Introduction to Materials Science and Engineering
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Lecture – 16
Close-packing of hard spheres

Hello and welcome today we are going to discuss closed packing of hard spheres. This is a essentially a geometrical or mathematical idea; however, it has an application in our study of materials. Because, closed packing of hard spheres also are models for the crystal structure of many metallic materials. We will see this in this particular video

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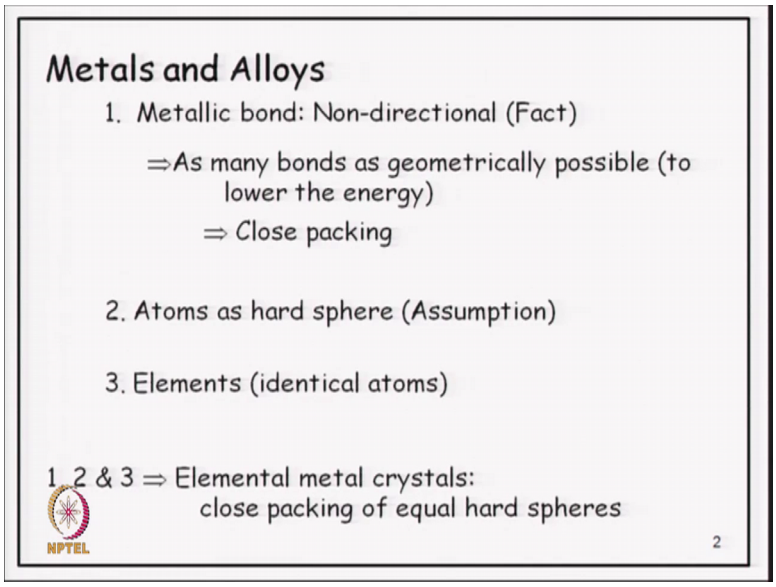

Now, if we look at the structure of metals and alloys their binding is metallic binding. Metallic binding or metallic bonds are non-directional by this we mean that if like you can contrast this with the covalent bonding of carbon. Where the angle between the carbon carbon bond is 109.5 this cannot be altered. Whereas, for metals there is no such metallic bonding there is no such pre-defined angle. Thus, you can bring in as many metallic atoms close together as possible. Non-metallic bonding give gives you the possibility of having as many bonds as geometrically possible.

Remember that each bond the formation of each bond lowers the energy of the material. Thus, as you form more and more bonds there is more lowering of the energy of the system and system is more stable. Metallic bond can give you this possibility of having

as many bonds as possible and that is why the idea of geometrical close packing comes in. If we have as many atoms packed around a given atom we will form more number of bonds in that case and there we will have a more stable structure.

Now, the second, the first one the metallic bond non-directional I have said as a fact and the second statement is to assume atoms as hard sphere. This of course, is an assumption. An assumption which is valid in many cases, but not of course, is strictly true. We will assume atoms as hard spheres.

The third fact is that pure metals or elements have all identical atoms. They will be represented by identical hard spheres. If we put these 3 things together we conclude that elemental metal crystals can be modeled as close packing of equal hard spheres that is why we essentially discuss the geometry of packing of equal hard spheres in this video.

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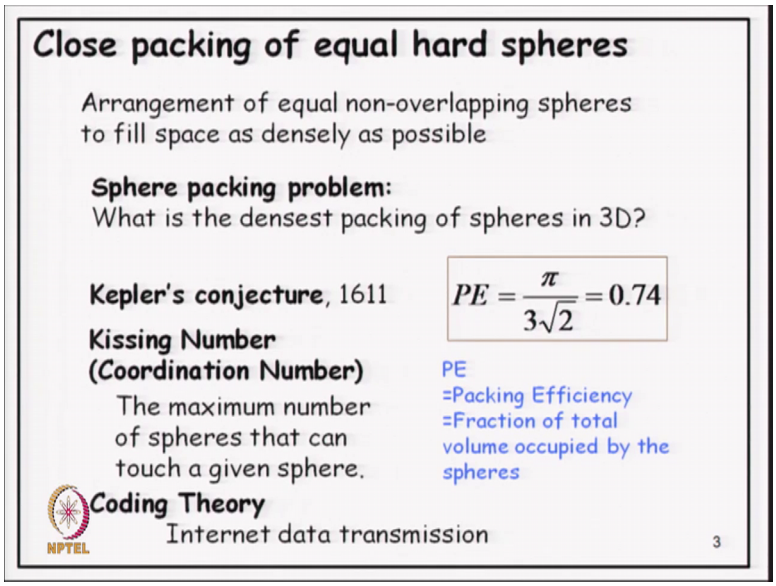

