An Introduction to Materials: Nature and Properties
(Part 1: Structure of Materials)
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Lecture - 16
Interstices
Solid Solution and Alloys

Ok. So now, let us get on to the next lecture which is lecture 16. So, in the previous lecture, we talked about packing in solids basically metallic solids. We looked at how do atoms pack in these materials? What is the atomic packing factor? What is the coordination number? And we also looked at in the beginning, we looked at other two type of lattices which are BCC and Simple Cubic Lattices which are not close packed ok. Close packed structures, i have CCN, HCP, BCC and simple cubic are non close packed structures, but they do have we do have certain metals which follow those structures. As a result, we need to know about them.

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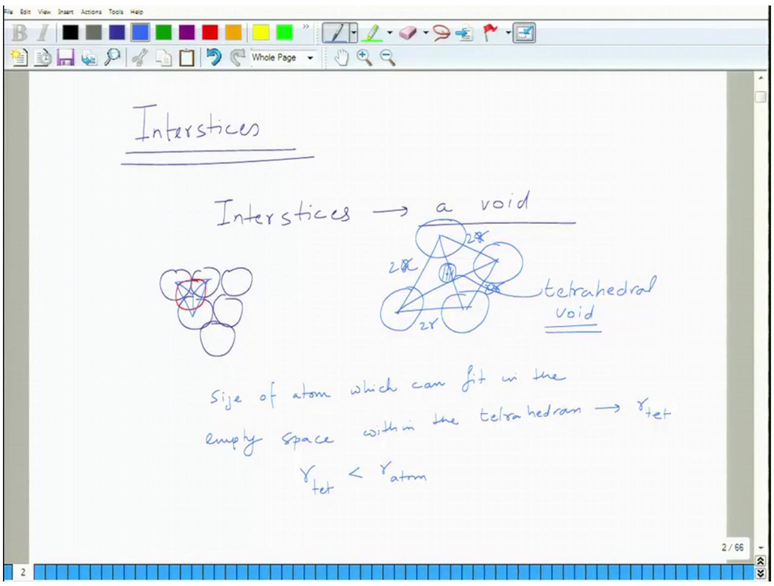

So now, we will talk about new topic in this metallic materials which is essentially Inter stices. Interstices is basically an Interstice is in is a void ok. We can see that, since atoms are spherical in nature, they do not completely they do fill their space but there are voids which are empty ah, there are empty spaces within the lattice.

So, as a result so, for example, if you see this particular kind of arrangement ok, you can see I can put an atom here on top. The next layer goes here, all are same atoms. The red is only for the sake of illustration, but you can see that within the within this body which is made by 3 atoms at the bottom and 1 atom on the top, this body is called as if all the atoms were of same sizes, I can create a body by connecting the centers of all the 4 atoms ok. 3 at the bottom, 1 at the top, this body is called as a Tetrahedra.

So, basically a tetrahedra is something like that you have a. So, I will have to draw a little oblique shape. This is sort of an tetrahedra where one atom is here, another atom is here, another atoms is here, another atom is here. And I mean, you have certain space lying at the center of the tetrahedra. So, the space which is available at the center of tetrahedra, you can fit a certain size of atom there so obviously, that atom is very small. So, the size of atom which can fit in the empty space within the tetrahedron is called as r tet. Let say and this r tet is much smaller than r, r of the radius of the host atom.

So, we will we will see what the size is. So, this size where you can make a smaller atom sit here, this is called as a tet the space in which an atom sit. This is called as a tetrahedral void. So, you have a tetrahedral void here. Similarly, you can have tetrahedral void underneath. So, various so, as long as you have this ford atom body which is symmetric in nature which is a regular tetrahedron you will have a tetrahedral void. Tetrahedral does not need to be regular. We will see in certain cases tetrahedra is not regular, but as long as it has a shape of a it is. So, you can see that how many sides does it have? It has 3 on the to the 3 on the top and 3 at the bottom right. It has total of 6 sides.

