An Introduction to Materials: Nature and Properties
(Part 1: Structure of Materials)
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Lecture - 15
Structure of Metals Packing Co-ordination Interstices

So, let us welcome to new lecture, lecture 15.

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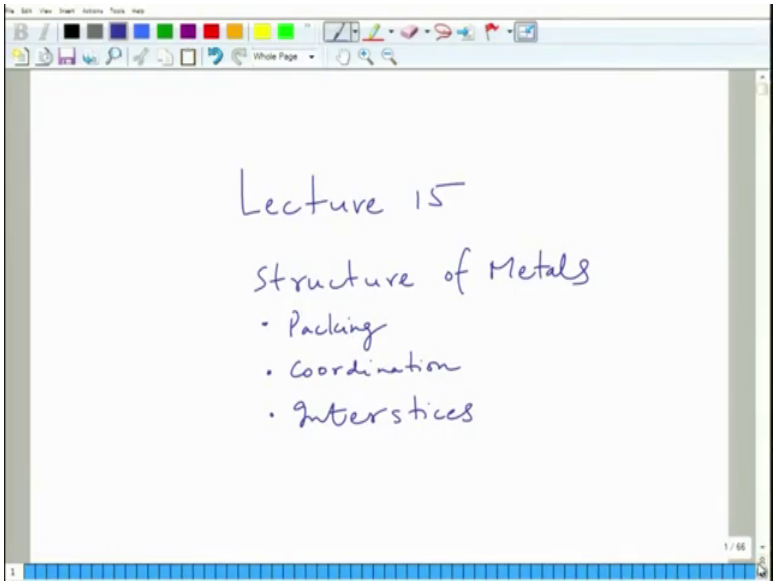

So, in this lecture we will again continue talking about structure of metals with a focus on packing of atoms in these structures, coordination's and interstices.

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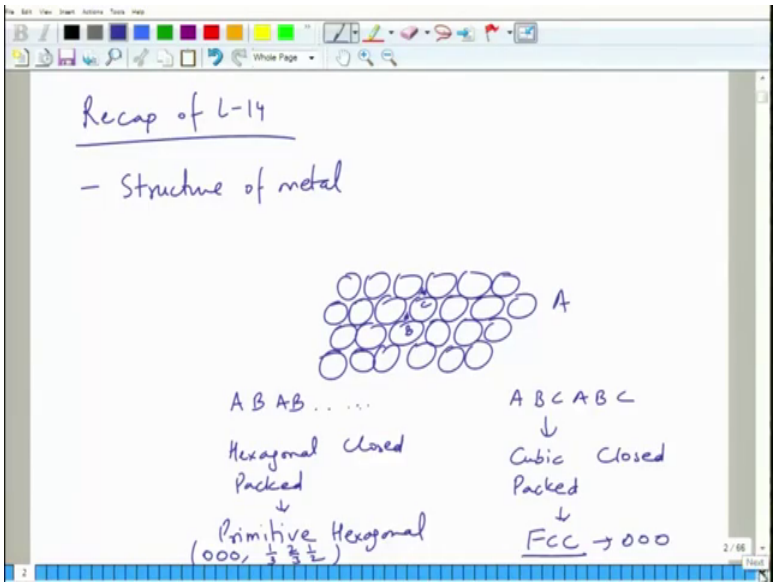

So, let me just recap the last lecture. So, in the last lecture we started about structure of metals. So, here we basically talked about how atoms packed closely in metallic structures, they packed themselves in face centred cubic or cubic closed packed structure and hexagonal closed packed structure the by the virtue of arrangement of layers in A B. So, each layer is hexagonal sort of layer in nature so, if you have a array of atoms like this and each layer underneath is like this. So, this is how and you can keep extending it in 2 directions.

So, this is how your first layer is going to be now if this is A layer when you put that B layer on top, the B layer can go on this type of interstices or this kind of interstices. So, if it let us say this interstices will give rise to B layer and this interstices will give rise to C layer. So, if you follow the stacking sequence of ABC ABC then what you come up within the cubic closed packed structure this can be described by a FCC lattice with a motif at 0 0 0.