Let us look at close packing of equal hard spheres. Now, this is in in mathematics or in geometry this is a famous problem and is known as a sphere packing problem. That is to find out what is the densest packing of spheres in 3Dimensions or for example, in any dimensions. Particularly, for 3Dimension Kepler long back in 1611 he has conjectured that the densest packing is have a density of 0.74 and is achieved by called cubic close packing or hexagonal close packing which we will see later in this course.

The packing efficiency is defined as the fraction of the total volume occupied fraction of the volume occupied by spheres out of the total volume. The number given here 0.74 is 74 percent. In Kepler's conjecture the spheres occupied 74 percent of the total volume available and this is the fact that this is the highest possible packing efficiency which one can achieve is what is Kepler's conjecture.

Another concept related to packing of spheres is what mathematicians interestingly called kissing number, but in science or in chemistry and physics coordination number is more common, is the number of spheres a given sphere touches in such a packing. The maximum number of spheres that a given sphere is in contact with or touches is the kissing number or the coordination number of that packing. In dense packing, both the packing efficiency and the coordination number will tend to be higher packing of spheres interestingly has applications in internet data transmission. Of course which is not a field of our interest in this course.

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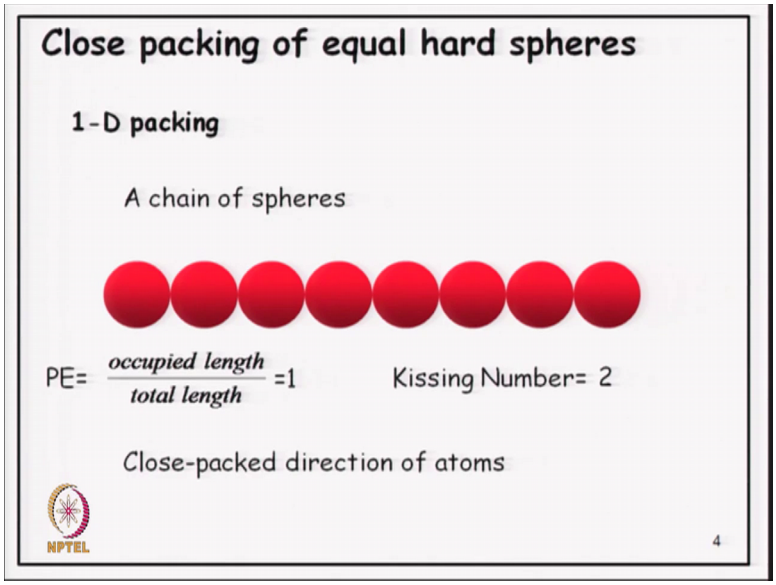

Now, let us look at close packing of hard spheres and we begin with one dimensional packing now this is a trivial case very simple. If we want to pack spheres a longer line then each sphere will be touching to it is spheres on it is left and right and we have a chain of spheres. Here, we can define packing efficiency since now we are talking of one dimension. The packing efficiency is not defined in terms of volume, but in terms of the

length that the total length of the line divided by the total length of line occupied by sphere.

This of course, in this one-dimensional chain the entire length of line is occupied by spheres. And we have a packing efficiency of 1 or 100 percent and the coordination number or the kissing number of course, each sphere is touching a sphere on it is left and a sphere on it is right. We have a kissing number of 2 such a row of atoms or such a row of spheres is known as closed pack direction of atoms or closed pack direction of spheres.