Now, as long as you have 6 sides body, which is which looks like a tetrahedral, it can be tetrahedral, it does not need to be regulated tetrahedral. In this case, it is a its let us say 2 r, 2 r, 2 r, 2 r, but in some other case all the directions all the dimensions may not be equal. So, we will need it to be careful about it, but in FCC and be HCP structures it is a regular tetrahedral.

So, this is the tetrahedral void. Then you might have something called as an Octahedral void.

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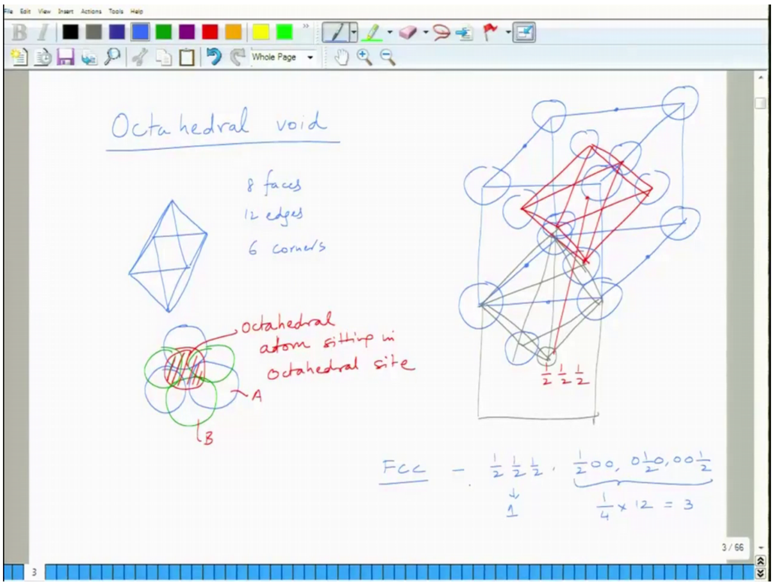

So, here in this case, you can see that this has 6 edges and 4 faces. In case of octahedral, oh octahedral is a body like that. Connect an edge, edge here, you connect edge there, you can edge here, you connect edge there, it has apex here. So, it has 8 faces and 12 edges and 6 corners.

And in this case, how many corners you had? You had 4 corners ok. This is the description. Now this Octahedra can be found in an in a ABC-ABC or AB-AB kind of packing. The configuration looks something like that. So, you have an atom sitting here, the next layer goes there and the next layer which comes on top, it does not need to go exactly on top of A, it can go to C. So, you will have this kind of a. So, this guy which is sitting at the center is surrounding by 3 at the bottom and 3 on top. It has 6 possibility of 6 coordination. So, this small atom, so this should be small actually, I have drawn it bigger, but this should be small. So, 1 bit. So, this is basically in octahedral atom sitting in octahedral site.

So, this is my A layer, this is my B layer, between the A and B layer, I have a octahedral void. How do you visualize this? You can visualize this. So, this octahedral is a little tricky to visualize. So, let me show you first the FCC structure. It is easy to visualize in case of FCC structure. It is difficult to visualize in case of HCP structure ok. The octahedral void in this case is made by connecting the sorry, one atom will be here as well. You connect these phases. This is the octahedral void in case of a FCC structure. And the location of octahedral void is half, half, half ok. Find out the size which we can do in a short while. So, this is the octahedral void that you can format half, half, half position. Are there any other octahedral voids present in a structure ? No, not on surfaces, on edges; so, this will be one octahedral void, this is another octahedral void. So, how do you form an octahedral here? So, because you can always, if I use a different color.

This is you will have an atom here sitting here, somewhere here and the neighboring unit cell right. This will connect to that you can again connect this to the atom at the face center. And the one at the bottom face will also be there right. So, this will again connect to. So, this will be octahedral void. So, all the edges will also be octahedral. Center of the edges will be octahedral void locations.