So, this is ABC ABC packing if you go think about if you pack in a or AB AB stacking kind of sequence where so, you put the next layer at B then the next layer again comes back on A you do not have to necessarily go to C which is again the alteration of ABC ABC type of packing, but both are closed packed structure this is called as hexagonal closed packed structure; however, in this case the lattice is primitive it is not primitive hexagonal with a motive fact 0 0 0 and one-third, two-third and half.

So, it is a 2 atom motif here in this case it is a single atom motif by which you can define the lattice single atom motif with FCC lattice will mean that you have 1 atom at 0 0 0 another at half of 0 another at half 0 half another at 0 half half that will automatically the moment you describe the lattice type as F so, that is the condition. So, this is where we were in the last class.

So, this class we will again look at some other structures so, not only your metals can in metals atoms arrange themselves in ABC ABC type of packing there are other structures as well for example.

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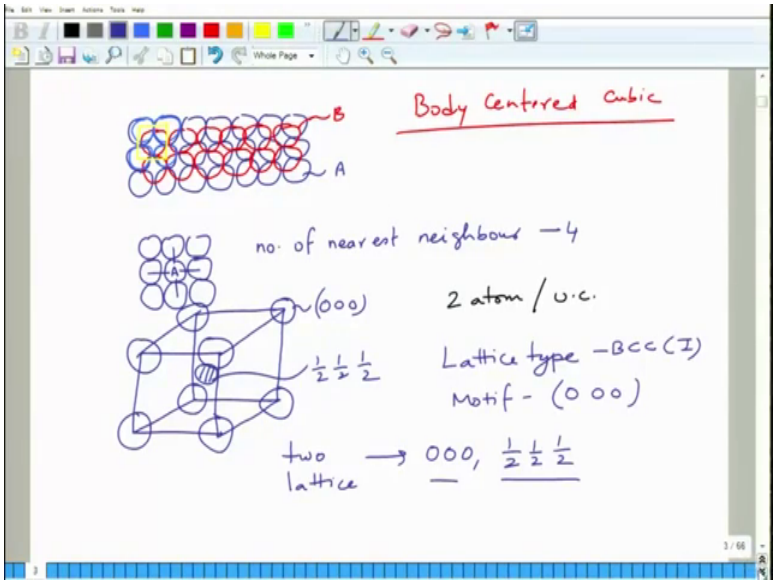

If you have atomic arrangement like this right and this is your next layer and so on and so forth. So, you can put the next layer if I use a different colour here like this now this is not the closed and the so this is your sorry. So, this will be B layer and the first layer will be A layer and then again. On top you can put a A layer. So, this is, but; however, in this case you can see that the A layer is not closely packed the number of atoms which surround each a atom in this case is different.

So, if you look at the if you look at the close number of nearest neighbours, number of nearest neighbours in A layer is each atom is surrounded by. So, if you have this kind of packing and if you talk about this particular let us say A guy. So, you have one this has a nearest neighbour, another one this has a nearest neighbour, another one this has a

nearest neighbour, another one this has a nearest neighbour. So, numbers of nearest neighbours are in the closed packed case, what was the situation, it was 6.

So, this means this is less closed packed so, you can find out also the atomic density in this layer by just calculating in the number of atoms per unit area and this of this sort of structure if you have this kind of stacking then what it gives rise to a structure which is look which is something like that try to remake it. So, for the sake of illustration the atoms are not touching here and 1 atom will be at the centre. So, these will be at 0 0 0 position and this will be at half half half position. So, this kind of lattices called as body centred cubic.

So, here you can see that this structure is less closely packed as compared to a hexagonal closed packed or face centred cubic structure we will see the atomic packing factor in a little while. So, this is another possibility that can occur in case of so, basically if you just want to look at it from the perspective of. So, if I just put another layer on top another layer on top would be something like that. So, the unit cell would be this unit cell the one in the yellow here. So, that would be the unit cell. So, it has it has 2 atoms at the centre, it has 2 atoms in the unit cell sorry, one at the corner at 0 0 0 so, 2 atoms per unit cell.

So, this lattice is lattice type is BCC which is I. So, when you define the lattice type as I the number then the motif becomes motif is 0 0 0 single atom motif at 0 0 0, when you define a lattice type as non primitive you do not need to define the coordinates of all the atoms in motif you just need to define only one atom which is at 0 0 0 it will. So, I symbol will ensure that the number of atoms in the unit cell one is at 0 0 0, another is at half half half and they are identical they are identical, they are identical lattice points. So, it has 2 lattice points per unit cell they are identical. So, these are this is 2 lattice points. So, I ensures that you have 2 lattice points, but to define the motif you can just choose single atom motif at 0 0 0.

