Structure of Materials
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Lecture - 15
Crystal Structures

We shall now take up the detail discussion of three important crystal structures, in which most of the metallic elements crystallize. The first one being the cubic closed pack crystal, second one being the BCC crystal, and the third one being the hexagonal closed pack crystal.

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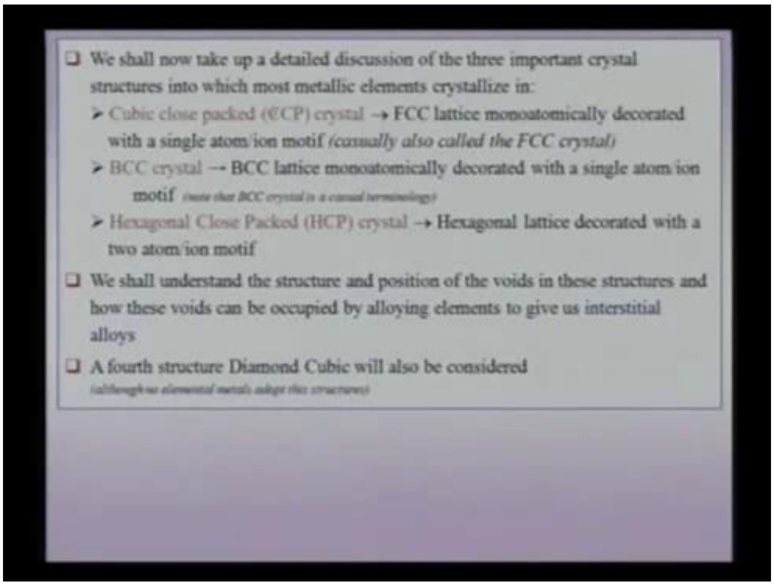

- We shall now take up a detailed discussion of the three important crystal structures into which most metallic elements crystallize in:
  - Cubic close packed (CCP) crystal → FCC lattice monoatomically decorated with a single atom/ion motif *(casually also called the FCC crystal)*
  - BCC crystal → BCC lattice monoatomically decorated with a single atom/ion motif *(note that BCC crystal is a casual terminology)*
  - Hexagonal Close Packed (HCP) crystal → Hexagonal lattice decorated with a two atom/ion motif
- We shall understand the structure and position of the voids in these structures and how these voids can be occupied by alloying elements to give us interstitial alloys
- A fourth structure Diamond Cubic will also be considered *(although no elemental metals adopt this structure)*

Often we call as we know, the CCP crystal, the Cubic Close Packed crystal also as see FCC crystal. But, we should note that this is what you might call rather casual usage and therefore, often we have to be differentiate this various kind of crystal structures, which are based on the FCC lattice. We should also consider the fourth crystal, the diamond cubic crystal even though there are no metallic element, which crystallize in this structure. Additionally we shall play importance to the interstitial positions, the voids in these crystal structures. And we will see how various for instance elements can fit into these interstitial voids, and give us interstitial a voids, so this will be the focus of next set of discussions.

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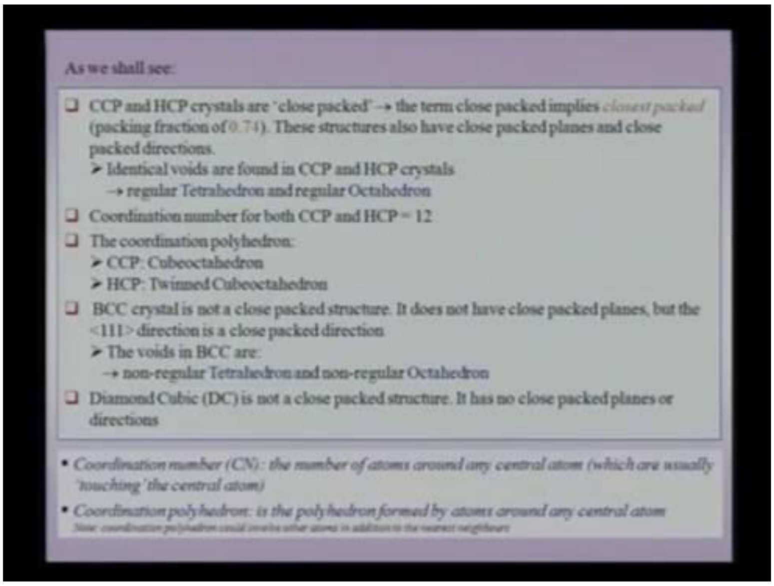

As we shall see:

- ☐ CCP and HCP crystals are 'close packed' → the term close packed implies *closest packed* (packing fraction of 0.74). These structures also have close packed planes and close packed directions.
  - ➢ Identical voids are found in CCP and HCP crystals
    → regular Tetrahedron and regular Octahedron
- ☐ Coordination number for both CCP and HCP = 12
- ☐ The coordination polyhedron:
  - ➢ CCP: Cubeoctahedron
  - ➢ HCP: Twinned Cubeoctahedron
- ☐ BCC crystal is not a close packed structure. It does not have close packed planes, but the <111> direction is a close packed direction
  - ➢ The voids in BCC are:
    → non-regular Tetrahedron and non-regular Octahedron
- ☐ Diamond Cubic (DC) is not a close packed structure. It has no close packed planes or directions

- *Coordination number (CN): the number of atoms around any central atom (which are usually 'touching' the central atom)*
- *Coordination polyhedron: is the polyhedron formed by atoms around any central atom*
  Note: coordination polyhedron could involve other atoms in addition to the nearest neighbours

And picking height, we will see what are the kinds of consideration we will keep in mind, we will see that the cubic close pattern and hexagonal closed factors crystal are closed packed. When I use the word or the term or the phrase closed pack, what I imply is that it is the closest packed, if you have sphere of all same size, the closest packing which you can obtain is 74 percent. That means, 74 percent space can be occupied, and these two crystal structures have that packing fraction or that percentage packing as 74 percent.

It is important to note as usual of course, see in detail later that the voids found in these two crystal structures are the regulated tetrahedron or regulated octahedron. The coordination number as usual see, the coordination number being the number of atoms surrounding e at any central atom, which are usually touching the atom and in some case they may not be touching the atom. Because, the coordination polyhedron is the polyhedron formed by the atom around any central atom, and it could involve atoms other than the nearest neighbors.

The coordination number for both CCP and HCP are is 12, and you can have no higher number than 12 for any configuration of ego size spheres. As we shall see the coordination polyhedrons for cubic close pack is the cube octahedron, and for the HCP is the 20 cube octahedron. We will also note the BCC crystal is not a closed pack crystal; that means, it is packing fraction is less than 0.74, it does not have any closed pack planes. But, the 1 1 1 direction in the BCC is actually a closed packed directions, the voids in BCC are not regular polyhedral like the tetrahedral, octahedral.

On the other hand they are neither fully distorted, so we can call them non regular tetrahedron, the none octahedron and you will see the shapes of these polyhedron. The diamond cubic structure is not a closed pack structure, it is no closed pack planes or close pack directions, we had mentioned this briefly, but we will revise in the concept again.