So, the octahedral voids in case of FCC are located at half, half, half; half, 0, 0; 0, half, half and 0, half, 0 and 0 half ok. And since each edge is shared by 4 unit cells, as a result since there are 12 edges, so, this will contribute to 1, these will contribute to 1 by 4 into 12, 3. 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12 but since each is shared by 4 unit cells, 12 divided by 4 is equal to 3. So, you have total of 4 octahedral voids within a FCC unit cell.

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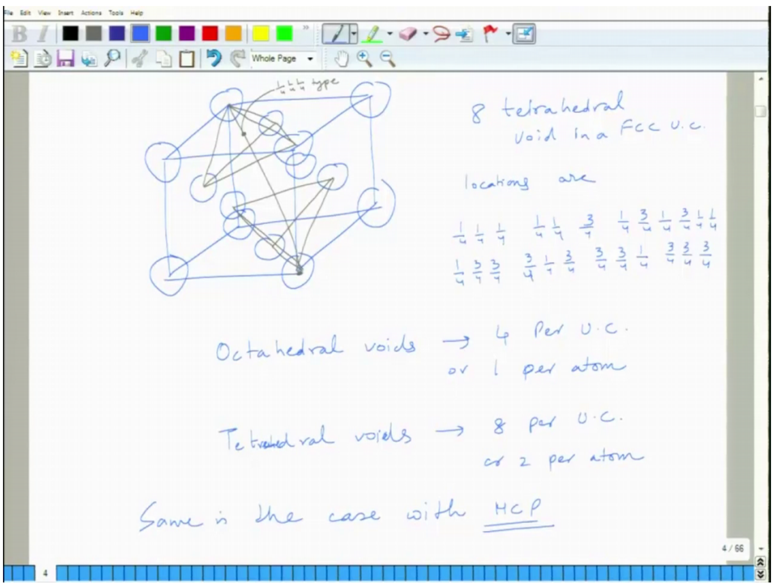

So, and tetrahedral void on the other hand in FCC structure lies at ok. Tetrahedral void lie lies at the position which I am going to show you now. If you connect this atom to the board then atom here, a atom here and with an atom here. And if you connect these places with each other, this will make a regular tetrahedral ok. Similarly, if you connect this atom with this atom, this atom and this atom and if you connect them with each other, you will make a tetrahedra. So, these are basically tetrahedral voids. They are located along a body diagonal. So, this position is 1 by 4, 1 by 4, 1 by 4 type. So, tetrahedral voids there are. So, you have 4 body diagonals and you have 2 on the each co near the each corner.

So, as a result you have 8 tetrahedral void in an in a FCC unit cell. Locations are 1 by 4, 1 by 4, 1 by 4, 1 by 4, 1 by 4, 1 by 4, 3 by 4, what else? 1 by 4, 3 by 4, 1 by 4, 3 by 4, 1 by 4 and 3 by 4, 1 by 4 and then you will have 1 by 4, 3 by 4, 3 by 4, and you will have 3 by 4, 1 by 4, 3 by 4 and then you will have 3 by 4, 3 by 4, 1 by 4 and then you will have 1 by 4, 3 by 4, 3 by 4 these are 8 locations that you will have. So, in a FCC unit cell octahedral voids are 4 per unit cell or 1 per atom because there are 4 atoms an FCC unit cell right. Tetrahedral voids or 8 per unit cell or 2 per atom same is the case with HCP.

Okay same is the case with HCP because both are close packed structures, they have same, but this are this is the arrangement is different. So, for example, for FCC.