Similarly, in case of FCC single atom motif will be at 0 0 0, but it ensures that you have 4 identical lattice points one at 0 0 0, another at half 0 half half 0 half, another at half of 0 and at 0 half half. So, this is another lattice type in metals which is quite common and the third one which is not so common could be in this kind of.

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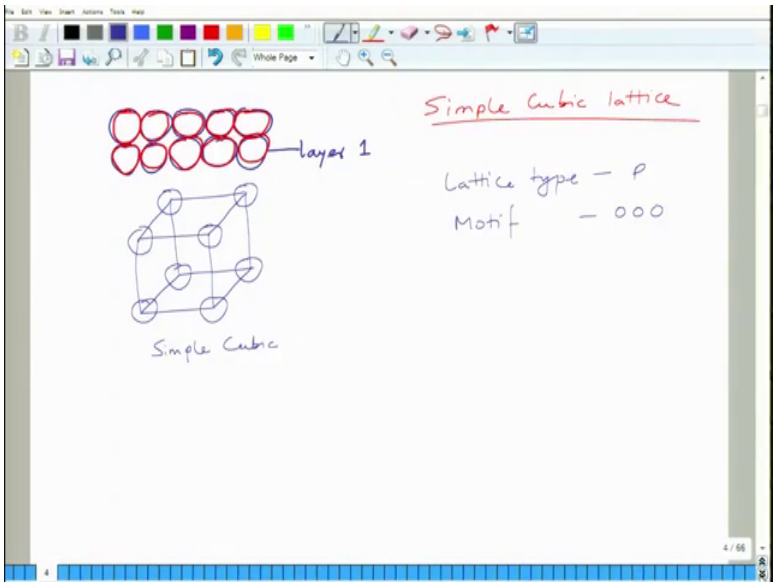

So, you have this arrangement sorry the fourth one. So, you have atoms in this fashion this is the layer 1, second layer goes directly on top of it. So, if you look at this structure it will look like all right. So, this is one atom, this is another atom, they are kept apart for the sake of illustration, but they do touch each other this is simple cubic. So, here each atom has how many nearest neighbours, 6 nearest neighbours, but within the within the plane it has only 4 nearest neighbours. So, likewise in case so BCC number of nearest neighbours were 8 in 3 D right.

So, this atom is surrounded by 8 of the atoms similarly this atom is surrounded by 8 atoms. So, one in the centre is same as so, I have all the dashed it, but they are both same atoms. So, this is called as a simple cubic lattice the lattice type is defined as P, which is Primitive and motif is at 0 0 0. So, these are the 4 type of lattices we typically find the examples of for example.

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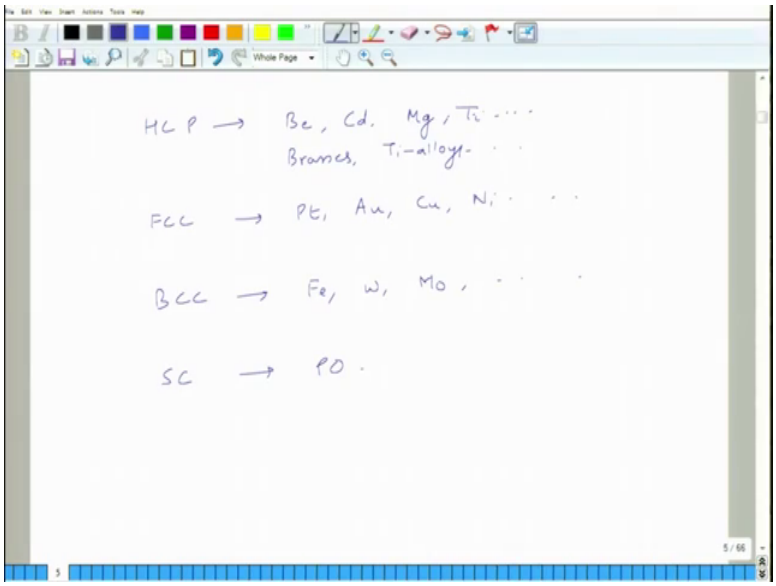

It is HCP based metals are beryllium, cadmium, magnesium, one form of titanium these are all metals some alloys for example, brasses titanium alloys they are also hexagonal in nature then you have FCC based metals. FCC based metals like platinum, gold, copper, nickel all of them are FCC based metals and then BCC based BCC structured metals are things like iron, tungsten, moly, molybdenum these are all BCC based material and then simple cubic is polonium PO, this is perhaps the only metal in the periodic table which is simple cubic structure.