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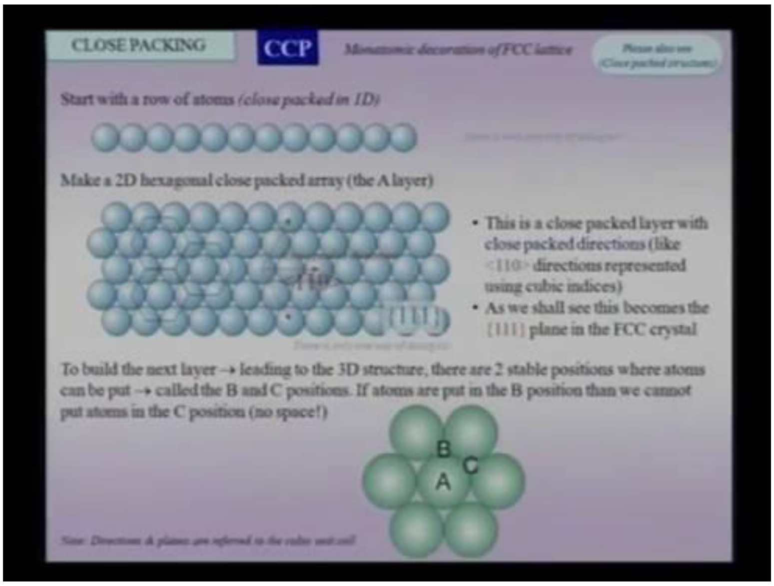

CLOSE PACKING

CCP

Monatomic decoration of FCC lattice

Please also see (Close packed structures)

Start with a row of atoms *(close packed in 1D)*

Make a 2D hexagonal close packed array (the A layer)

- This is a close packed layer with close packed directions (like <110> directions represented using cubic indices)
- As we shall see this becomes the (111) plane in the FCC crystal

To build the next layer → leading to the 3D structure, there are 2 stable positions where atoms can be put → called the B and C positions. If atoms are put in the B position than we cannot put atoms in the C position (no space!)

Note: Directions & planes are referred to the cubic unit cell

So, let us.try to understand how do we form the cubic closed pack structure, starting with for instance single atom. Then with the row of closed pack sphere, then going on to planes of closed packs spheres and finally, to the three dimensions structure which is the cubic closed pack structure. So, we already have noted that the CCP crystal is obtained by the mono atomic decoration of the FCC lattice, so let us start with the row of atoms of course, with single sphere then make the close pack row of atoms.

Then starting with this row by putting these rows one below the other in a fashion shown here, I can obtain a hexagonal closed pack layer. Of course, I call it has hexagonal because, this layer has got hexagonal symmetry, and you can see once the layer has been formed, it has got closed pack direction. And as we shall see later that these closed pack layers when you correspond it to the cubic directions, then this will be corresponding to the 1 1 0 type of directions.

So, this is the closed pack direction, this is the closed pack direction, this is the closed pack direction. And this layer has got hexagonal symmetry, and for instance around this point if I rotate 60 degrees and the structure will remain in varied, now this layer itself we will see that actually becomes what according to the cubic indices will be the 1 1 1 plane of the cubic crystal. Now, to build the next layer which will actually lead to the three dimensional structure, there are two stable positions for in suppose I call all the atomic positions in this layer as the a layer.

That means, this green sphere or functions in this case the blue sphere is A position, this will also be A position, this will also be A position and, so far. Now, once atoms are presented in the A position, there are two other table positions where I can put atoms to make the second layer for instance this will be the B position, and then this could be the C position. Now, suppose I start putting the atoms in the B position suppose I put a sphere here, then I will not have enough space to actually put an atom of the same size or the sphere of the same size in the C position.

That means, if I chosen B in the second layer then I can put one sphere here, one sphere here and one sphere here, which all the B positions. Alternately I could put sphere in the second layer in C position, which means that I cannot put sphere in the B position I can put one in this C position here, I can put one in this C position here I can put C position here. So, I have two choices for the second layer and I can construct a second layer by putting atoms in the way I have told. We will actually show these things revising these things again with physical modals, so that the concept of space fillings becomes absolutely clear, but we have these choices for the second layer.

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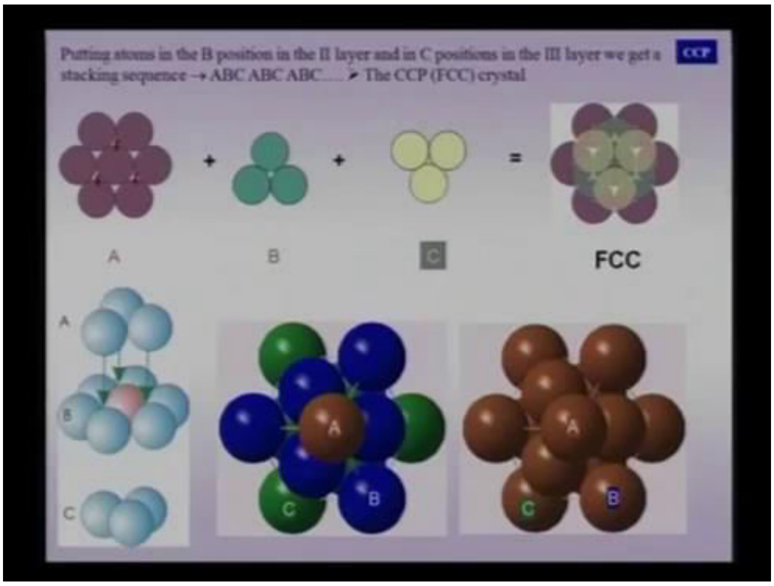

Putting atoms in the B position in the II layer and in C positions in the III layer we get a stacking sequence → ABC ABC ABC...... ➤ The CCP (FCC) crystal

Now, having constructed an A layer suppose I choose my second layer to be the B layer; that means, I have put atoms in this position, this position and this position. So, I have put atoms in the B layer then and I have marked them in green color, then I have I can propagate this entire two dimensional planes. And each one of this planes independently not in combination, but independently has a six fold symmetry.

So, I even though I shown this as triangle actually this layer, and this layer are no different, they are both hexagonal layers. And I can put this layer, having put the B layer again I have two choices I can put a sphere directly above the sphere, which I have put in the A layer. That means, the sphere will sit in the A position or I have alternative that I could actually put sphere in vacant in C position.

That means I have already put an atom in the A position, the second layer is in the B position, for the third layer either I can go directly above the A layer or I can put it in the vacant C position for the to obtain the cubic close pack crystals I will have to use the alternative C. That means, the first layer I call the A, the second layer B, third layer C and therefore, my packing would look something like this.

So, this is my A layer this is look at the diagram right hand side, the B layer is the green layer, and the C layer is a layer which is the originally was left vacant. So, each one of these layers is actually a hexagonal layer, exactly that I have shown in this diagram, the blue layer here, and I can put these three layers together. Now, this kind of packing of three layers I can repeat again; that means, fourth layer I put out the exactly about the A layer, the fifth layer exactly about the B layer, the six layer would be exactly about the c layer and, so forth.

Therefore, such a packing would be called the A B C, A B C, A B C packing, and the crystal I obtain in this case would be called a cubic close pack crystal. Now, the same thing is shown in certain projection here for instance you have the C layer, then you have the B layer and have the A layer. So, in the A layer for instance the sphere could be go into the voids from by the B layer of course, this atoms shown in different color just for identification, all sphere are identical as far as the crystal goes.

And the C layer would go into the white which is now form the B layer, but in a different void, if you look down the directions. That means, now looking like the exactly the way I did down this direction, which is perpendicular what as we see the 1 1 1 layer of the cubic crystal. So, this is my 1 1 1 planes which is I am constructing now, so this will be my A layer, the B layer would be the once shown in the blue color here, and final the C layer would be the layer shown in the green color. And finally, you have layer below as the A layer, so if I color all my sphere identically which is what they are, they are identical spices then I would have a packing along 1 1 direction which looks like this.

