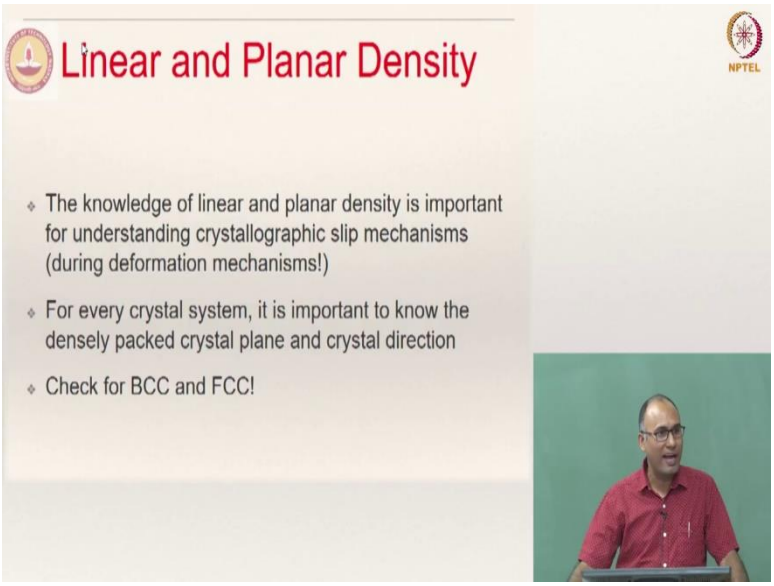
Basics of Materials Engineering
Prof. Ratna Kumar Annabattula
Department of Mechanical Engineering
Indian Institute of Technology, Madras

Lecture – 08
Crystal Structure - 6 (Planar density, Close-Packed Structures, Stacking Faults)

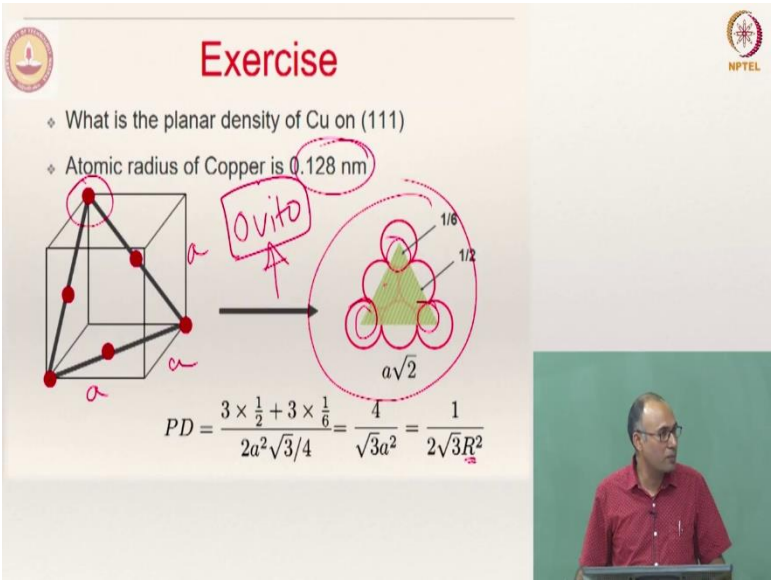
(Refer Slide Time: 00:24)



Alright, so in the last class we have seen the definition of linear density and planar density. Linear density means the number of atoms sitting on a crystallographic direction, divided by the length of the crystallographic direction vector. And similarly, we have also defined planer density.

So, we will see in the next module, we are going to talk about imperfections.

(Refer Slide Time: 01:08)



So, we have defined this linear density and planar density. If you see we have also discussed what is the most densely packed plane in FCC; and I said it is the (111) plane. I have asked you to go back and then check what will be the most densely packed plane in BCC. I hope you have done that.

So, how do you go about calculating the planar density, say for instance copper? Copper is an FCC crystal, and what is the planar density on (111) plane, given the radius of the atom to be 1.128 nanometers? Alright. So, that is our (111) plane. And if you look at the actual structure; in this case we are only representing the position of the atom; given the size of the atom and the lattice parameter, if you would actually look at the real scale, this is what you will see.

And then of course, when you are doing planar density calculations, you will realize that only 1/6th of this atom falls in that plane. As a result, you will have these three areas contributing to only 1/6th of it, and remaining three are $\frac{1}{2}$. So that is 1/6th, and the lattice parameter here is $\frac{a}{\sqrt{2}}$, by knowing this *a* and this as *a*. It is a cubic crystal, so we know that this is *a*, and this is *a*, and this also as *a*.

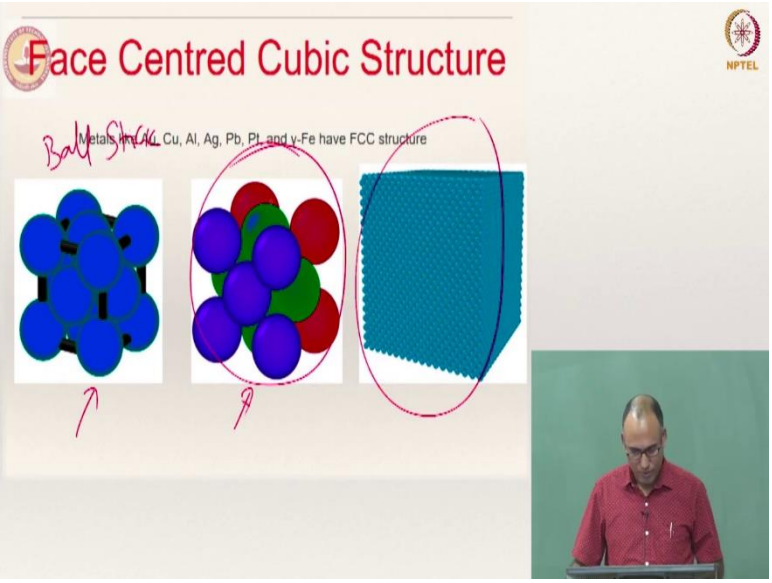
I suggest you guys to do is go back and try to choose an atom size, and all of you guys know Fusion 360, right? Try to construct this structure and then you will realize that is the closely packed plane. This can be better understood by doing it and if you are even more

enthusiastic, I suggest you guys to use this open source visualization tool called Ovito. It actually means open source visualization tool.