So, in this case of FCC structured materials we define a closed packed plane the plane which is absolutely closed packed.

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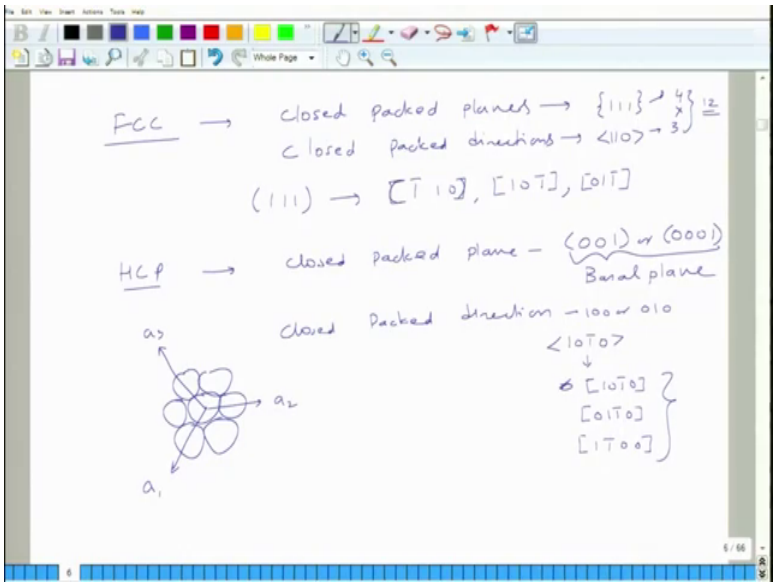

So, this plane is 1 1 1 plane and in this plane lies a closed packed direction which is of 1 1 0 type this can be illustrated by this bracket. So, of course, if you take this type of 1 1 1 plane then the directions which will lie in this will be bar 1 1 0, 1 0 bar 1 and 0 1 bar 1. The dot product of the direction which lies in the plane should be equal to 0. So, there are these closed packed planes and directions in case of FCC in case of HCP the closed packed plane is 0 0 1 or 0 0 0 1 which is also called as basal plane and the closed packed directions you have only.

So, if you look at hexagonal system this is right this is the plane the directions closed packed directions are this is a closed packed direction, this is the closed packed direction and this is the closed packed direction. So, if this is a 1, this is a 2 and this is a 3, you can write in 2 coordinate system, 3 coordinate System so, this is 1 0 0 this is 0 1 0 direction. So, you can have 1 0 0 or 0 1 0, but since this is also a direction which otherwise will turn out to as a as a 1 1 0 direction. So, you need to you need to modify this so, what will that direction b.

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So, you will have 1 0 bar 1 0 type of directions. So, this will ensure this will ensure 1 0 bar 1 0 0 sorry 0 1 1 bar 0 at 1 bar bar 1 bar 1 0 0 these three directions will lie within this plane. So, there are only 3 sets one plane and 3 directions in case of FCC there are multiple choices 1 1 1 planes are there are 4 types of 1 1 1 planes finally, we have 8, but

equivalent if you do not consider equivalent planes and there are these 4 and then you have three types of directions in each of them. So, total possibilities are 12 in this case so, this 4 into 3 will be 12.

So, we will see this in the mechanical behaviour this is called a slip system. In case of mechanical properties we consider this as a slip system because on this plane the mechanical deformation happens in FCC structure materials. So, there are 12 slip systems in FCC in a in case of HCP there are only 3 slip systems one multiplied by 3.