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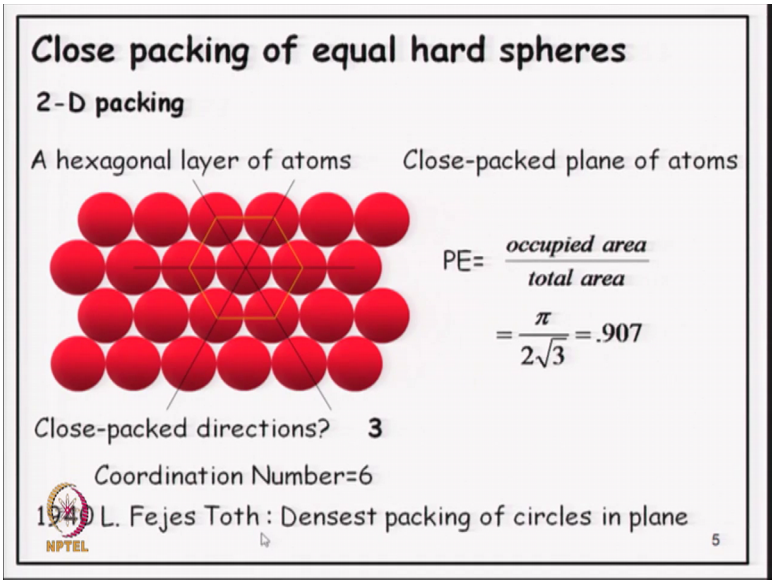

Now, let us look at this way we build that in 2Dimensional case by packing such rows. We begin with first row which is a single row of close packed spheres and we want to now add to it the second row of atoms; obviously, the best way if we want a dense packing is to put the second row in the crevice of 2 atoms in the row below. If we keep doing this we do get the second row which is as closely packed as possible as the first row and the 2 rows together are as closely packed as possible. Then we can similarly add the third row and the 4th row and continue in the 2Dimension.

Now, we have a so-called hexagonal layer of atoms or spheres in which each sphere is touching 6 other spheres around it. The coordination number in this case becomes 6 and the number of directions in which the atoms are touching the close-packed directions also now becomes more and we can see that in this structure there are 3Directions in

which the atoms are touching. The horizontal direction of course, in which we started with, but 2 more directions came up due to the structure of the or the geometry of the structure along this direction also atoms are touching and along this direction also atoms are touching.

Assuming our hard sphere model of atoms I am using atom and sphere interchangeably. There are this is one direction there is a other direction and this is a third direction starting from any central atom. We can we have 3Directions in which atoms are closely packed. There are 3 close-packed directions if we want to find out the packing efficiency of this structure. This is an interesting exercise and we can do it very simple by simple geometry first of all we have to identify a region of this 2D which repeats itself. A repeating unit in this case a nice repeating unit will be a hexagon. This is a hexagon and the entire since the entire plane can be decomposed into identical hexagons we can take the packing efficiency in the hexagons as the packing efficiency of the entire 2Dimensional plane

In this hexagon, it is easy to compute the packing efficiency by first counting the number of spheres which belong to the hexagon you can see that one is sphere is totally included in the hexagon and the corners sphere each of them contribute one third because of the one 20-degree angle of the hexagon each sphere one third part of each sphere is inside the hexagon. One third times 6 corners gives you 2 spheres effectively 2 spheres from the corners and one sphere from inside. They are totally 3 spheres inside this hexagon.

The area occupied by them will be 3 times the area of the circle and this can then be divided by the total area of the hexagon I leave this as an exercise for you can do this and find a ratio which is equal to pi by 2 root 3 which is 0.907. Around 90.7 percent 90.7 percent of the area in a 2Dimensional plane is occupied by the spheres in a 2D packing. It is a very dense packing of spheres which is there.

The coordination number I had already said that this is a 6 here because each sphere contacts 6 spheres in this particular packing. The fact that this is the densest packing of his spheres in 2D was proved in 19 forty by a mathematician talk.

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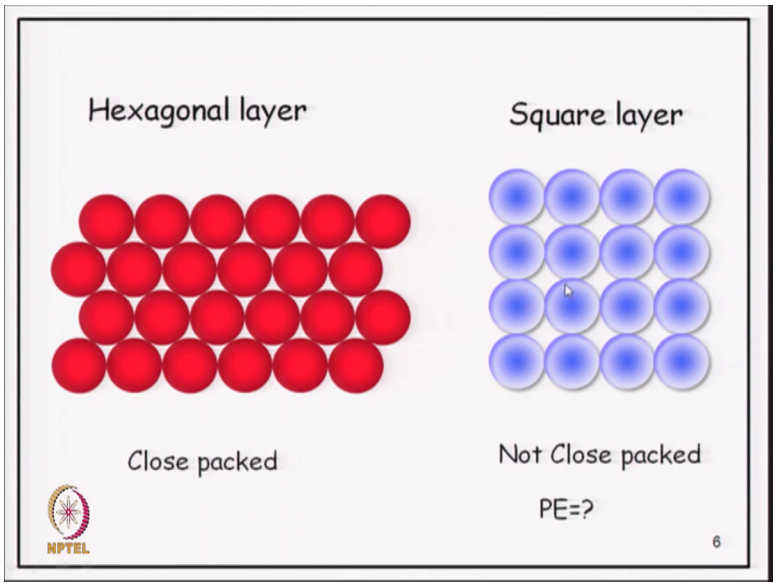