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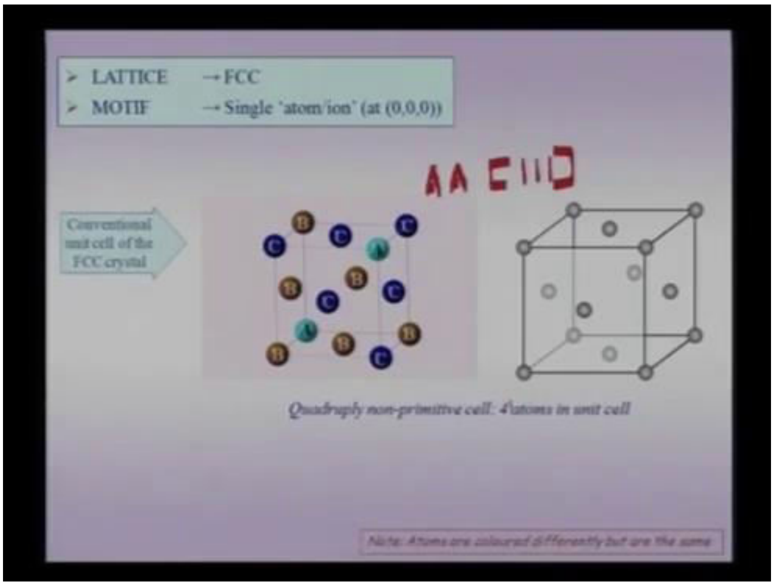

- LATTICE → FCC
- MOTIF → Single 'atom/ion' (at (0,0,0))

Conventional unit cell of the FCC crystal

AA [110]

Quadruply non-primitive cell: 4 atoms in unit cell

Note: Atoms are coloured differently but are the same

Now, as I said we will look at this construction once again in the detail using models, but before that let us look at what we call the conventional unit cell, and corrected to correspond to the packing which we are just now consider. Now, we already know the lattice FCC, and the motif is a single atom or ion at for instance 0 0 0, now I want now correspond my picture of A B C packing with the conventional unit cell of FCC, where in which already consider before.

Now, the way of constructing is actually constructing along the vector connecting the A to the A atom, which is now my 1 1 1 directions. So, the A A direction connecting my A to A this the 1 1 1 direction, and I am trying to construct my crystal along the direction. So, you can see that the A exists then there is a B layer, which is now made by this B spheres and there is a C layer and finally, there is one more A layer.

So, in another words I am constructing my crystal with respect to this orientation, the standard orientation of the FCC crystal along the 1 1 1 direction. And what I get as you know quarterly non primitive unit cell, which has 4 atoms per unit cell.

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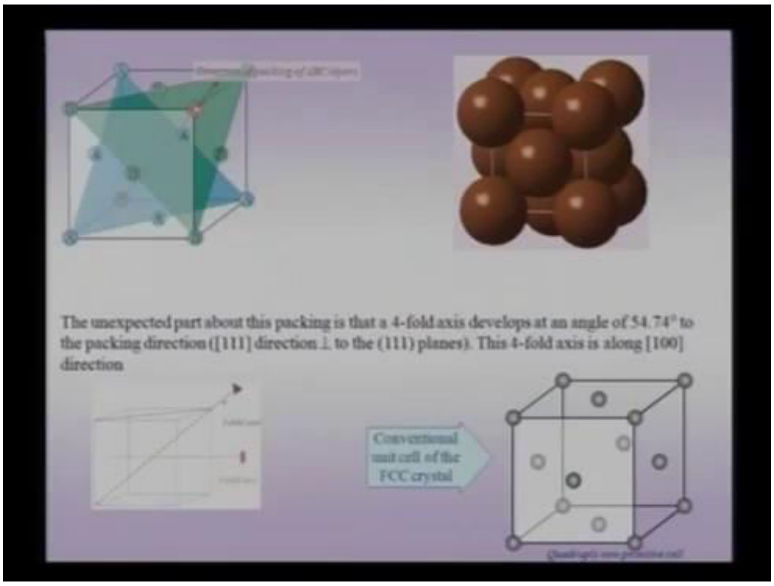

The unexpected part about this packing is that a 4-fold axis develops at an angle of 54.74° to the packing direction ([111] direction ⊥ to the (111) planes). This 4-fold axis is along [100] direction

Now, this diagram again tries to clarify the same point that have a C layer of course, in this case that I called that the A layer, but just a common lecture. Therefore, I have a layer here, then I have next layer which is the blue layer, again contacting sphere and hexagonal configuration. Then I have this green layer which again consist sphere here hexagonal configuration, and there is a final layer which also a center of this, but also got atoms in hexagonal configuration.

Now, when I do this kind of a packing it is not surprising that crystal high generate has got not 6 fold, but 3 fold. The 6 fold original layers has 6 fold symmetry, but this A B C packing has destroy the 6 fold, and has left only with a 3 fold rotational symmetry, in fact, you can also visualize this symmetry as not just crystal mere in simple rotation is 3 fold, but in terms of a rotor inversion actually itself 3 bar axis.

So, this C C axis actually the 3 bar axis and if you want to look at the simple rotational axis, it is a 3 fold axis. Now, so far it is easy to understand because, 3 fold is the sub group of 6 fold symmetry and therefore, that is what survives during the packing, but what is surprising which arises during the kind of A B C, A B C kind of packing is the existence of the 4 fold. Now, we are doing the packing along this 3 fold direction which this is the vector we shown here, which is the direction of the packing A B C layers.

But, surprisingly at a angle of the bottle 54.74 degrees to this 3 fold axis, you get a 4 fold axis. This aspect is not obvious when you try to do this packing, but this is generated purely by this kind of packing which is the A B C, A B C, A B C kind of packing, before we take up primitive unit cell of the FCC crystal structure, you will try to understand to same concept which mention here using models.

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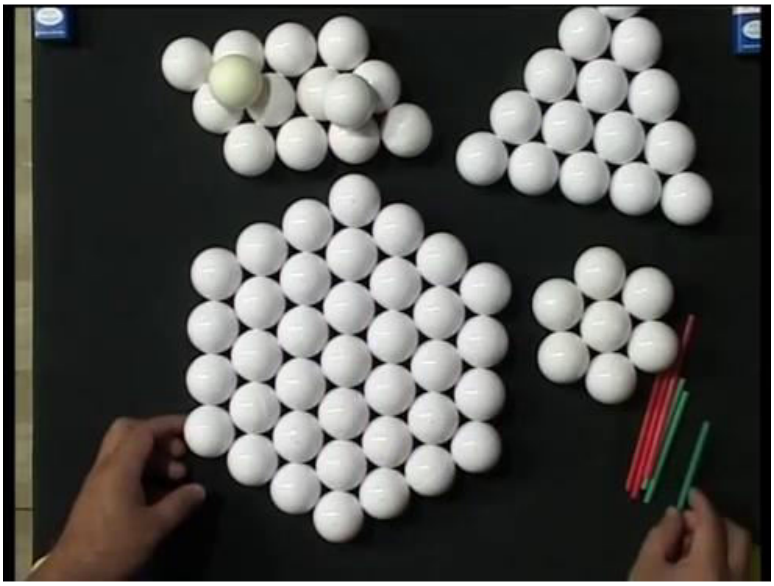

What I have got here, as you can see is a hexagonal layer of atoms, this is closest packing I can get in two dimensions, and also we have touching each other and as you can see this axis for instant is an axis 6 fold symmetry. To understand my A B C packing

I will take part of this hole hexagonal structure which is not nothing, but a small section here, which just got 7 atoms. Now, this 7 atoms I call the A layer, so this atoms belong to the A layer.

Now, I have two options either I can put sphere here which I will choose for instant green sphere to show you or I can put sphere in this position, the other position which is remaining here. So, option for the second layer here or here, but not both, so let me level those, so let me level this three as the B positions, so I got three B position and then additionally there is possibility of putting atom in C positions. So, let us look at the structure, so got the A layer then for my second layer I can either put atoms in the B position or the C position.

But, I cannot put atoms in both positions because, now if we put atoms for instance in this position then there is not enough space to put it here. Therefore, if I put atom in the B position for instance for the second layer, then I can put atom continuously in the B position. So, this is my B position has been defect, still my C position are vacant like you can see here, and I can put an atom in the third layer either directly about the A layer which is one option.

In which case I would take for instances sphere like this, and put try about the A layer or the other possibility is to put an atom in the vacant C position which is right here. So, in the case for the generating the cubic close pack crystal have an A B C kind of packing; that means, this is my A, this my B the third layer would to be the C layer which would be try about the vacant area, which is generated by this straw put by atom right atom right here in the vacant position.