This is a really a nice tool wherein you can actually construct crystal structures, you can download the input files for FCC, BCC and other kinds of crystal structure. And look at how they are written and then you will be able to visualize them and you can cut the planes of your choice. You can actually visualize (111) plane, how the atoms look like and (110), (111), (100), and all the planes and then you can rotate. So, you will get a better feeling how all the different kinds of crystal structures look like i.e., BCC, FCC and HCP.

It is really a nice tool. We will see in one of the tutorial classes, I will show you how to use this, ok? Alright, so you can calculate the planar density by playing with number of atoms divided by the area of the plane. And then that will be your planar density, and you substitute the value for *R* given here and then you will get the planar density of (111) plane in copper crystal.

(Refer Slide Time: 04:34)



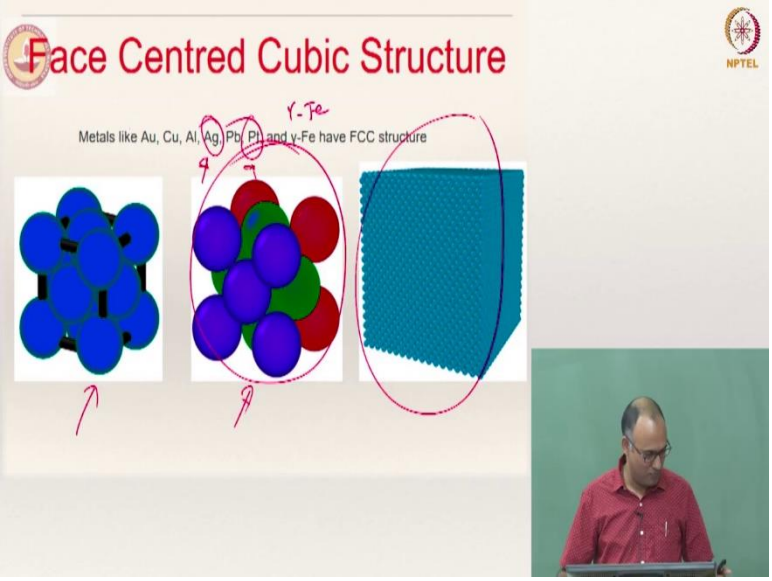
So, this is what we call the ball stick model. This is something that you can actually construct very nicely in Ovito. This is actually constructed in Ovito, this is also constructed in Ovito. And here this is an FCC crystal, but I have given three different colors.

I am showing you different planes. You can color that in that fashion so that you will get a good feeling for how the real crystal structure looks like and you can actually go inside

and see how the gaps are there, what kind of the free spaces are available, if you have an FCC structure and a BCC structure and so on. I seriously encourage you guys go back and try this; it will really enhance your understanding of these structures.

So, now you take this unit cell and stack it in 3D. Translate in *x*, *y* and *z* directions, and you will construct an FCC crystal lattice.

(Refer Slide Time: 05:51)



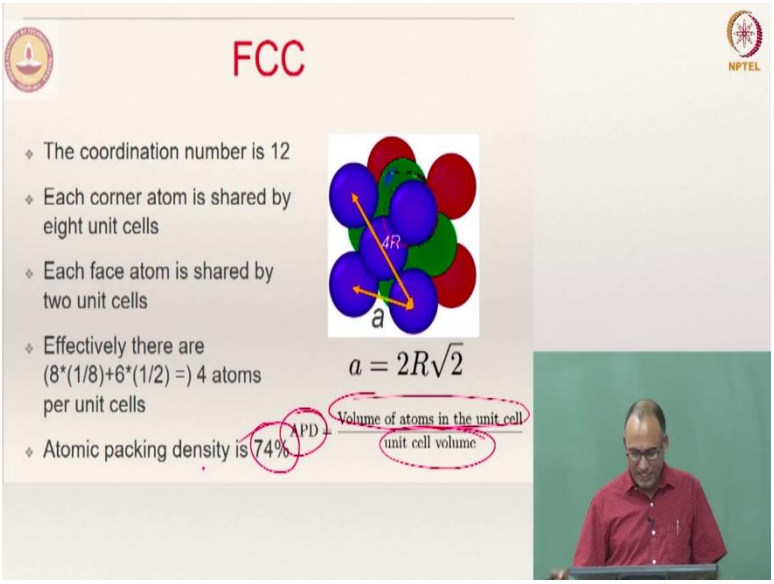
That is how it looks like in full 3D. Alright, what are the different kinds of materials or elements that you have in periodic table that have FCC crystal structure. I have only written couple of them. You can see gold, copper, aluminum, silver, lead, platinum, and γ-iron. They all have face centered cubic structure. It is good to remember what are the elements that have FCC, BCC and so on; at least the popular metals that you have familiar with.