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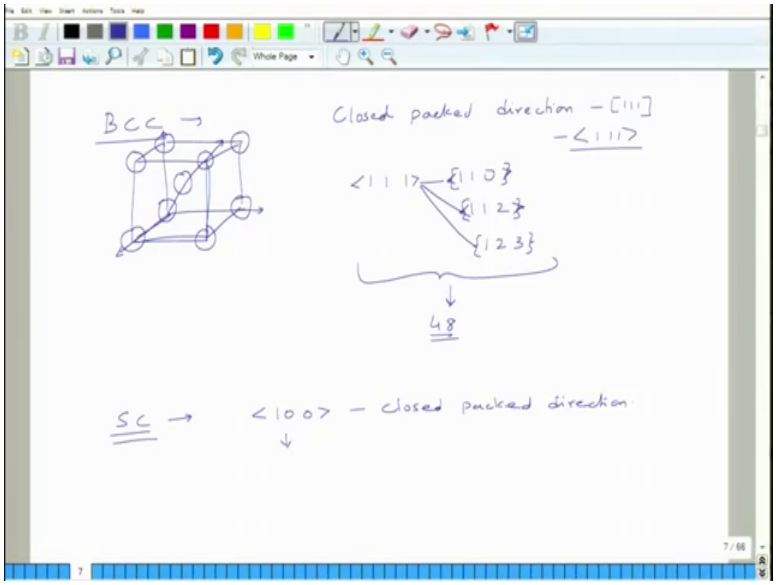

Now in case of BCC there is no closed packed plane the plane which has the highest density of atoms which is like this. So, there is no closed packed plane, but there is a closed packed direction all right sorry not this let me just draw the BCC cell again just this is the BCC cell so, closed packed plane means plane having highest atomic density. So, there is no since there is no hexagonal packing of atoms in BCC structured there is no closed packed plane, but there is a closed packed direction in this direction the atoms touch each other. So, BCC has a closed packed direction which is.

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1 1 1.

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1 1 1 1 1 1 and there are multiple types of this 1 1 1. So, basically since it is a cubic structure you can write this as 1 1 1. So, 1 1 1 types of directions are closed packed directions, there is no closed packed plane because there is no there is no plane with that hexagonal arrangement of atoms which the highest possible density of atoms in a plane. However, in this case in metals in single atom case; however, what may happen is this direction may lie within the plane. So, if you just take the so, this direction lies in a few types of plane.

So, 1 1 1 there are few possibilities 1 1 1 direction may lie in a plane which is the 1 1 0 type of plane, it may lie in a plane which is 1 1 2 type of a plane, it may lie in a plane which is 1 2 3 type of plane. So, this is a possibility that may exist sorry not this kind of this is the plane. So, for plane we use this symbol and this is there. So, if you work out the combinations the combinations will be total of 48. So, this is again something which is used in mechanical behaviour of materials, in case of simple cubic the closed packed direction is nothing, but.

Student: 1 0 0.

1 0 0 type of direction this is the closed packed directions along which the atoms touch each other and by the virtue of that it lies in it may lie in several types of planes all right. This is basically you can find out the type of planes in which it can lie why it is not a closed packed structure is only 1 metal. So, we just generally do not consider the slip system this in this case. So, now, once we have seen the 4 types of these lattices with their closed packed planes and directions we will now move on to what is called as coordination number.

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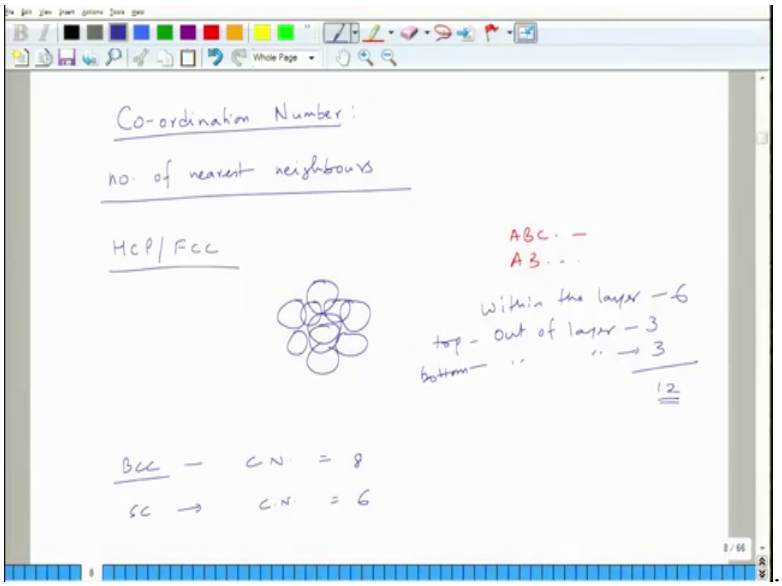