Now, I propagate this structure in finitely and I get and A B C, A B C kind of a packing, as I mention by important then surprising fact is the generation of the 4 fold. So, let us see how the 4 fold is generated by putting together A B C layers, so for instance suppose I call this the A layer or let me start with a single atom in the A layer I called as the A layer my second layer. So, you can see here, you can see from the other camera angle this is my A position and this is my B position.

So, I got a B position here and I put the next layer with atoms in the C positions which would be like this. I specifically cut this planes along I am not taken infinite planes, what I have done is that I have taken certain section of this planes. Actually as you can see this planes are infinite planes with this kind of orientation running across in the two dimension in finitely, but I have taken portion of this to illustrate to the point. Now, I have A layer, I have this B layer, have this C layer, and finally, I put on A layer above that.

Now, I am just using this single ball to generate the A layer, but it we know difference from this layer, but the origin of this layer would be at this atom. Now, I have done this A B C, A B C, A B C packing I can go to infinitely, but illustrate the important point now you can see this configuration has a 3 fold symmetry. So, now my axis which is coming out towards from this at as got a 3 fold symmetry and more preciously it has got 3 bar kind of symmetry.

Now, to understand that how the fourfold was generated I rotate this 4 configuration I can clearly see this is now unit cell of the cubic close pack structure, which is conventionally drawn where in now my central atom is this atom coming outward is the 4 fold axis and this was the original 3 fold or 3 bar kind of an axis. So, this is my 4 fold axis, as it is clearly seen now I can actually visualize the A B C, A B C packing as the conventional unit cell of the cubic close pack structure.

And show the wire frame model of the same thing, which have you seen before which has a show from different camera angle.

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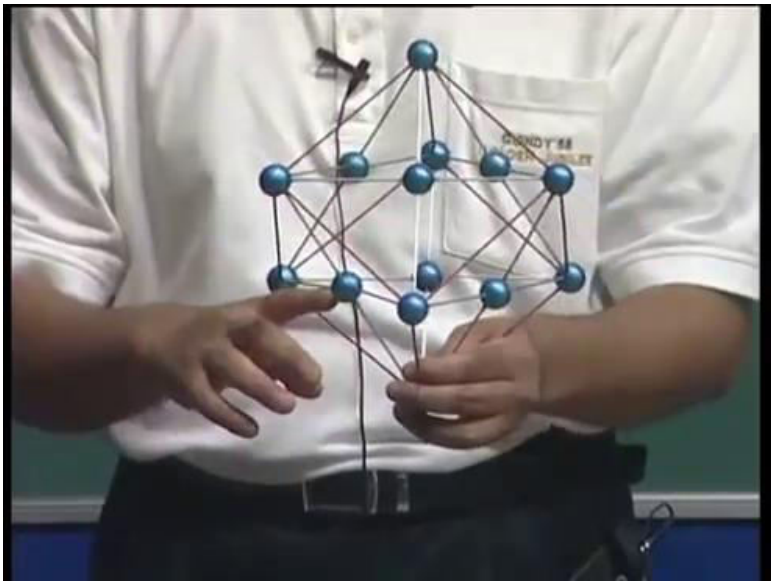

So, you can see this is my structure which have an generating A B C, A B C kind of structure, but I have to look along that structure along my body diagonal. So, the A B C, A B C packing was along the body diagonal of this cube, which runs like this, this is my body diagonal of the cube. And therefore, I got A B C, A B C packing around this directions, and these are the 1 1 kind of planes you can see this plane here, and the next plane is this connecting this atoms finally, the top one is another.

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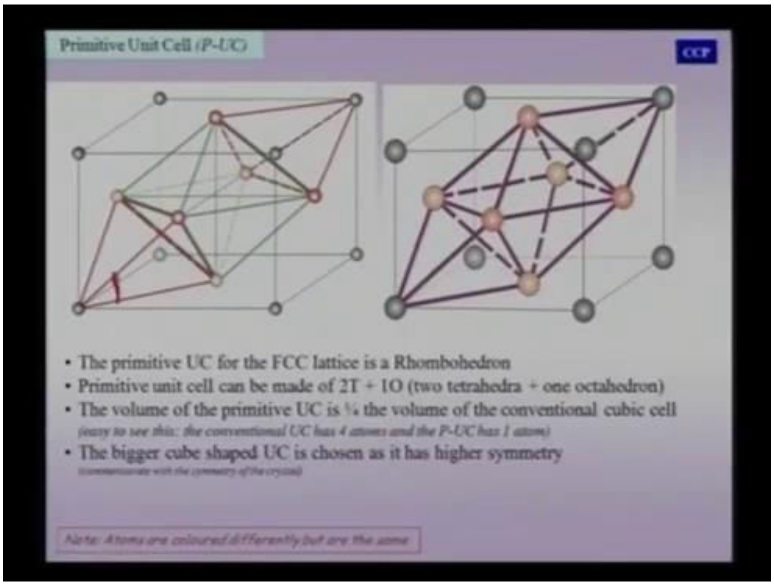

Primitive Unit Cell (P-UC)

- The primitive UC for the FCC lattice is a Rhombohedron
- Primitive unit cell can be made of 2T + 1O (two tetrahedra + one octahedron)
- The volume of the primitive UC is ¼ the volume of the conventional cubic cell
  (easy to see this: the conventional UC has 4 atoms and the P-UC has 1 atom)
- The bigger cube shaped UC is chosen as it has higher symmetry
  (commensurate with the symmetry of the crystal)

Note: Atoms are coloured differently but are the same

Let us next consider the primitive unit cell of the FCC crystal structure, in another word this the cubic close pack crystal structure. The primitive unit cell is shown by this red and green outlines, if I have to consider the lattice parameters of such unit cell, you see that A is equal to B is equal to C, and what are these factors now the A vectors, they cannot the atom at the 0 0 0 position to an atom in the half 0 0 positions.

So, A equal to B equal to C and all the angles for instance the alpha angle which should be the angle between the this, and this vector, the alpha the beta and the gamma all will be equal, but will not equal to 90 degrees. So, merely based on the shape of the unit cell, one might to be template to think this is actually diagonal or rumba hydrant unit cell, but actually this is the primitive unit cell of the cubic close pack structure. Now, the important point to be note is that this; obviously, has an 1 4 the volume as there as the primitive, non primitive quadratic non primitive unit cell.

Because, the quarterly non primitive unit cell has 4 atom per unit cell there is 1 atom per unit cell therefore, it has 1 4'th the volume as the that of the conventional unit cell for the FCC structure. Now, the other important point to note that we already seen that his look likes a very distorted kind of parallelepiped, but we have seen that all parallelepipeds are space fully. So, this camp hydrant though it may not of obvious from this picture is actually base filling solid.

Now, another important point to be noted which we use later to understand this structures is the fact that this unit cell, and without off as made of one regular tetrahedron with vertices as this, this, this and this point. And octahedron a regular octahedron with a center at 0 0 0 this is the center of octahedron with the atoms making of the octahedron as this vertices of this screen lines, so this can be thought of as 2 tetra hydra plus 1 octahedral.

Now, the reason we choose usually do not choose this unit cell for the cubic structure is because, unit cell itself has lower symmetry. Then the crystal, which as you can see has a 4 fold symmetry, and actually has a 4 by m 3 by m 2 by m point group symmetry, so we will take up the same structure using the model. So, that we can understand it the same slightly better. So, I have a here with me wire frame model of the same structure showing the primitive unit cell of the cubic close pack structure.

So, as you can see here that the cubic primitive unit cell is made up is oriented along the 1 1 1 direction of the cube, and the 1 1 1 is the direction along which has center of the tetrahedron which is now in the blue and red outlines, the other tetrahedron which is also in blue and red outlines. So, let me take my little bit, so in the background you can see this is my blue outline, this is my red outline, so this is tetrahedron with and then you have a center octahedron, which is conscience of 8 faces and which center at the 0 0 0 positions.

So, later on we will see that these octahedron and tetrahedron can be the centers or the wide center cubic close pack structure. So, you can clearly see this is now the new rhombohedral or the unit cell, which is has just got triangular kind of geometry, in these slide we should note often the colors the atoms differently, but all atoms are the same. So, they are not different atom which is having color only for better visualization of this structure.