In some sense, if we have to remember as Indians, the most expensive once are FCC, right? This guy, this guy; and if you want to take a gift or want to give a gift this is what you prefer, right? So, they are usually FCC.

(Refer Slide Time: 06:51)

In addition to what we have discussed in the class, I encourage you guys to go through these two YouTube links; they give a really nice explanation of the FCC, BCC and HCP; all three crystal structures that we are discussing in this class. I am sure that if you have patience and go through this video, you will have much better understanding of these systems.

(Refer Slide Time: 07:21)



So, we have discussed linear density and planar density. 1D is over, 2D is over and then 3D, right? Then we have talked about planes and then you need to talk about volumes. So,

that is what is called atomic packing density. It is a volume fraction in some sense. How is the packing density of this crystal structure? So, for instance, if we take FCC, what you need to look at is the volume of atoms in the unit cell divided by the unit cell volume.

What is the volume of this unit cell? The volume of this unit cell is a^3, $a = 2\sqrt{2}R$. So, you know the volume of the unit cell now by knowing the radius of the atom that you are taking. And if it is FCC you need to know volume of the atoms in the unit cell. How many atoms are there in a unit cell of FCC? When you are looking at the unit cell, if you want to find out how many atoms are there in one FCC unit cell, you also need to think about the surrounding environment.

You have to imagine a full 3-dimensional crystal lattice, and then see how each atom is shared by other unit cells. For instance, if you take one corner atom, one corner atom is shared by?

Student: 8.

8.

So, effectively you only have 1/8th of the atom belonging to a unit cell. How many such corner atoms are there? 8 corner atoms. So, all the corner atoms together will give you effectively 1 atom per FCC unit cell. And how about the face centered. Each face center is shared by?

Student: (Refer Time: 09:17).

2 unit cells.

So, effectively you have one-half an atom per face centered position. So, how many such face centered atoms are there in FCC? How many?

Student: 6.

6, very good. So, effectively you have three atoms. So, totally?

Student: 4.

4 atoms. You know the radius of the atom, so the atomic packing density for an FCC crystal is

$$\mathrm{APD}_{\mathrm{FCC}} = \frac{4 * \frac{4}{3}\pi R^3}{a^3}$$

For an FCC crystal what would that be? I want you to give me a number. How much? Louder.

Student: 80%.

Above 80% ok. So, she is saying 80%. You guys do not want to say anything!

Student: (Refer Time: 10:22) 70.

70.

Student: 72.

70 percentage ok. Any other numbers?

Student: (Refer Time: 10:27) 74%.

Student: (Refer Time: 10:28).

Why don't you just do a calculation and tell me Why do you have to guess?

Student: (Refer Time: 10:37).

It is a simple calculation right. 9?

Student: (Refer Time: 10:41) 7.

37?

Student: (Refer Time: 10:45).

37 you got?

Student: 73.

73 you got? 74 somebody get.

Student: (Refer Time: 10:53).

Simple multiplication and division seem to have different answers.

So, are you doing the fraction properly? The numerator should be total volume of atoms in the unit cell and the denominator should be volume of the unit cell. How many 74's? Just now changed. 68's? 73's? No. You change your mind?

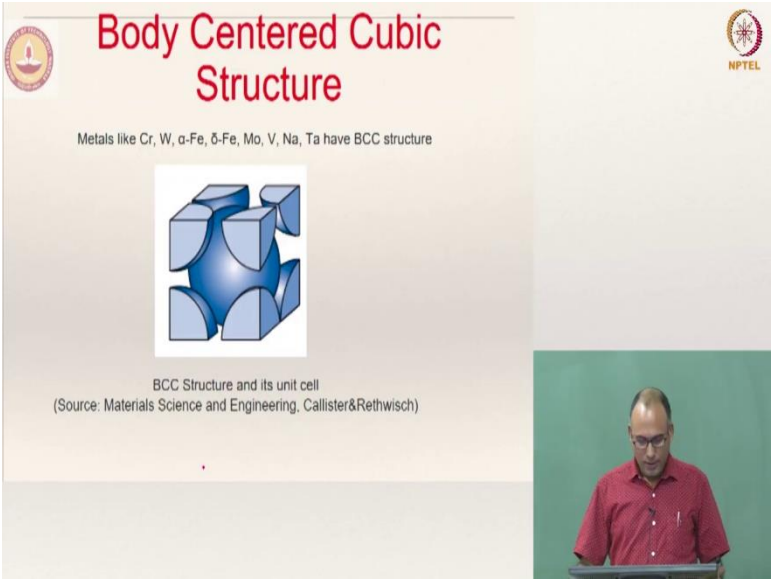
So, we need to think about certain properties of this crystal lattice. So, what is the coordination number? For FCC the coordination number is 12. What do you mean by coordination number?

Student: (Refer Time: 11:46).

How many nearest neighbors that a particular atom has in an FCC structure? Every atom in a FCC will have twelve nearest neighbors, that is what is called coordination number; you need to verify that, ok?

We have just now discussed each corner atom is shared by 8 unit cells, each face atom is shared by 2 unit cells, effectively you 4 atoms per unit cell. And then if you calculate atomic packing density, you should get 74 percent. FCC is known to be a close-packed structure. Amongst all the crystal structures that we have looked at, FCC is one of the closely packed structures. So, this is the maximum packing density that you can get for any crystalline material.

(Refer Slide Time: 12:47)



If you take BCC what would that be? So, this is your body centered cubic structure, right? How many atoms are there per unit cell?