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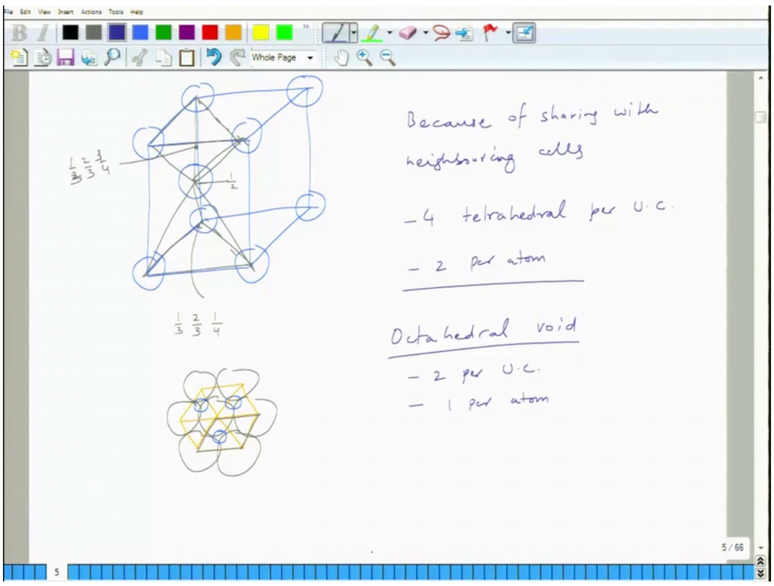

So, for FCC, HCP a tetrahedral void this is one atom, this is one atom, this is one atom, this another one and now if i just make sort of a within this somewhere you have one this atom sitting. So, one of the tetrahedra which is made is this.

So, I. So, this is one of the tetrahedra that you have; another tetrahedra of course is this. Though this is one tetrahedral void, this is another tetrahedral void. So, what is the sa what is the location of tetrahedral void in this case; this tetrahedral void is that 1 by 3, 2 by 3 sorry, this is at half this is half; what is this location? 1 by four 4, this is at 1 by 3, 2 by 3 and 3 by 4 now, but there are only 2 tetrahedral voids here. Where are the other 2 tetrahedral voids. Now if you look at that top view of a hexagonal unit cell; this is the top view of hexagonal unit cell. So, the unit cell is you have one atom sitting in lets say if this is the if this is my first unit cell ok, I am saying that one atom is sitting here; the second atom got to be sitting here and the third item is got to be sitting somewhere here.

So, you can see that these 3 give you 1 tetrahedral void, but remember these 3 these atoms also share that a tetrahedral voids on the sides. They are sharing tetrahedral void of the neighboring unit cell. So, those 2 neighboring unit cells contribute to the oct tetrahedral void of this unit cell. So, as a result you have because of sharing with the neighbors just like an FCC right because of sharing with neighboring cells, we have 4 tetrahedral voids per unit cell and each unit cell has 2 atoms, as a result its 2 per atom. Similarly, octahedral void is 2 per unit cell or 1 per atom. So, let me show you how the octahedral void looks like I show you it is a little difficult to draw.

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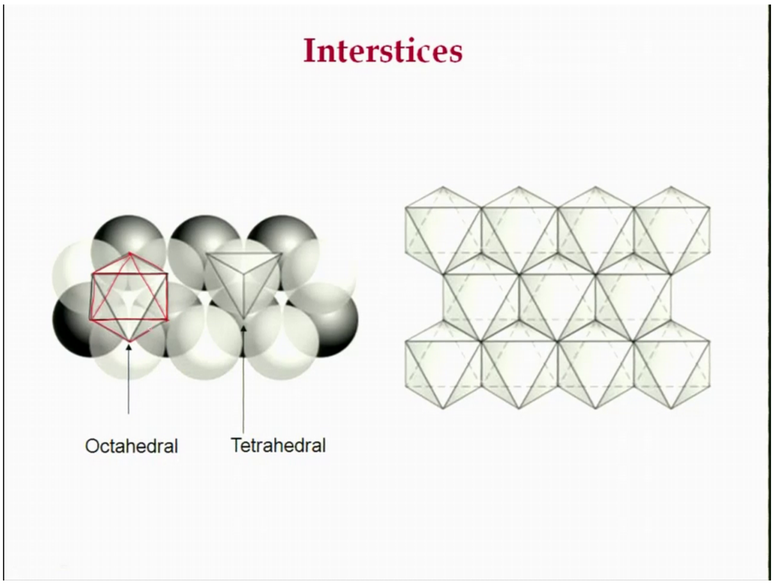

So, this is how the octahedral void looks like in FCC. So, this is the bottom one is the first layer, the lighter one is the second layer the top layer. So, you can see 3 atoms at the bottom; 3 atoms on the top between them there is octahedral void. So, this octahedra is a bit tilted octahedra.