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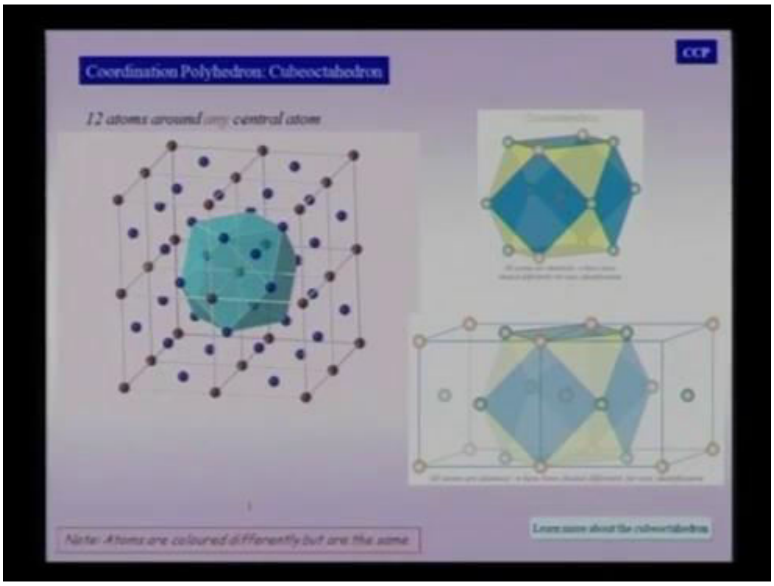

CCP

Coordination Polyhedron: Cubeoctahedron

12 atoms around any central atom

Note: Atoms are coloured differently but are the same

Learn more about the cuboctahedron

Now, let us get to the next stage which is the coordination polyhedron, and the coordination polyhedron for the cubic close pack structure is a cube box hydrant. So, two aspect come in when we talk about the coordination polyhedron number of course, coordination number which is 12, and as pointed out around the given sphere, if you want to touch maximum number of spheres of the same size, the number cannot exist to 12.

Therefore, this is the maximum number you can get and therefore, that is what is achieved in both the cubic close pack structure, and as we see later the hexagonal close pack structure. The second thing is the of course, what the shape of the coordination polyhedron, the shape for the coordination polyhedron is a cube octahedron, a cube octahedron is got such a name. Because, it is exactly between a cube and octahedron I can take a cube, and then I truncate one of it is faces; that means, I cut one of faces; that means, I can take cube like this, and then I can cut it vertices.

Now, if I cut deep enough then I will be cutting into the these a just which are the original vertices of the cube. I cut deep enough then you will see that this faces which is cut faces become triangular. And the remaining face which if I cut little bit this face blue hexagonal, but I cut deep enough they will be squares and therefore, I get a cube octahedral. Now, in terms of the simple rotation symmetry, the cube octahedron is exactly identical to the of a cube and is the coordination polyhedron in the cubic close pack structure.

Now, if you want the visualization cube octahedron here it has been shown between 8 unit cell, you can see take any atom in the FCC lattice or any lattice position and place and atom, and when you see that you find a cube octahedron around it. So, it could be atom setting on the vortex of the cubic unit cell or it could be the atom setting the face centering position. As we know the this are both lattice point and therefore, they are exactly equivalent and you get a cube octahedron, as the coordination polyhedron.

Now, before we go to the hexagonal close pack structure I will show you models of how this close pack cubic octahedron or the coordination cubic octahedron is formed.

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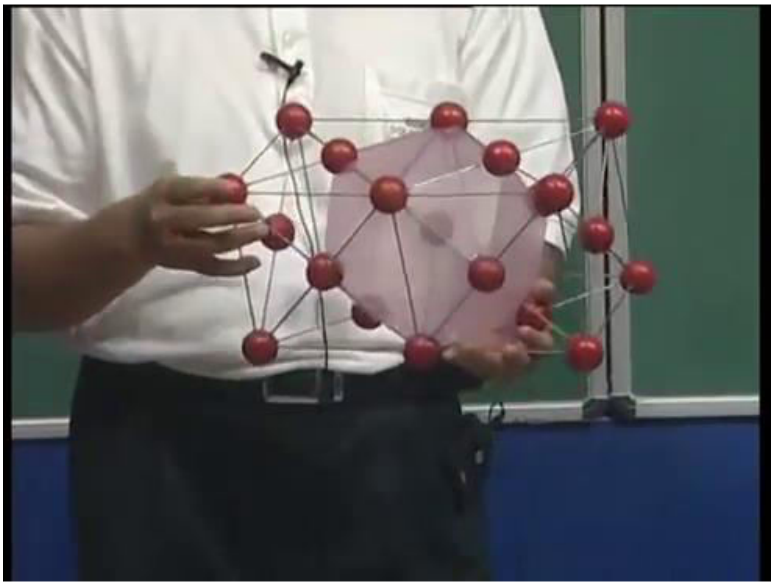

So, I have here two unit cells of the cubic close pack structure in the conventional representation. And you can see that, the center sphere which is located exactly between the two unit cells has a coordination polyhedron which is the cube octahedron, and as you can see the cube octahedron has square, and triangular faces. These triangular faces are the centers the opposite centers triangular faces with a center of the 3 fold axis, and this will continue to be the sense shed of the 4 fold axis, as you can see this is the seat of the 4 fold axis, and this is seat of the 3 fold axis.

Now, even though I choose an the set the central atom here, the atom between the two unit cell to be the center of cube octahedron, I can choose any atom in this cubic close structure. And the coordination polyhedron I would be obtain would be a cube octahedron, another point to be noted here which we should see in some other isolate violated is every atom is exactly located at the same distance from the central atom which is root 2 a by 2.

So, this atom located root 2 a by 2, this located at root 2 a by 2 and this located at root 2 a by 2, and this also located root 2 a by 2. So, all them are located at the same distance from the central atom, and the coordination polyhedron is a cube octahedron this kind of structure later on as usual see will be useful in some other calculation, we can make with the cubic close pack crystal.

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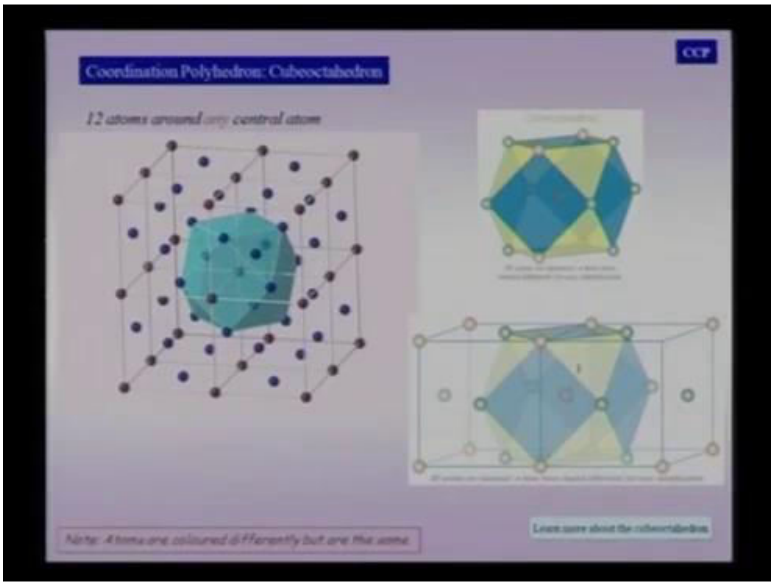

Coordination Polyhedron: Cuboctahedron

CCP

12 atoms around any central atom

Note: Atoms are coloured differently but are the same

Now, returning into the picture here we have to again note that all atoms are identical, we just color them for better visualization of the structure.