Coordination number is basically the number of nearest neighbours. So, for HCP or FCC case as we have seen in the closed packed structure so, you have arrangement like this right. Next atom goes let us say this is the atom which is the next layer atom and then again the next layer if it is the next layer will go either it will go on top of A.

Student: (Refer Time: 18:50).

Or it will go on top of.

Student: (Refer Time: 18:52).

B so, either it will be ABC ABC or it will be no matter what the case is this atom will be surrounded by. So, within the plane how many neighbours will it have 1. So, within the, and let me just show. So, this is let us say 1 layer within the layer it has 6 neighbours within the layer within the layer 6 and if it has a layer upward town then it can have one atom here one atom here and one atom somewhere here how many it will have.

Student: (Refer Time: 19:39).

It will have out of the layer 3 3 on top.

Student: (Refer Time: 19:48).

And 3 on bottom; So, how many nearest neighbours it will have, 12 total of 12 nearest neighbours it will have I will just give you a short animation of that.

Let me see if I have a slide so, if you just look at this animation.

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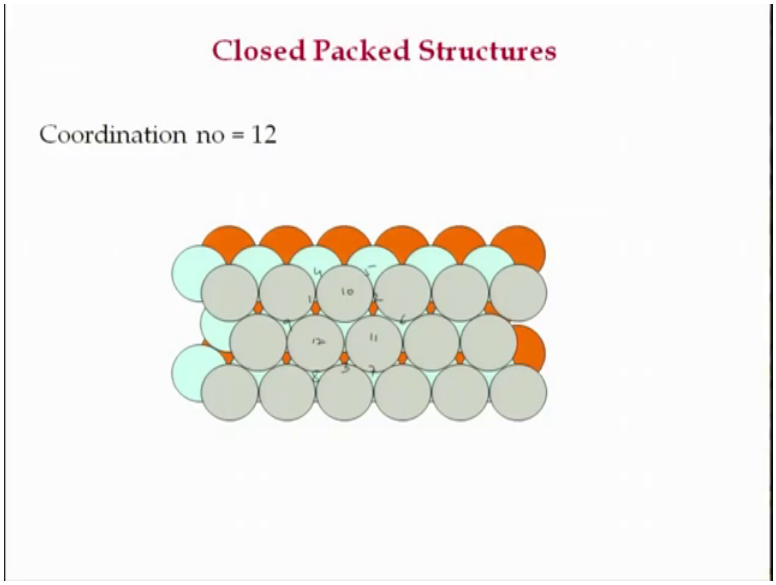

This is the first layer this is the second layer so, it has 3 below, 6 within plane, you can see that 3 below are the ones which are 1 2 3 all right 6 within the plane 4 5 6 7 8 9 and 3 on top 10 11 12 and you can just fill it now. So, each atom has 12 nearest neighbours in FCC or HCP structure. This will have 12 nearest neighbours.

So, coordination number in case of this is 12 in case of BCC the coordination number is 8 which were obvious in case of simple cubic the coordination number was 6 we can see that number of nearest neighbours is largest in case of a closed packed structure.

As a result there is a quantity called as atomic packing factor which is highest in case of FCC.