Now, just to emphasize this fact that why we are calling a dense packing or densest packing of spheres we should look at another packing which is not so dense. If we pack this spheres in a way such that another sphere is exactly above the sphere on which it is sitting unlike here where each sphere went into the crevice of the 2 spheres. Now, here it is sphere on sphere. Instead of a hexagonal layer you get a square layer each sphere is now in contact with only 4 spheres.

Coordination number drops from 6 to 2 and we have a square layer of spheres and you can see by calculating it is packing efficiency I have given you hint of how to calculate the packing efficiency of hexagonal layer, you can do this as an exercise and find the packing efficiency of a square layer and you will find that it is much less compared to the packing efficiency of hexagonal layer intuitively you can see that now you have larger crevasses. There are more area which is left unoccupied.

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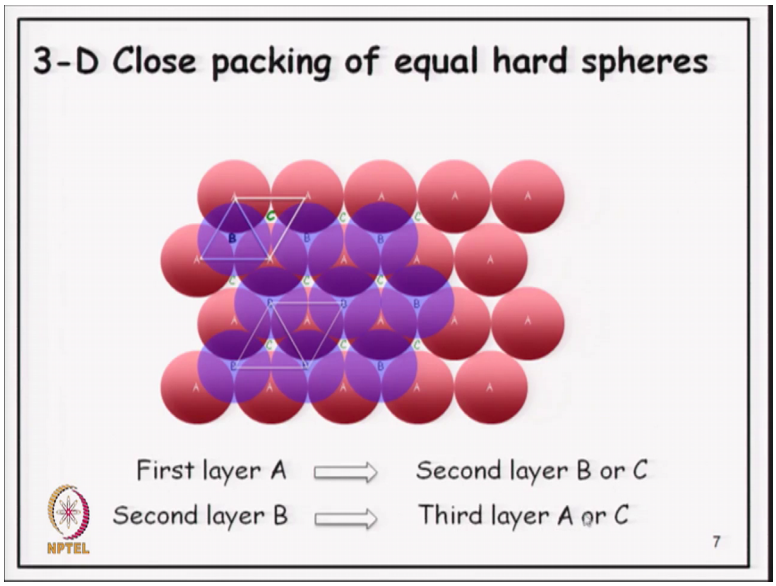

We now come to the 3D close packing of hard spheres for this we begin with the close pack layer which we have already constructed. We know that this is the densest packing of spheres in 2D and by packing such layers we want to now create a 3D close packing. Where shall the next layer of atoms go? If we look at it carefully, we call first of all we designate this layer has an air layer and all these positions or the centers of these atoms has the A positions. We are beginning with an A layer.

Now, if we look at a triangle of 3A atoms. The next layer of atoms can sit in such triangular crevices. It will not like to sat if or if we do make a sphere A next layer is sphere to sit exactly above A. The packing will not be so dense. For dense packing or for stable packing the next layer of atom will go into crevices like this this is one kind of crevice which is formed by 3A atoms which are forming and upright equilateral triangle. There is a crevice here and the next layer of atom can sit there.

I call such site the centroid of this A triangle as B. The atom which will be placed there will be called AB atom. I place AB atom this is I am showing in projection, but you have to imagine that this blue atom is sitting above the layer of these 3A atoms. If you now just see next to this a triangle another triangle of 3A atoms. These 3A atoms are forming an inverted triangle and an atom can sit in this crevice also and we distinguish this crevice made by the in triangle of inverted triangle by the other crevice which is made by

an upright triangle by giving them different designation. We have already designated the upright triangle as B the inverted triangle we designate as C.