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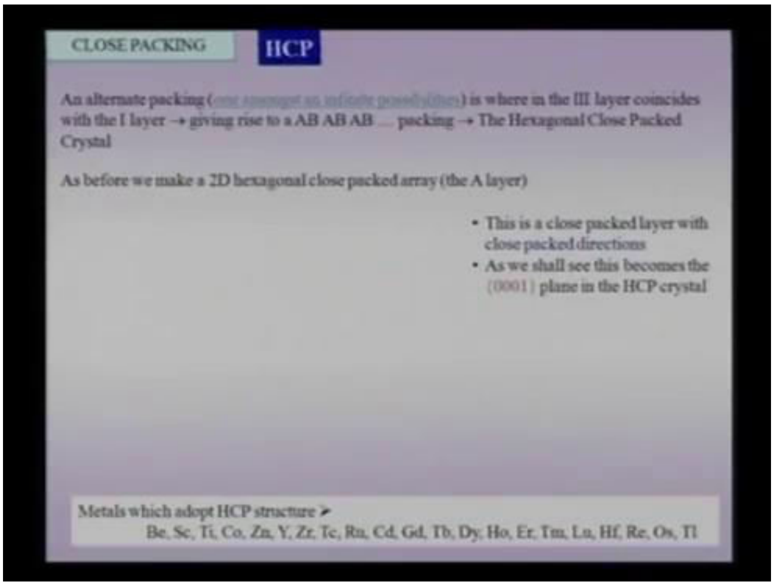

CLOSE PACKING **HCP**

An alternate packing (one amongst an infinite possibilities) is where in the III layer coincides with the I layer → giving rise to a AB AB AB … packing → The Hexagonal Close Packed Crystal

As before we make a 2D hexagonal close packed array (the A layer)

- This is a close packed layer with close packed directions
- As we shall see this becomes the (0001) plane in the HCP crystal

Metals which adopt HCP structure ➢
Be, Sc, Ti, Co, Zn, Y, Zr, Tc, Ru, Cd, Gd, Tb, Dy, Ho, Er, Tm, Lu, Hf, Re, Os, Tl

The second kind of structure which we can generate by packing of this close pack hexagonal layers is the hexagonal close pack crystal structure. Actually these two crystal structure though we have pick up in this particular lecture are nothing, but two of the infinite set up possibilities.

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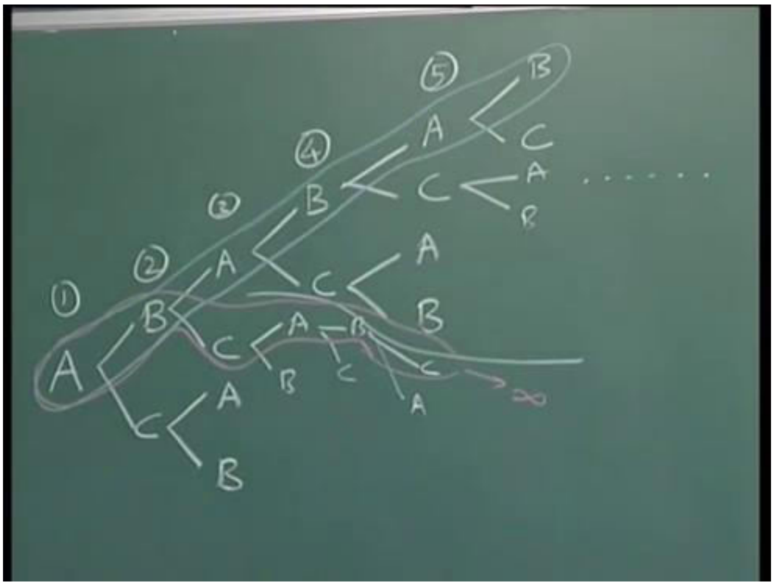

So, why are the infinite set up possibilities let me explain them on the board for instance suppose I start with in A layer I have two choices for the second layer which are B and C. Having chosen B as a second layer I would have two choices for the third layer, which will be A and C formally for this C layer I would choice of A and B, having chosen the third layer as, so this is my layer 1, this my layer 2, and this is my layer 3 I have again choice for the fourth layer as B and C and for the fifth layer function having taken this part would be an and I can go add infinite term in my choice of various layers.

But, the most common crystal structure which are found in nature are these two kind of packing which is nothing, but my A B, A B packing which is this branch of my tree and the second kind of packing is one which starts here. So, I have let me draw border here is second kind of packing which is the one we already seen is A B C, A B C kind of a packing going to infinity. So, this are the two common structures, but by no means this are only two possibilities, though often you find that many of this other possibilities actually do not exist in the nature.

But, these are the two common possibilities the one outline blue and one outline line in red. But, in general we have infinite set up possibilities of close pack crystals which we form by staring with the hexagonal close pack layer.

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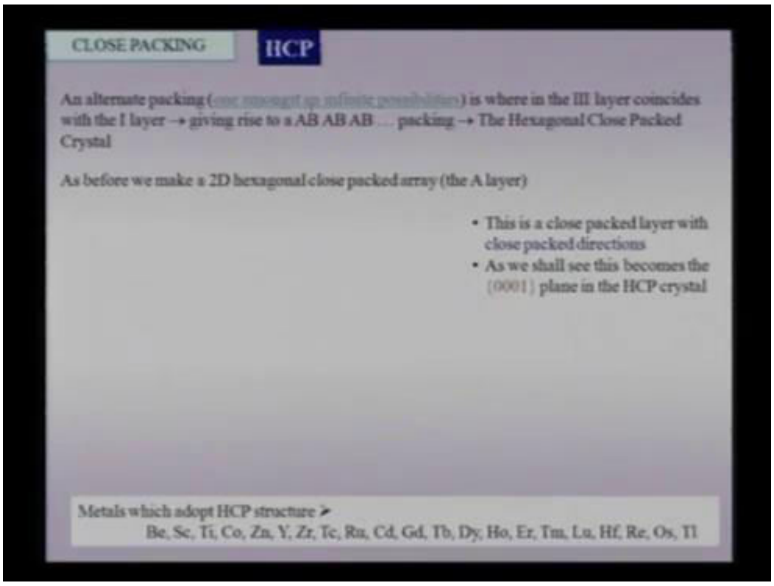

CLOSE PACKING

HCP

An alternate packing (one amongst an infinite possibilities) is where in the III layer coincides with the I layer → giving rise to a AB AB AB …. packing → The Hexagonal Close Packed Crystal

As before we make a 2D hexagonal close packed array (the A layer)

- This is a close packed layer with close packed directions
- As we shall see this becomes the (0001) plane in the HCP crystal

Metals which adopt HCP structure ➢
Be, Sc, Ti, Co, Zn, Y, Zr, Tc, Ru, Cd, Gd, Tb, Dy, Ho, Er, Tm, Lu, Hf, Re, Os, Tl

And the one which we are now considering simplest the lord, which is outland in the board in blue color which is the A B, A B, A B kind of packing, and the crystal structure we obtain is the what is known as the hexagonal close pack crystal. So, as before we should take of the hexagonal layer to close pack layer which we call them A layer and then we will generate the whole structure. Later on we will see that this structure actually this layer is actually the 0 0 0 1 kind of a plane in the hexagonal close pack crystal.

And we have already seen that many crystal actually adopt the HCP structure and some of the common example is as zinc, titanium and cadmium.