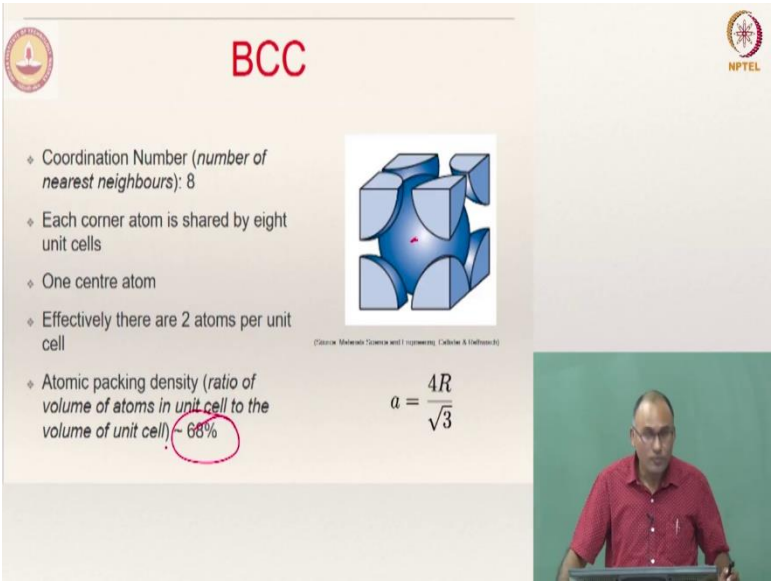
Student: 2.

2 atoms, very good. So, what are the elements that have BCC structure? Chromium, what is W?

Student: Tungsten.

And α-iron, δ-iron, molybdenum, vanadium, sodium, tantalum and many more.

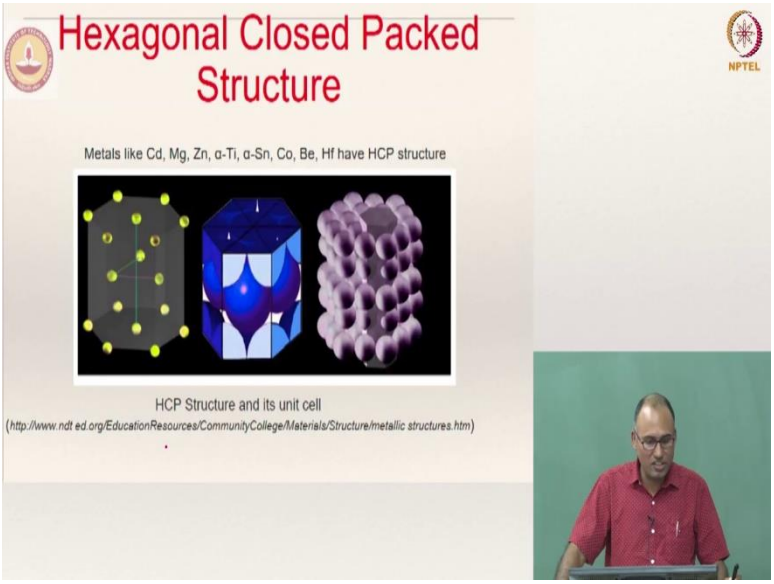
(Refer Slide Time: 13:14)



So, what is the lattice parameter for BCC? It is $\frac{4R}{\sqrt{3}}$ because only the body diagonal atoms are touching each other, right? The coordination number for BCC is 8. So, if you take a full 3D lattice; you can see any atom as a body centered atom or a corner atom depending upon how you choose.

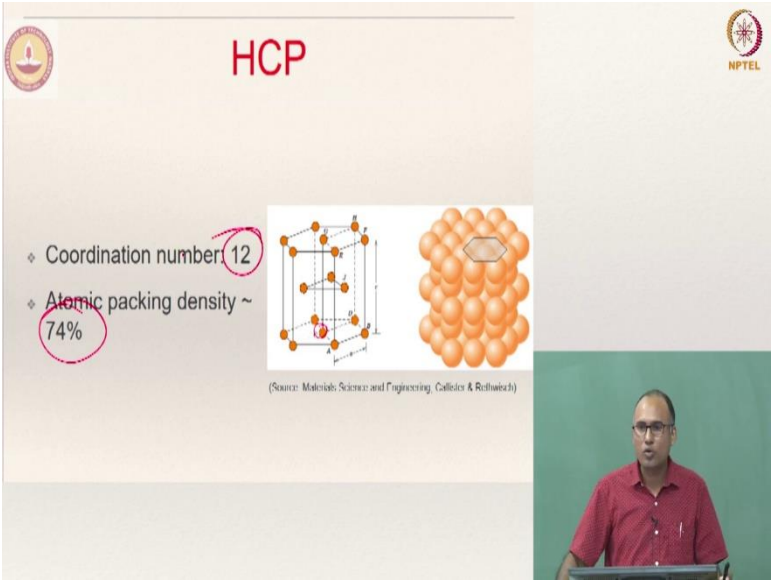
So, now you look at this body centered atom, it is surrounded by 8 atoms. So, that is how it is easy to say that is there are 8 nearest neighbors, ok? One center atom, effectively 2 atoms per unit, and the atomic packing density is 68%. So, FCC is more densely packed than BCC; which means, there is more free space in a BCC unit cell compared to FCC unit cell, keep that in mind. The packing densities of FCC and BCC you should be able to calculate on your own, if you cannot remember.

