, we will look at it little later, it means a little complicated here the conversion is not as simple in case of a direction, as in case of plane.

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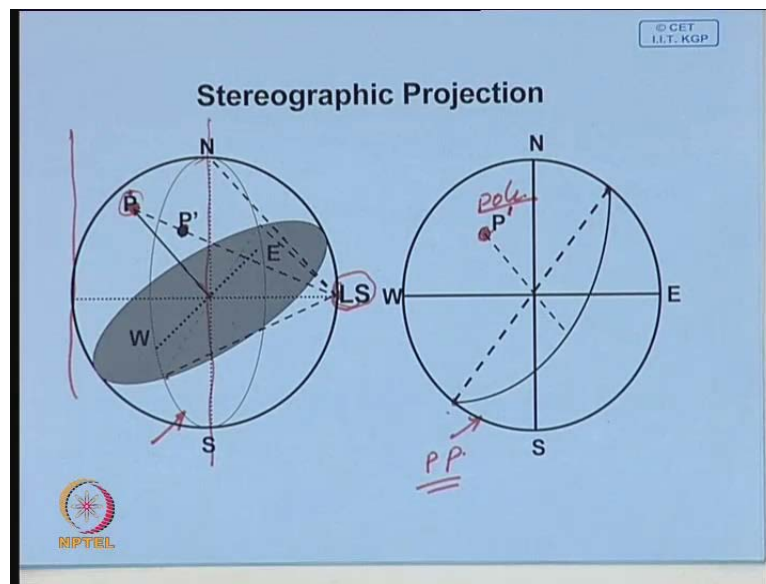
Now with this, we now have some idea about the crystal structures **in if** in common metallic materials. And we also looked at the atomic arrangement along different planes, and how these layers are arranged. But to solve crystallographic problem like engineers we need to develop a concept, where we can represent different crystal directions in a two-dimensional figure, or in a two-dimensional plane. And engineer often you know to represent a 3d object we make use of projections, we take look at any solid. May be from the top if you look at you get a top view or plane; if you look at from the front you get elevation; if you look at from the side you get the side view.

Now here, when you represent large object three-dimensional object in this type of 2d diagram, what you do. You draw a scale down model, and you give these three views to represent that particular object. And here you follow certain rule that the distances between two points are exactly same, you scale it down, but all these distances they are proportional. So, these are this engineering projections, you know the distance relationship between distance or maintain. Now in crystallography often it is more important to know that angles between different crystallography directions.

So, here you need a different kind of projection, and we call this projection stereographic projection, which is shown over here. What you do you imagine that you have a small

crystal, crystal is so small that it occupies the center of this reference sphere, it occupies the center of this reference sphere. What does it mean? It means that any plane that you draw in the crystal will pass through the origin; say, suppose if you draw one plane it passes through the origin, you draw the vertical plane this also will pass through the origin. So, this sphere we call this large sphere is reference sphere, it is radius is much larger than the crystal.

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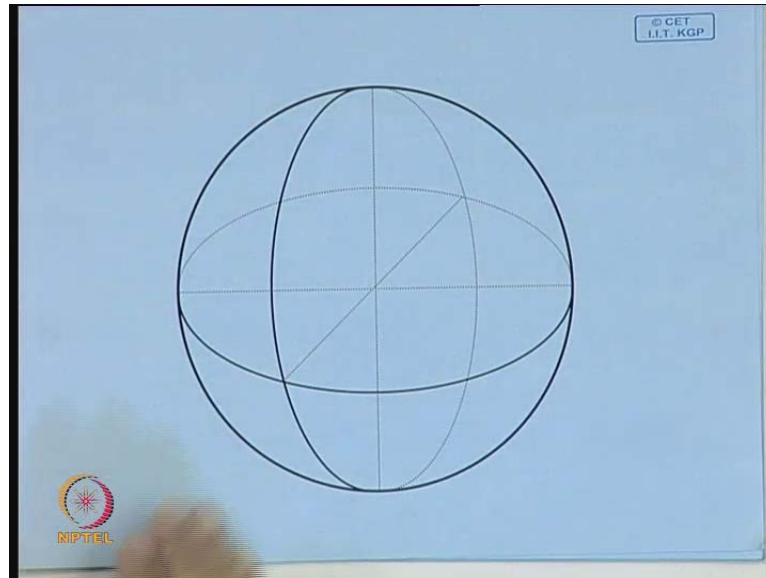
And now what you will do is, you look at a particular plane in the crystal, this plane as I said will pass through the origin. And now draw a line which is perpendicular to this plane, and extend it to intersect this reference sphere.