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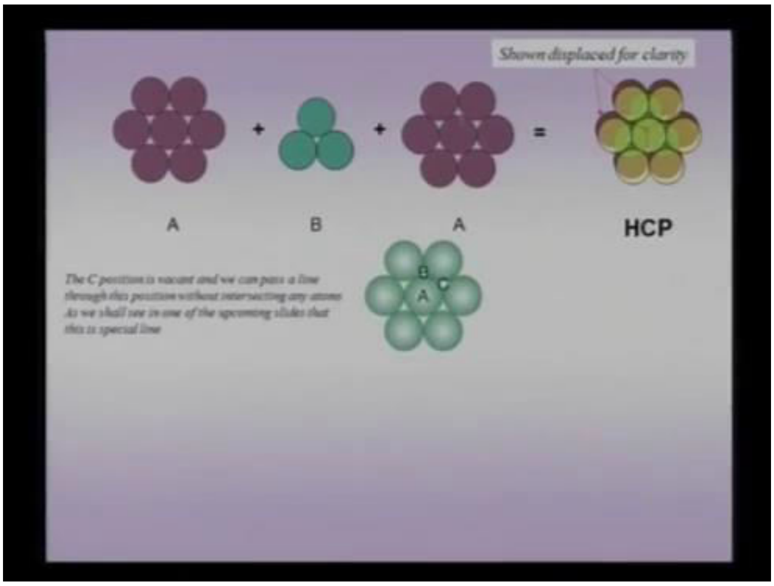

The C position is vacant and we can pass a line through this position without intersecting any atoms As we shall see in one of the upcoming slides that this is special line

So, let us see how the structure work out, you got this round layer which is the A layer, we chosen next layer is B layer. But, third layer I go directly about the A layer and therefore, is the same color and therefore, I get an A B, A B kind of packing which is the hexagonal close pack crystal. So, we start with the A layer put a B layer, but then instead going to the C layer we put the layer right above the third layer, right above the third about the A layer.

And therefore, we get A B, A B kind of packing and we will notice in this case that the C layer remains completely vacant. That means, if you get a pass ray of light through the C layer it will completely pass through the C layer.

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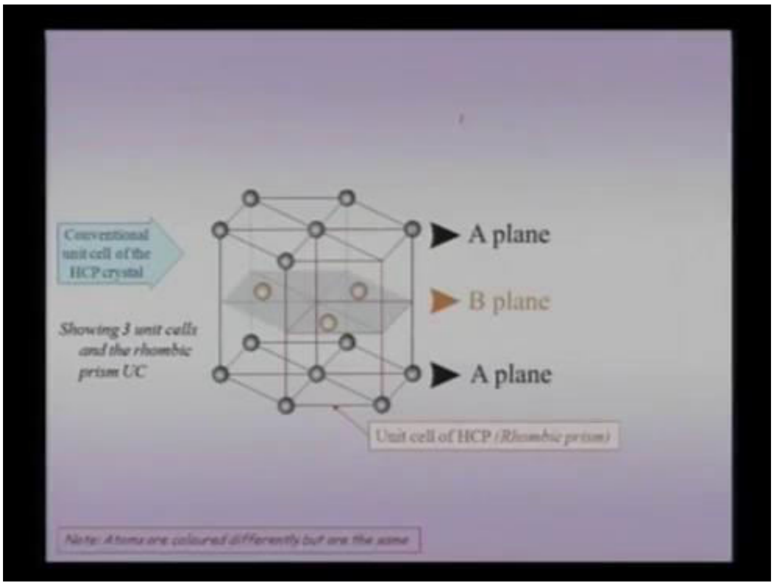

Conventional unit cell of the HCP crystal

Showing 3 unit cells and the rhombic prism UC

A plane

B plane

A plane

Unit cell of HCP *(Rhombic prism)*

Note: Atoms are coloured differently but are the same

And this vacant position C layer as we shall see as a important from the point of view, why the hexagonal close factors is actually called an hexagonal close pack crystal. Now, before I take up the conventional represent unit cell, let me go down to the modal to explain the concept here we just, now seen which is the A B A B kind of packing.

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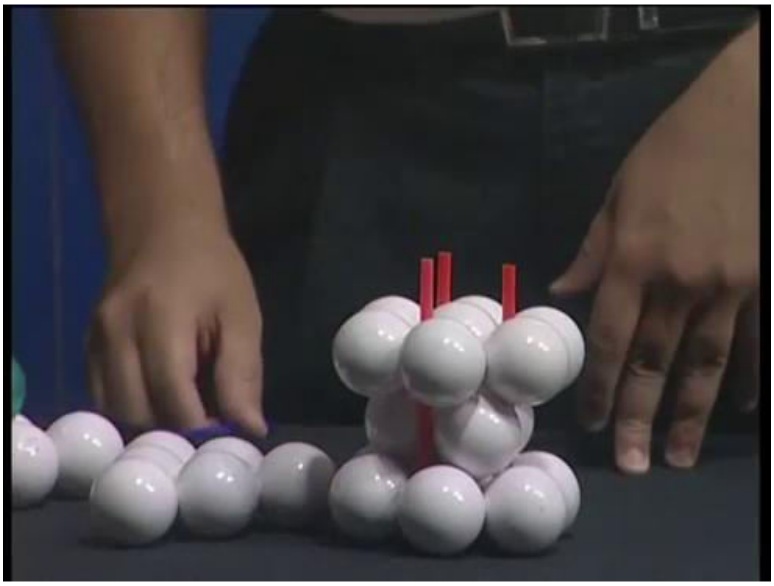

So, here we have as before a layer I trunked part of the hexagonal layer, and I call this the a set up of atoms. So, I put my atoms in the B position and; that means, that I leave my C position here which is vacant, now for the make the third layer I will take the same set up planes, and put exactly about the A layer. And therefore, I get an A B, A B kind of packing I will continue this infinite up in another words the fourth layer would be exactly about the layer about that, and the fifth layer would be again which is about the A layer just one to do like this.

But, let me look at this structure little more carefully which is shown by alternate model just kept here, which shows the A B, A B kind of packing. Now, as I mention when you do an A B, A B kind of packing the C position which I mark with the red straw remains completely vacant and actually you can see that the vector can pass right through to this C layer, so all my C position are completely vacant.

Now, an important point to be noted this stage is that even in the A B A B kind of packing, my original hexagonal symmetry with 6 folds symmetry has been just destroyed. Because, just now this are additional atoms in the central positions and therefore, what I have here the rotational axis at the passing through this is merely 3 fold. That raises an important questions that even though I have only a 3 fold axis why do I called this un hexagonal close pack crystal, and why do this function called trinomial close factors.

Because, it is only got a 3 fold rotation axis, so this A B C and both A B C, A B C packing and also the A B, A B packing destroy by 6 fold symmetry present in the individual layers, like an individual layer like this and I got only 3 fold symmetry left. So, why do I called this an hexagonal close pack crystal, and as we know that crystal are name based on the symmetry, and not base on the geometry unit cell, and why is still called the hexagonal close pack crystal, so this the questions we will answer later.

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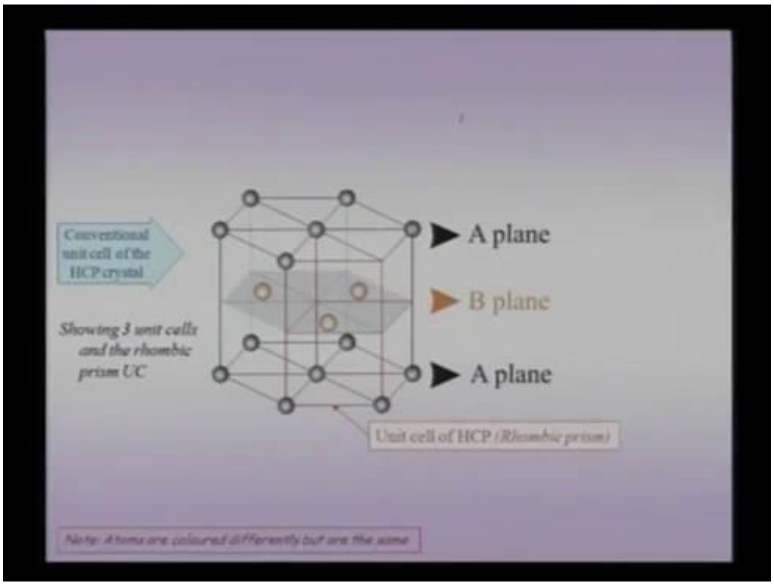

Conventional unit cell of the HCP crystal

Showing 3 unit cells and the rhombic prism UC

A plane

B plane

A plane

Unit cell of HCP *(Rhombic prism)*

Note: Atoms are coloured differently but are the same

So, this is the conventional unit cell of the hexagonal close pack crystal, where we have in the A layer, the B layer and again the A layer right about the A layer which was the first layer which as a started off. Now, as I told before this actually shows three unit cells of the hexagonal close pack crystal, and the actual unit cell is nothing, but this rhombic prism. Now, few things have to be noted we have seen already that there is only one kind of hexagonal lattice, the simple hexagonal lattice.