So, the first 2 atoms here, so let me just now draw. So, this is the square shaped body this one alright and this is one apex and this is second apex ok. So, if you connect now; you connected here connected here and of course, you can connect have to you will have to connect there as well and then you connect to here and you connect to here. So, its octahedra which is a tilted octahedral. It does not look like as if it is a standing octahedral; it is a tilted octahedra within the unit cell right. So,. So, this is how the octahedral are arranged you can see on the right; these are the various octahedras within the hexagonal unit cell. So, you will have total of 2 octahedra is per unit cell.

So, now these octahedral and tetrahedral voids are of lot of importance. So now, we need to consider what is the size of these octahedral tetrahedral voids. Let us take the example of.

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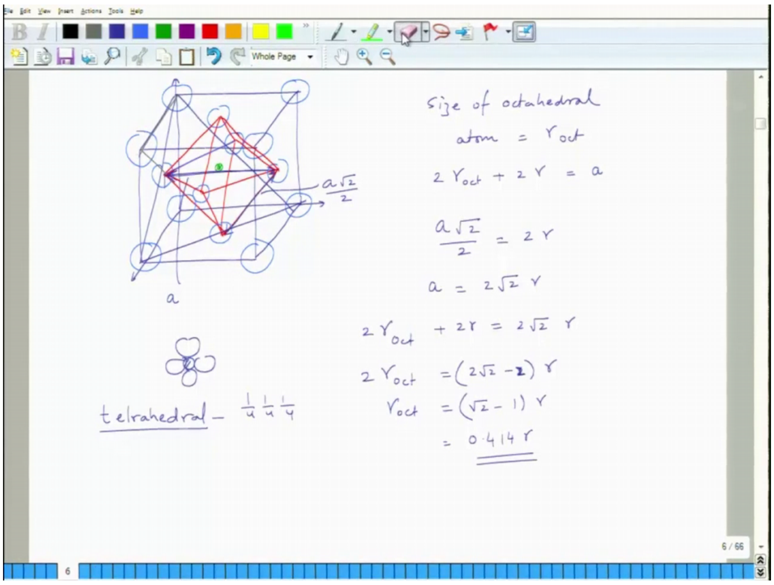

Let us take the example of FCC unit cell because what will go in them is determine quite a lot quite strongly by the size of this, size of the atom which is dependent upon the size of octahedral void. So, let us say, we have these atoms at various locations ok; one atom here, another here, another here, another here; we are saying that my octahedral is sorry this is my octahedral void.

The atom which goes in there is some where there. Now if you of course, atoms are not touching here; if you make a 2D view of this. So, what is this length.

Student: a.

A this is a, very good. And these lengths are a root 2 by 2 there is nothing but phase diagonal right. So, the size of let us say the size of atom which fits in the octahedral interstices is equal to r oct and so, I know from this is that this is equal to then will become. So, since these atoms are not touching each other, you will have situation like this, you will have a atom sitting here, smaller atom here; you will have an atom here. So, you can say that r oct plus 2 r that say just r is equal to a. And what is the relation with respect to r and a, we know that these two atoms touch each other right. So, or if you, so this is the 1, 1, 1 plane.

. So, if that is the case then the distance between this and that atom, this distance the distance between this and that atom is nothing but a divided by root 2 by 2; this is equal to 2 r. So, I can now find. So, there is a relation between. So, I can write this a to be equal to 2 root 2 div into r. So, r oct plus 2 r is equal to ok. So, r oct is equal to 2 root 2 minus 2 into r and this will work out to be.

So, this is how you will determine this 2 r yeah this is 2 r yeah, this is the mistake that we have made. So, this is 2, two 2's will cancel each other. So, this will be r oct will be equal to root 2 minus 1 r root 2 is 1.414. So, this will be 0.414 r. So, thats what I was wondering that number have gone somewhere wrong. So, this is 2 r oct.