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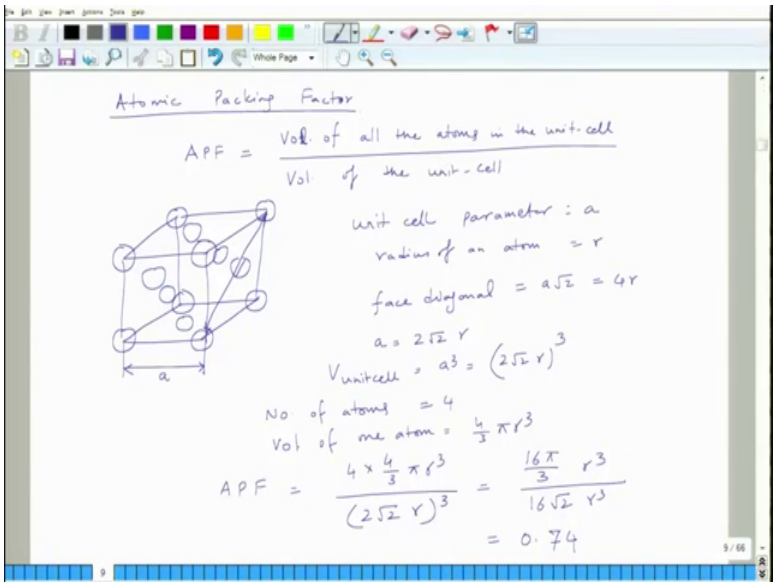

What is atomic packing factor which is A P F is basically volume of all the atoms in the unit cell divided by volume of the unit cell. So, let us say let us see in case of FCC, in case of FCC you have situation like this. So, I will not draw the atoms touching with each other, but they do touch each other for the sake of illustration. So, this is the scenario you have all right now what is so in case of FCC.

Let us say the unit cell parameter is a, so unit cell parameter is a radius of an atom is r. So, I can see that the atoms touch along the faces I know that the atoms touch along the faces if they touch along the faces then what is the relation between r and a. So, face diagonal length is equal to a root.

Student: 2.

2 this is equal to this is 2 r, this is 1 r, this is 1 r, this becomes equal to 4 r. So, a is equal to 2 root 2 r. So, volume of unit cell V unit cell is equal to a cube which is equal to 2 root 2 r cube all right now volume of so, and how number of atoms are 4.

Student: 4.

Volume of one atom is 4 by 3 pi r cube. So, APF can be worked out as 4 into 4 by 3 pi r cube divided by 2 root 2 r cube. So, this will be 16 by 16 pi by 3 r cube this will be equal to 18 2 16 root 2 r cube and this will work out to be point nearly 0.7 4 I think. So, this is how you determine the atomic packing factor.

So, as an exercise you can take determine the atomic packing factor of BCC simple cubic and HCP structures.

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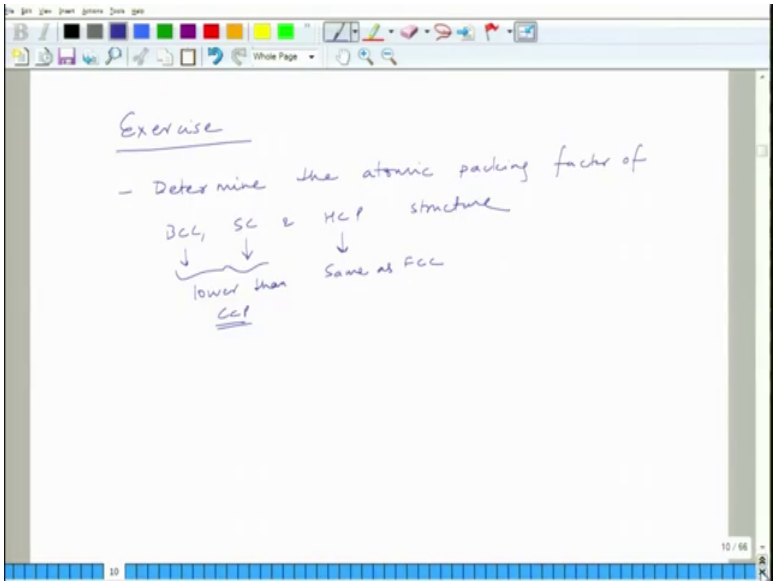

HCP you can see it will come out same as FCC because both are closed packed structures. So, FCC it will be same as FCC, but it is determined in a different manner it is not it is not the same manner as FCC simple cubic and BCC will be lower than CCP, but you need to work out what these numbers will be you can see by intuition that FCC HCP is the highest, BCC is the second highest and HCP is the a simple cubic is the lowest.

So, this will be the atomic packing factor of these materials the last thing I wanted to cover in this perhaps if you would not to be able to go to interstices is in case of HCP crystal HCP lattices.