The next layer atom can of course, sit at this site C also; however, if you compute and I leave this again as an exercise if you compute the distance between B and C. This distance is less than the diameter of this sphere. Thus, simultaneously u and this distance can be easily computed because all you have to do you have to equilateral triangles sharing the common edge and you have to find the distance between the centers of these triangles.

In terms of the edge of the triangle, what you will find? That the distance BC is much less than the distance A A of the site of the triangle so; obviously, if I have put A sphere at C simultaneously, I cannot put A sphere at B also. I show this by this visual where I placed I deliberately placed A sphere both B and C and you can see that they are overlapping and with hardest sphere such overlap is not possible. We have to choose when we when we have an a layer, we have a choice of either B site or AC site, but we have to choose one of them. We can not put sphere on both of them.

Let us choose B. We keep a sphere at the site B. Now, this is not if we look at the entire layer there are many such sites which are formed by upright triangle. We call all those sites B. This is B this is B centre of upright triangle, this is also centered of an upright triangle. All such sites are called B. Similarly, all sites which are formed by inverted triangle I label them C. These are the C sites and I as I have said I am choosing B as my preferred site and the next layer of spheres I will place at B. I place another sphere next to this. There are now 2 spheres and they are contacting as you can see. If I keep placing spheres at all the B I will again get a close pack layer of spheres just like the a layer only it is now above a and sitting on the atoms A.

I have now 2 layers of spheres A and B packed as closely as possible. What we see here? That the first if first layer was a the second layer we could have chosen either as B or C now look at the B spheres itself. If I look at this B triangle a triangle of 3B atoms forming an upright triangle the center of that itself is C. The third layer atom can be located at this C site, which was not occupied by the first layer or the second layer. This is one possibility, but you can see also that the 3B atoms here.

The adjoining triangle that is forming an inverted triangle and the center of these in this inverted B triangle is exactly above A. I can the third layer again can go on these 3B atoms which will be exactly on A. If I choose the second layer as be the third layer can either be A or C. On A I can put B or C and on B I can put A or C.

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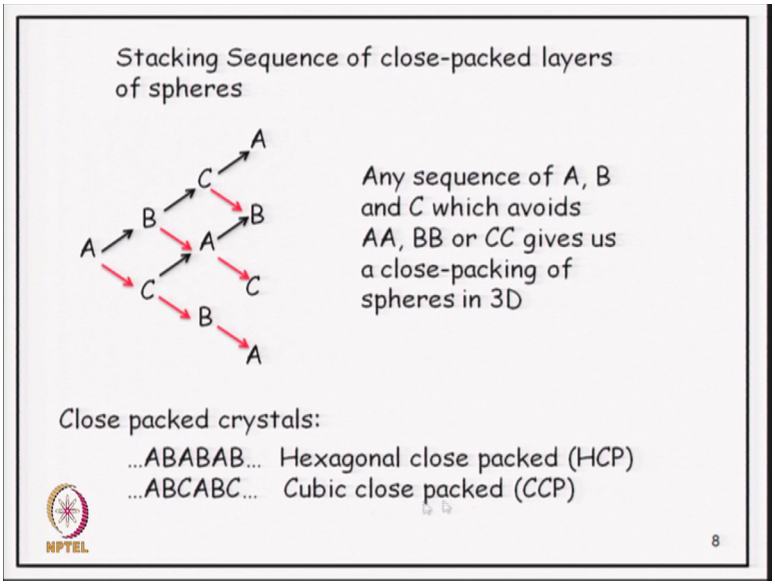

Let us summarize this, the stacking sequence of closed pack players on A. I can put either B or C on B. I can put either C or A on C I can put A or B and similarly on C A or B. Essentially, our rule is that any sequence of A or BAB or C is possible which avoids similar. Similar stacking AA BB or CC should not be there should be avoided. If we write any sequence of the letters A B and C that will give us a sequence of close practice fair with the same packing efficiency of 0.74.

All these structures will be closed packed structures of spheres out of which 2 of them are very important for closed packed crystals and they are very simple sequence AB AB AB which gives us hexagonal close-packed structure and ABC ABC ABC which gives us cubic close packed structure.

Thank you very much for your attention and in the next video, we will take up in more detail the close packed structure of hexagonal and cubic crystals.