Because remember this is 2, 2 of r which is diameter. So, 2 r oct plus 2 r is equal to a and we know that a root 2 by divided by 2 is equal to 2 r by the geometrical relationship FCC unit cell yes the replace a in terms of r and what you get is r oct. So, the maximum size of the atom that can fit in octahedral void is 0.414 of the radius of the host lattice and the same is true about hexagonal lattice as well.

Similarly, if you now need to find out the size of octahedral atom, size of octahedral atom in case of HCP its easier because the atom sits at tetrahedral sorry, in case of tetrahedral void, since its at 1 by 4, 1 by 4, 1 by 4, the distance between this point and the apex is. So, let us say if this is the tetrahedra I will, I will probably do it on the next page.

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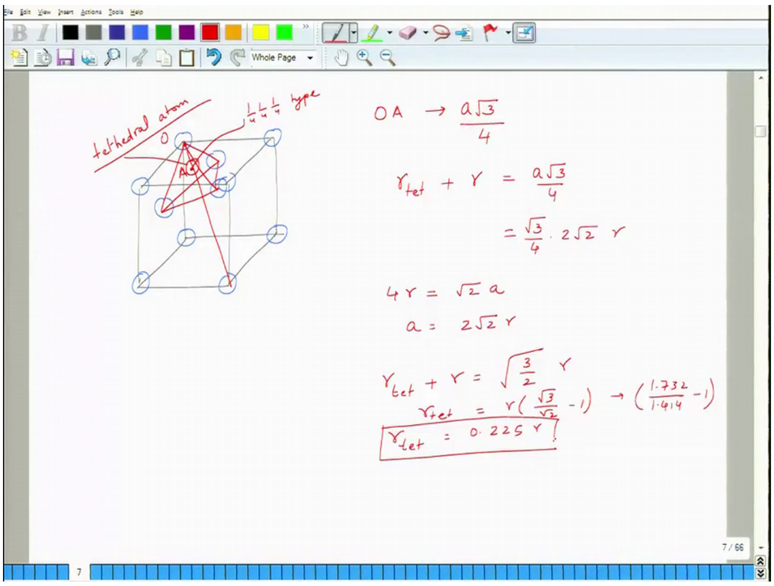

So, I will just draw these 3 atoms ok. One at the center tetrahedra is made by connecting this atom with this atom, this atom and this atom. This is tetrahedra all right. Our atom is sitting somewhere here this location is 1 by 4, 1 by 4, 1 by 4 type and this connects the body diagonal. So, if this is O, this is A, that distance OA is diagonal is a root 3 and this will be 1 by 4 of a root 3. So, if you have an atom here which is small atom this is which is tetrahedral atom which does not distort that tetrahedral just sits in there snuggly without distorting the tetrahedra. So, then this r of tetrahedral atom plus r of host is equal to a root 3 divided by 4. And what is a in terms of r? Root 3 divided by 4 in to in case of FCC, we know that 4 r is equal to root 2 a. So, a is equal to 2 root 2 r.

So, r tet plus r is equal to root 3 by 4. So, sorry I have I am doing it again. So, I just substitute this by and this equation as 2 root 2 r. So, this will be r tet. So, r tet plus r is equal to root 3 by 2 div into r. So, as a result you can write this r tet to be equal to if you just work this out this will be nothing but is equal to. So, r tet will be equal to r into root 3 by root 2 minus 1 which is nothing but 1.732 divided by 1.414 minus 1.

So, you can see that this is more than uh. So, this will be 0.225 r. So, this is the maximum size of atom that can fit in a tetrahedral void without distorting that tetrahedral void ok. So, the similar size of atom you can also do tetrahedral void calculation just by drawing a tetrahedron. So, if you just make the simple picture of tetrahedra.