Let us say it intersect this at point P. Now you put a light source here, look at this point from this particular point. So, maybe you put a light source here, and put a either a projection plane here, or put a projection plane here; imagine that. Say, suppose you take a projection on this, what you do? You join this with this; it will intersect this point at p. So, this particular plane is called the projection plane, and which is shown over here this is the projection plane, and this point is shown here this point is called pole. Whereas, this particular plane will intersect this reference sphere at certain points; so, which is shown here, it intersect somewhere here and here.

So, these intersection points will come here like this, and this particular plane will get projected like this. And in this case we call this point p is a stereographic projection, this

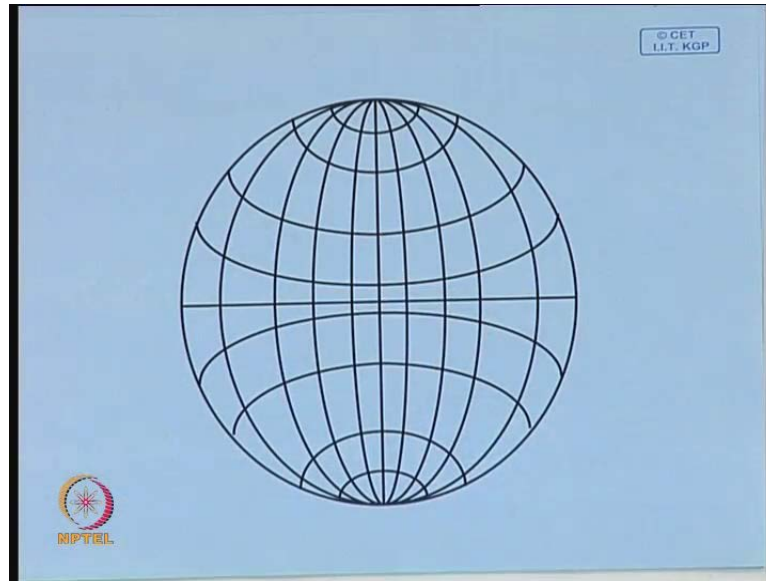
P is a stereographic projection of this pole P. And this particular type of projection what is retained is the angular relationship. And this angular relationships are maintains so, that is why we call this as an angle true projection, and you are very familiar with globes.

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If you look at the globe, you have the geographical globe; if you look at you have certain great circles which are drawn. So, equatorial plane another plane vertical plane which course through the center of the globe is like this. We call all these great circles wherever the diameter of the great circle is equal to the diameter of the reference sphere. And we also have a set of line in the globe, which goes like this we call these latitudes.

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So, here also you can think about a similar situation, and look at a projection of this kind of a rule globe which we call wolf net. And wolf net a typical figure is like this, here all these are the great circles and these have diameter, which is equal to the diameter of the reference sphere. And you can clearly see that distance relationship is not maintained, but angular relationship will be maintained until, and you will have this kind of projections of this small spheres, a small circles like this; they are called latitude. It will exactly similar to the globe, and this type of reference net one uses it is called wolf net. And this is use to measure to perform angular measurement on stereographic projections.

So, in this class, I just introduced to you the concept of stereographic projection at the end, this projects this concept is little abstract. And maybe we will next class we will talk about it in a little detail. And apart from that, we also looked at the atomics arrangement in different crystals, which you find in metals little critically, and given you some of these exercises, I hope you will try to solve them. Thank you.