(Refer Slide Time: 14:29)



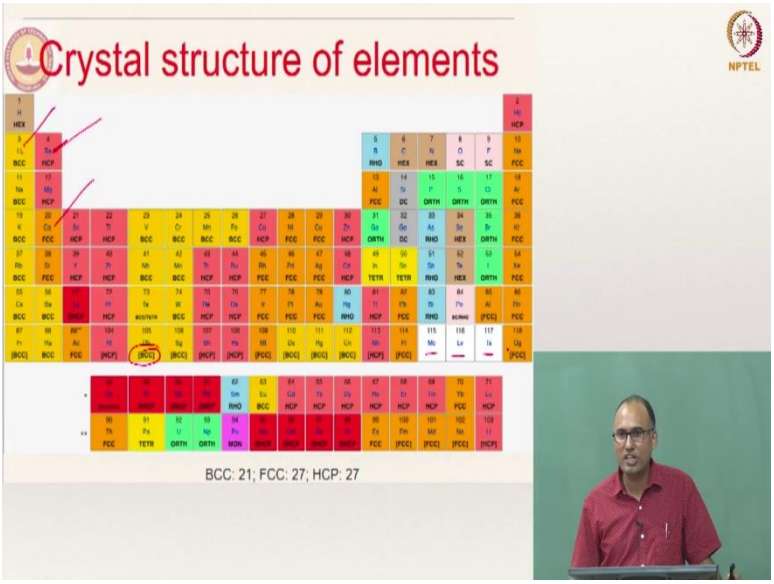
So, then you have hexagonal close-packed structure. The elements cadmium, magnesium, zinc, α-titanium, α -tin, cobalt, beryllium, hafnium, and so on, ok? They have hexagonal close-packed structure.

(Refer Slide Time: 14:47)



Again, HCP has a coordination number of 12 and atomic packing density of 74%, same as your FCC structure. You can calculate that and show. You can see that if you take this atom surrounded by 6 here and the next lattice 6. So, that that is why you can see that it has coordination number 12.

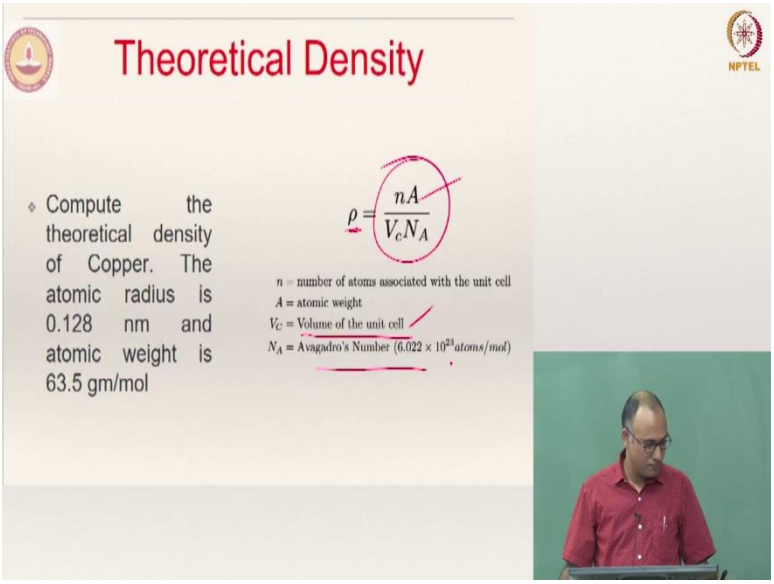
(Refer Slide Time: 15:13)



If you would look at the periodic table, these orange color elements are BCC and the -- this is pink right? The pink color is HCP. I am bad at colors; so, if it is not pink whatever it is, ok? And this is actually yellow and this is orange I think ok. All the yellow colored elements are BCC, orange colored elements are FCC, and whatever this color is that is HCP.

And I have actually tried to calculate how many elements are BCC, FCC and HCP. There are 21 elements which are BCC, 27 are FCC and 27 are HCP. And in this, you see that there are certain elements whose crystal structure is written in brackets, right? So, they are the predicted crystal structures, we probably do not know exactly their crystal structure. They are predicted theoretically, and they turned out to be BCC. That is why they have been written in brackets. For instance, we have no knowledge about the crystal structure of these elements.

(Refer Slide Time: 16:34)



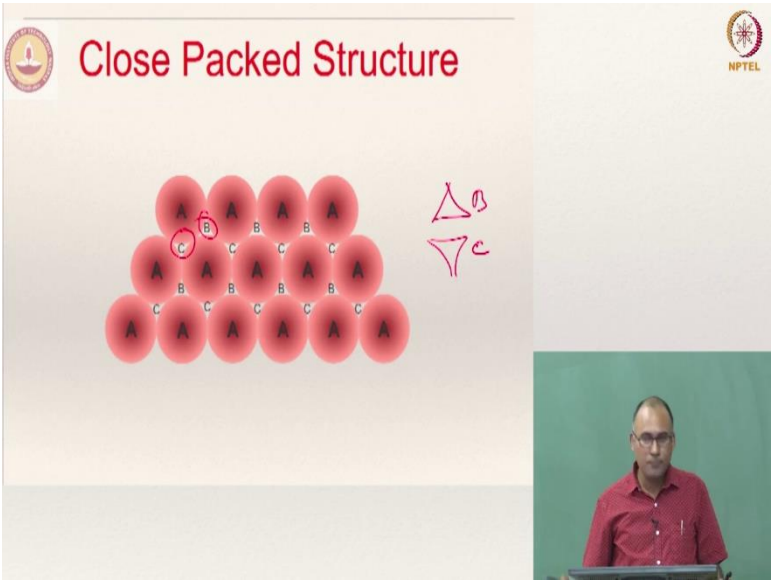
And then, how do you go about calculating theoretical density? This is something that you would have done in your plus 2, right? For instance, if you have to calculate the theoretical density of copper whose atomic radius is 0.128 nanometers and atomic weight is 63.5 gram per mol, you can do that calculation using the formula

I am not deriving this formula in the class, but I think this is something that you have learnt in your plus 2. If you did not please go back and verify your textbooks. It is also available in Callister.