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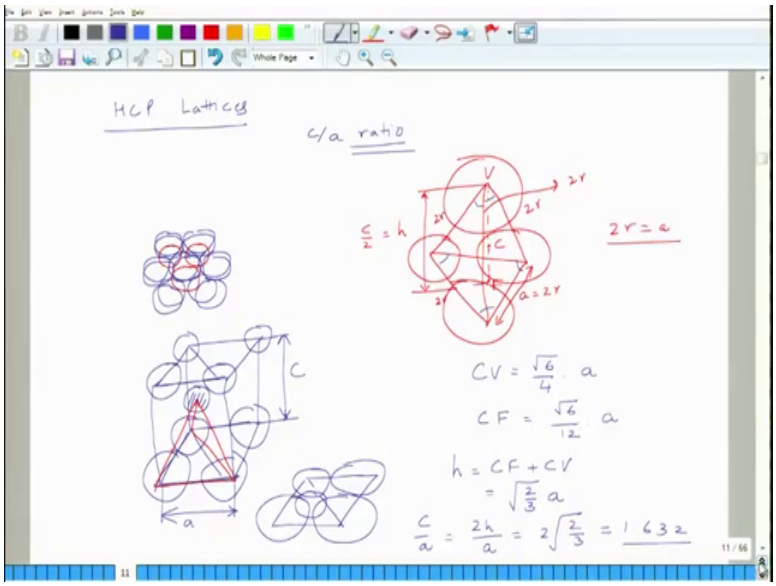

There is something called as c by a ratio, now in case of a hexagonal closed packed we know that there is a and the next set of atoms goes one goes here another goes here and another goes here this is the b layer and the another next layer will again be it will be this layer and slightly displacing it. So, that it is clearer to you it will be this layer, it will be this layer, this layer and it will be this layer.

So, basically what is the a parameter in this case if you just take the now if you just draw the unit cell, the unit cell is something like that you have one atom here, one atom here, one atom here, one atom here, another here, another here, another here, another here and one in between, between these 3 atoms and these 3 atoms right between these 3 atoms you have one atom. So, this is the atom so, this is one triangle if you just draw the top view top view would be like this, this is one atom, this is another atom these are all become little and this will be sitting here.

So, what we need to determine is if this is a, this is c, when atoms are touching each other what is the ideal c by a ratio in a FCC structure. So, basically we need to find out so, if you look at the structure now ideal c by a ratio if this atom if you connect this atom with the atoms below, if you connect this with that, this with that, this with the, what does it make, it makes a tetrahedron right it makes a regular tetrahedron.

So, basically what you have here is you have something like that a regular tetrahedron like this which was a height let us say this is the. So, if I just draw so, this let us say is

the centre of this tetrahedron. So, let us say this point is a, the distance between these 2 is h, which is equal to c by 2 all right.

So, we need to determine these points this is V let us say this is F and the centre and the centre of this octahedra tetrahedra is somewhere which is called as c. So, by geometry now you need to work out that. So, you know that these distances are, what is this distance, this is a which is equal to 2 r because you have an atom sitting here right, you have a atom here, you have a atom here, you have a atom here and you have a atom here, they are all touching each other right. So, all the sides are 2 r and this is 2 r, this is 2 r, this is 2 r and even this one is 2 r all of them are 2 r and 2 r is equal to a, we need to find out what h is which is c by 2.

So, by geometry you can work out this distance CV is equal to root of 6 by 4 into a and CF will be equal to root of 6 divided by 12 into a and we know that h is equal to CF plus CV. So, this will be root of 2 by 3 into a and ideal c by a ratio in this case will be equal to 2 h divided by a, which is equal to 2 into root 2 divided by 3 and this will be equal to 1.6 3 2. So, I will leave it to you as a homework to work out this analytically what will CVV, it is simple geometry nothing else these are all equilateral triangles, but the angles between the apexes being 60 degrees.

So, this is the 60 degree angle, this is 60 degree, this is 60 degree, this is 60 degree, this is 60 degree, this is very simple straightforward geometry and try to work it out and there are plenty of books from which you can take the help. So, CV will you need to first determine what is CV and then you need to determine what is CF and once you determine these two using geometry you can determine, what is the height of the tetrahedron all right.

So, this is where we will end this lecture in the next lecture we will talk about interstices in these in these structures and the structure of some common metals and alloys.