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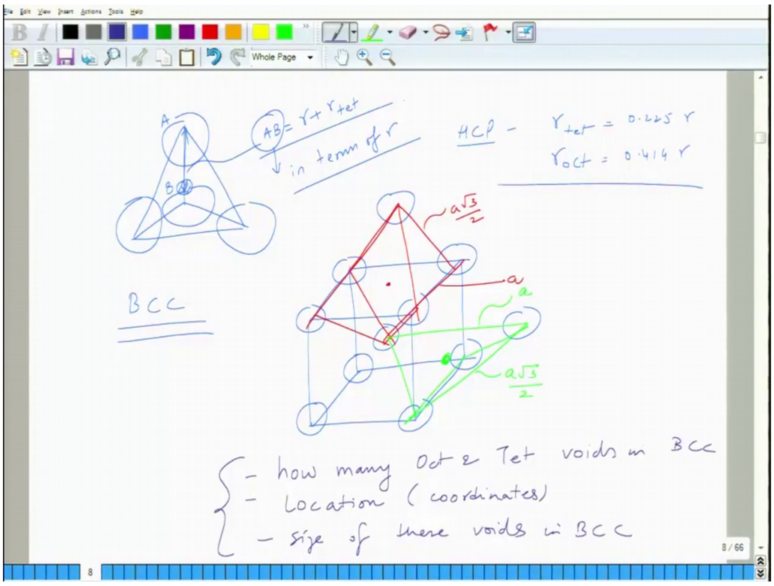

So, this is your tetrahedra for example, and the atom which will fit somewhere here at the center of the tetrahedral, these are all touching atoms there.

So, just like you do that calculation for c by a, you can do the simple calculation of. So, that if you if you remember we worked out two distances c v and c f ok. So, you just have to work out this distance from the center to center. So, this distance is equal to lets say if this is A, this is B, AB is equal to r plus r tet. So, you need to work out a in terms of AB in terms of small r using the geometrical methods of a simple tetrahedron.

So, this will again give you the same relation; octahedral void remains the same and so, in case of HCP also r tet is equal to 0.225 r and r oct is equal to 0.414 r. Things are not same; now this is about the close packed structures. Things are not same in case of BCC. In case of BCC, since BCC, is a it is not a closed pack structure, but it does have voids; you know it is not a closed pack structure as a result it has voids. You have one atom here, here, here, here, here, here and one here. It has voids, but these are their all distorted voids. So, for example, the octahedral voids in case of BCC, these are the octahedral voids.

So, this is the octahedral void, but this is not a regular octahedron because all the sides are not equal. This is a root 3 divided by 2 and this is a as a result its not a regular octahedron ok. So, this is these kind of octahedral voids are present in BCC, what is that tetrahedral void? The tetrahedral void is basically if I draw another atom on this side and tetrahedra by different drawing by different color maybe this color. So, this is a tetrahedral, this is a tetrahedra center of this will be tetrahedral void, but this is a again a irregular tetrahedra because you can see that this length is a this length is a root 3 divided by 2.

So, as a result sizes are not the same. So, I will leave it to you as a homework that how many octahedral and tetrahedral voids in BCC locations, determine the exact location in terms of coordinates and the size of these voids in BCC. So, by it is a fairly straight forward thing to work out because you remember that you have to take the shortest size you do not have to take the longest size. There will be two sizes one; so depending upon which distance you take it will be long and short, the smallest that can fit is the given by the shortest ok.

So, these are the octahedral and tetrahedral voids which are present in metallic structures these voids are useful because the impurities go in them and because nothing is pure in nature; steel contains carbon. So, as a carbon is smaller atom it goes to interstices and that makes the steel stronger than pure iron. So, it is neat it is good to know about these interstices; these interstices is also important when we consider the ionic solids.

Because in ionic solids anions are bigger; cations has smaller; cations occupy the interstices sites. So, that is where the knowledge of these interstices is very useful. So, in this in the next lecture, we will talk about the solid solutions and alloys of metals and once we finish the metal part, we will move on to covalent solids and ionic solids ok. So, we have we have we have spent quite a bit of time on packing of solids the packing fraction coordination number and then the interstices and this has formed the basis of studying the substitutional interstitial solid solutions and alloys in metallic structures ok, finish it.

Thank you.