Here, n is the number of atoms associated with the unit cell and A is the atomic weight of the particular atom that we are looking at. V_c is the volume of the unit cell. By knowing the crystal structure, you will be able to calculate the volume of the unit cell.

For instance, this is copper. Copper is which structure? Copper is FCC. By knowing the radius of copper atom, you can calculate the volume of the unit cell, and N_A is Avogadro's number that you know, right? So, you can actually calculate the theoretical density of copper.

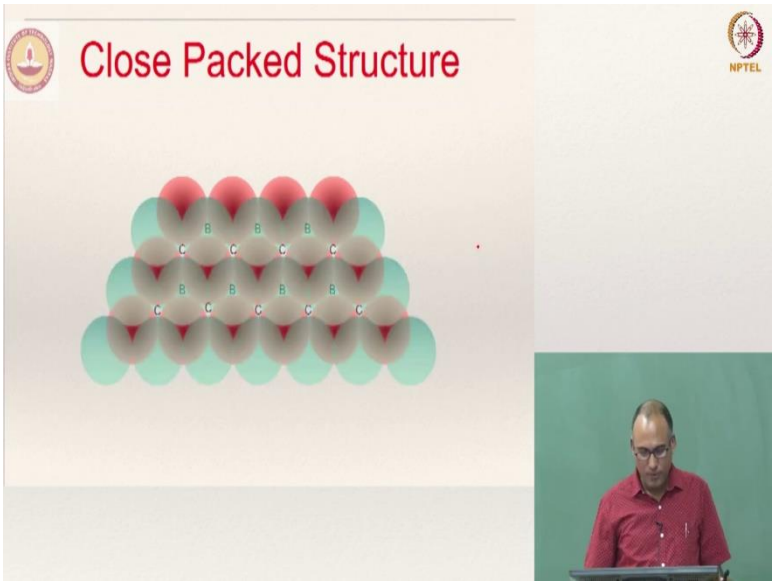
(Refer Slide Time: 17:51)



So, when we are talking about close-packed structures, we have said that both FCC and HCP are close-packed structures, but they are different in a subtle way. So, how are they constructed -- FCC and HCP structures? So, for instance, if you have all A's are atoms. So, you have constructed them in a close-packed way.

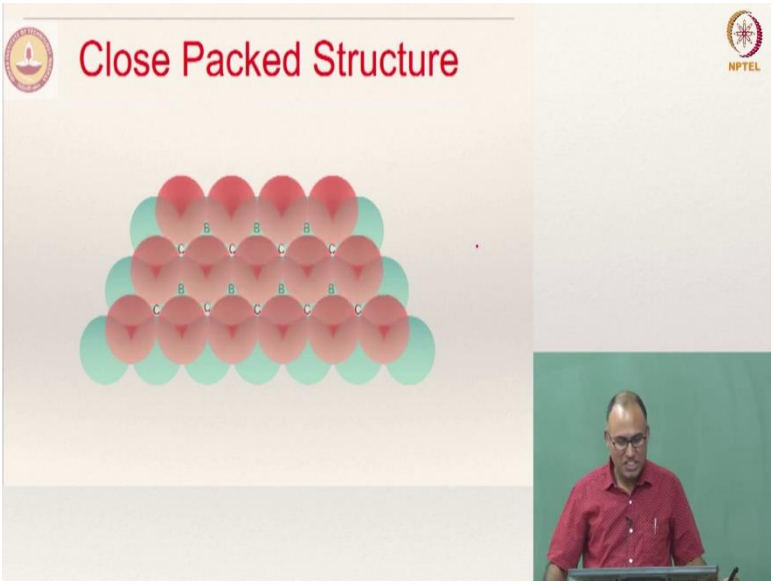
And now, you have 2 kinds of free spaces here. They are B type free spaces and C type free spaces. The B type free space is like that and C type free space is like that -- that is B type that is C type, right? Basically inverted. Are you able to see that?

(Refer Slide Time: 18:44)



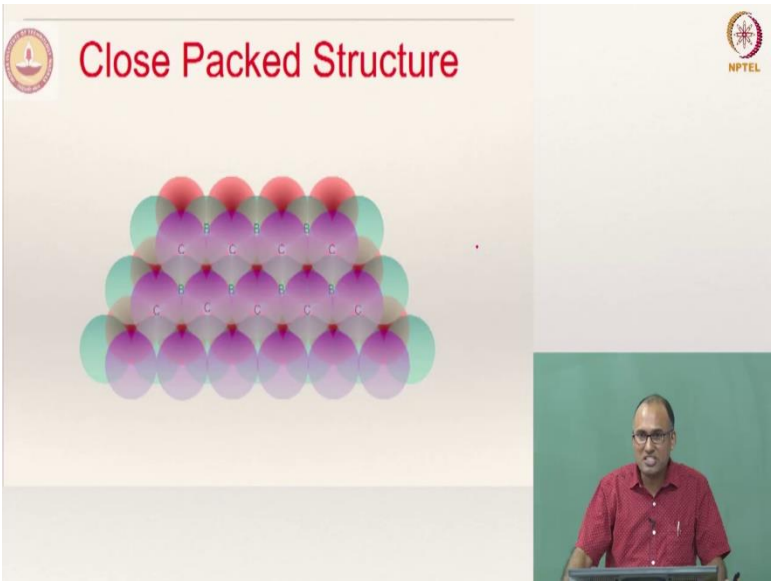
Now, this is the first layer of atoms. And now if I pack the next layer of atoms at B; now I have A and B. So, first I have stacked the A layer, and then the next layer of atoms are stacked at B position.

(Refer Slide Time: 18:59)

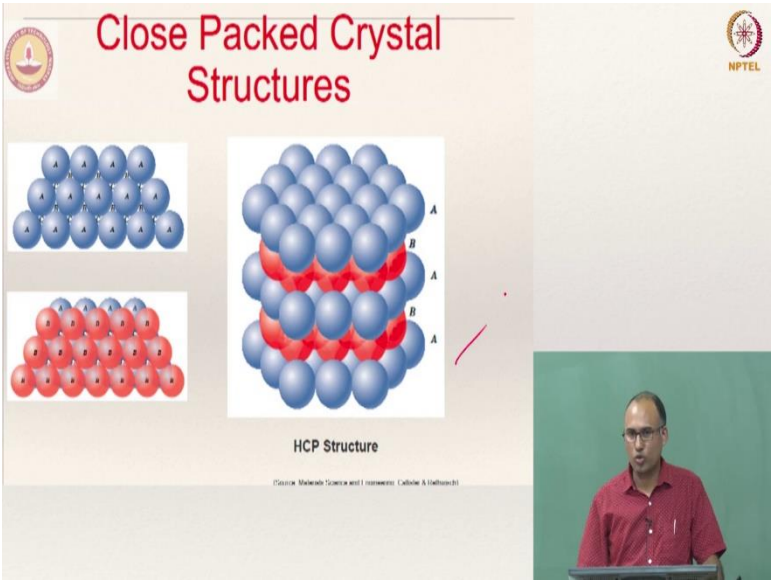


And if the next layer is stacked at again A position, then what you will get is ABABAB. Instead of doing that, if you do A then B and then C, then you will get ABCABC -- if you continue that, then you will have ABCABC. One of them will be HCP another one will be FCC.

(Refer Slide Time: 19:21)

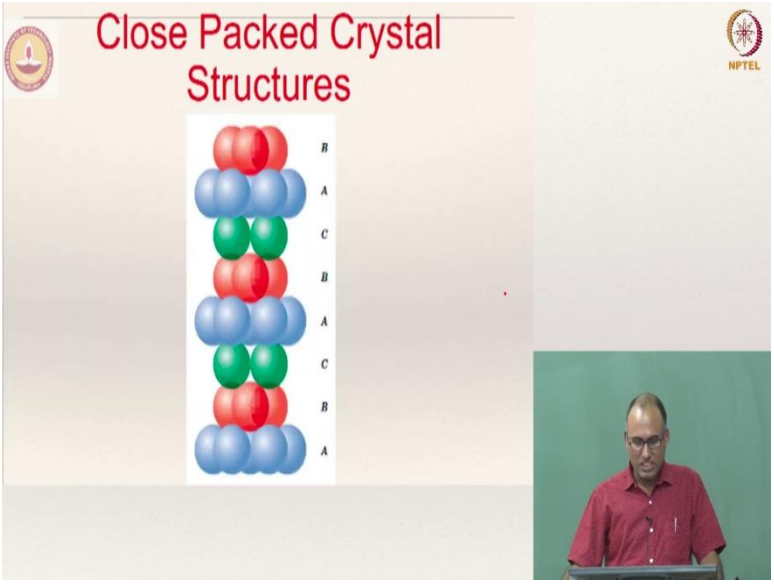


(Refer Slide Time: 19:27)



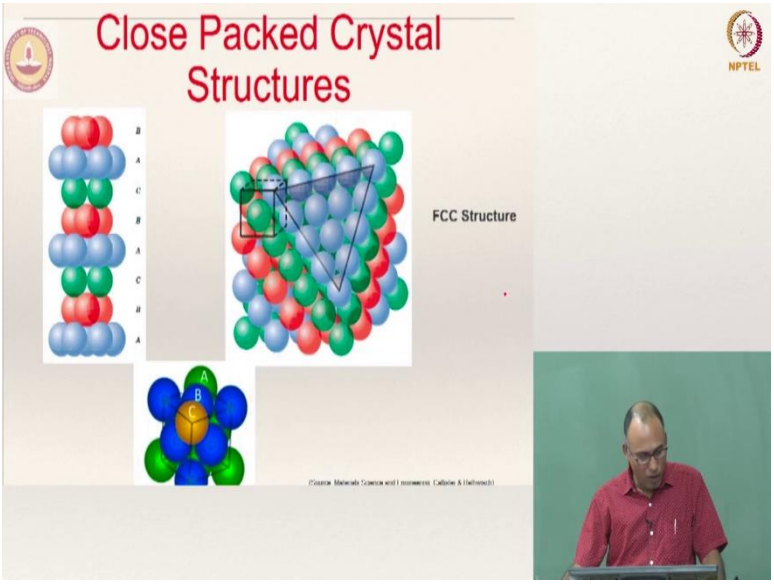
That is ABC. Previously we have seen ABABAB, now ABCABCABC. If you see that, this is your ABAB structure that leads to your hexagonal close-packed structure. If you have ABCABC, you will get face centered cubic structure.

(Refer Slide Time: 19:46)

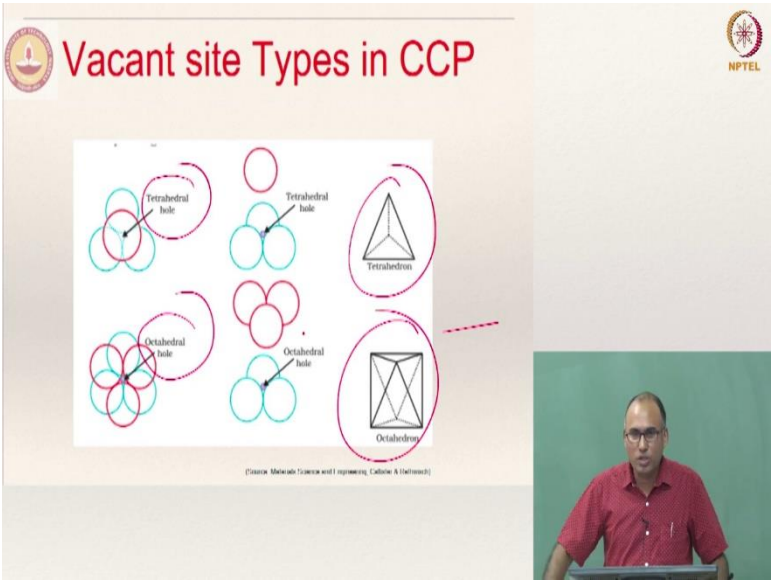


Again, I suggest you please go back and try to do this on your own, ok? So, this is your ABCABC structure.

(Refer Slide Time: 19:50)



(Refer Slide Time: 19:57)



So, you can actually construct these close-packed structures and then see how one can generate FCC and HCP structures. If you want to generate these -- if you want to saw your hands, all that you can do is you can have the steel balls and some neodymium magnets, right? And then use these two things together and then construct this AB, ABC lattices, and then you will be able to see the difference between FCC and HCP structure.

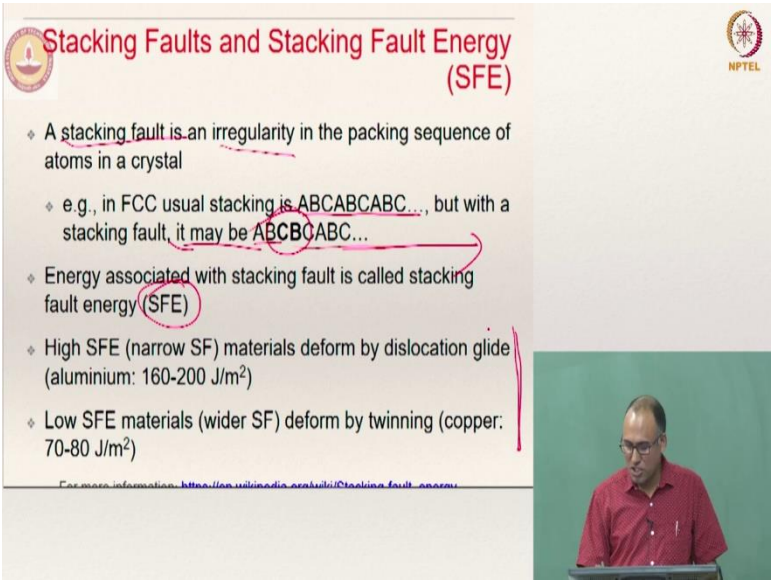
Alright, so this I will discuss at a later stage when we need to discuss about the vacant sites. So, we have just now discussed that in FCC and BCC you will have some free space,

right? There are different kinds of free spaces. One type of vacancy or vacant site is called tetrahedral site, and another type of vacancy is called octahedral site i.e., tetrahedral space and octahedral space.

This is your tetrahedral void space and this is your octahedral void space. And the volume of the tetrahedral void space is going to be different in different kinds of crystal structures and vice versa. And in some crystal structures, you may not have both the void spaces available, you may have only one kind of them available.

I think right now I am not going to spend time on here, but when we are talking about defects, we will try to look at that, ok?

(Refer Slide Time: 21:34)



We have discussed about the stacking of atoms in order to generate the close-packed structures; ABCABCABC and ABABAB. Suppose if you make a mistake in the stacking; that means, you are introducing a stacking fault in the crystal lattice. So, stacking fault is nothing but an irregularity in the packing sequence of atoms in crystal.

For instance, in FCC the usual packing is ABCABCABC, and instead of doing this packing, if you do ABC and then forgot to put A and then BCABC and so on; here it is perfect, here it is perfect and here you made mistake. So, that is sort of a defect in the crystal, right? This is what you call stacking fault.

So, the fact that you have introduced a stacking fault, there is an energy associated with the stacking fault and that energy is going to be called as stacking fault energy. Depending upon the kind of stacking faults, you have materials which have high stacking fault energy and low stacking fault energy.

At this point of time it suffices for us to know that there is something called stacking fault, which is due to a missing layer of atoms in the close-packed structures. And because of the introduction of that kind of a stacking fault, the internal energy of the crystal is going to increase. And the energy associated with that particular fault is called stacking fault energy.

So, depending upon the width of the stacking fault, you can call them as narrow stacking faults or wider stacking faults, and then there is an energy associated with them. We will discuss about this in the next module. What is the implication of having a high stacking fault energy system and a low stacking fault energy system, how does that lead to the different kind of deformation behavior in materials, ok?