So, now, how do I accumulate this presents of the additional atom within the unit cell, and there is exactly this is additional atoms located within the unit cells, so this are couple of question we can ask.

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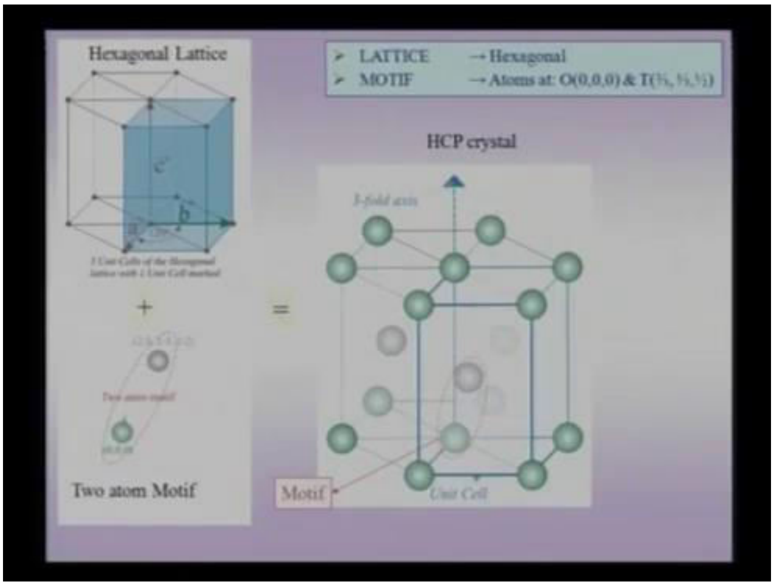

- LATTICE → Hexagonal
- MOTIF → Atoms at: O(0,0,0) & T(⅔, ⅓, ½)

But, before we do that we note the lattices hexagonal, and now the motif is an atom at 0 0 0, and also another atom which is located at the 2 3'rd along the x axis, 2 3'rd that is A 1 axis 1 3'rd along the a 2 axis and half along the C axis. So, this is the an additional atom and that atom goes part of the motif and is not part of the lattice itself. Therefore, if this is my lattice point, then this atom here goes part of the motif.

And my conventional unit cell as you can see here is the rhombic prism which is outline in the blue color. So, I have my simple hexagonal lattice and a 2 atom motif and as before I have to put exactly this kind of motif, and identical orientation at each lattice point to get the hexagonal close factors crystal. And as a point the hexagonal close pack crystal if I look at pure rotation symmetry has got the 3 fold rotation only.

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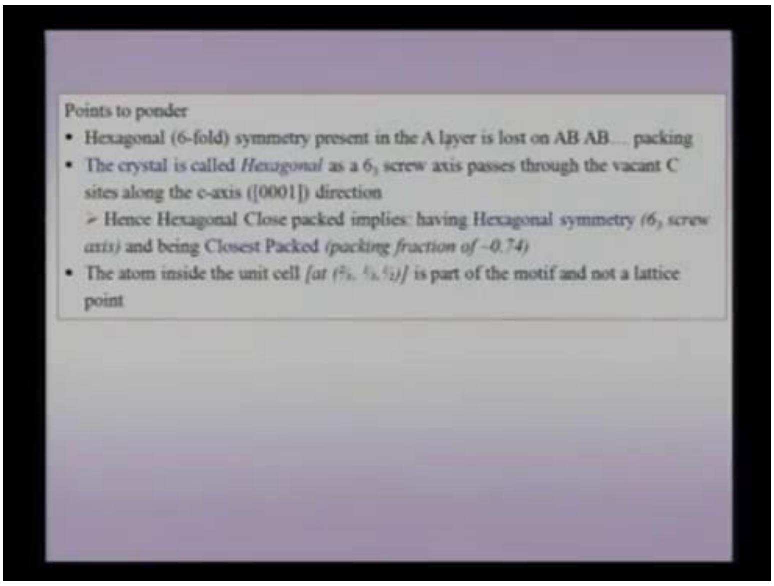

Points to ponder

- Hexagonal (6-fold) symmetry present in the A layer is lost on AB AB… packing
- The crystal is called *Hexagonal* as a 6_3 screw axis passes through the vacant C sites along the c-axis ([0001]) direction
  - Hence Hexagonal Close packed implies: having Hexagonal symmetry *(6_3 screw axis)* and being Closest Packed *(packing fraction of ~0.74)*
- The atom inside the unit cell *[at $(^2/_3, ^1/_3, ^1/_2)$]* is part of the motif and not a lattice point

Now, just to improve size some other points which we consider, so far the hexagonal 6 fold symmetry present in the A layer is lost on a layer A B, A B packing, the crystal now the answering the important question, the crystal is called hexagonal crystal. Because, there is 6 3 screw axis which passes through the vacant C sites, as I mention the vacant C site was an importance for our consideration, and there is an I mention that was this reason that actually you got 6 3 screw axis with passes through the vacant C sites and you can you already seen that vacant C site in the 0 0 0 1 projection.

Now, even though this is not a pure rotational 6 fold axis it has still has 6 and 8 that is this why these crystal which have an 6 3 screw axis are classified under the hexagonal class. We also seen that this is one of the close crystal pack one of the close crystal packing possible which is 74 percent packing of volume, an additional point to be noted is the atom inside the unit cell is no part of the lattice and it is; that means, center of that atom is not a lattice point, but it actually part of the motif.

So, this are the some important one consideration and we can take a further view to understand the same crystal structure, here presenting nothing no new time to be visualization the crystal structure in various ways.

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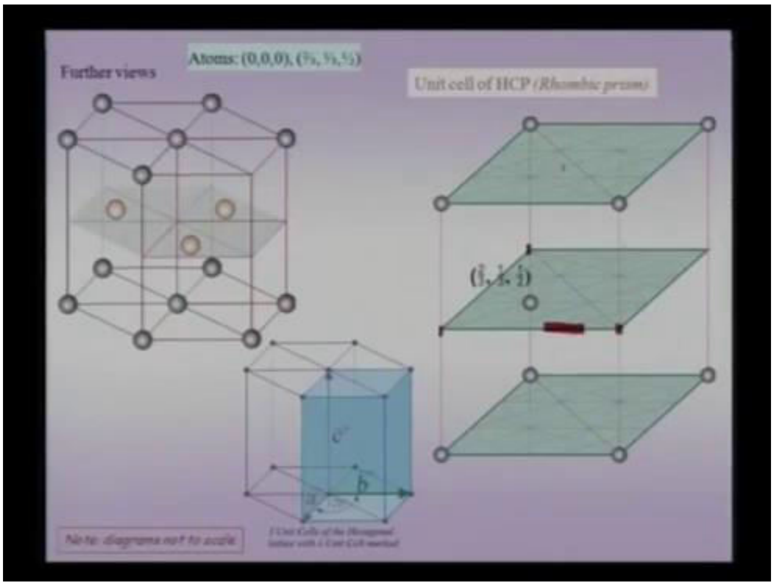

Further views

Atoms: (0,0,0), (⅔,⅓,½)

Unit cell of HCP (Rhombic prism)

Note: diagrams not to scale

And another important way to see where exactly the additional atoms located, so you can take my wrong represented divided into 4 first into half therefore, that I get my triangular prism. And this triangle prism I can divided into half along the C axis therefore, I get the meet plane of the this my meet plane of the triangular prism, and this atom is located on the mid plane and at this center out of triangle, which is vertices as marked here. So, this atom is located at the center out of this triangle which is nothing, but the mid plane of the half of the triangular prism.

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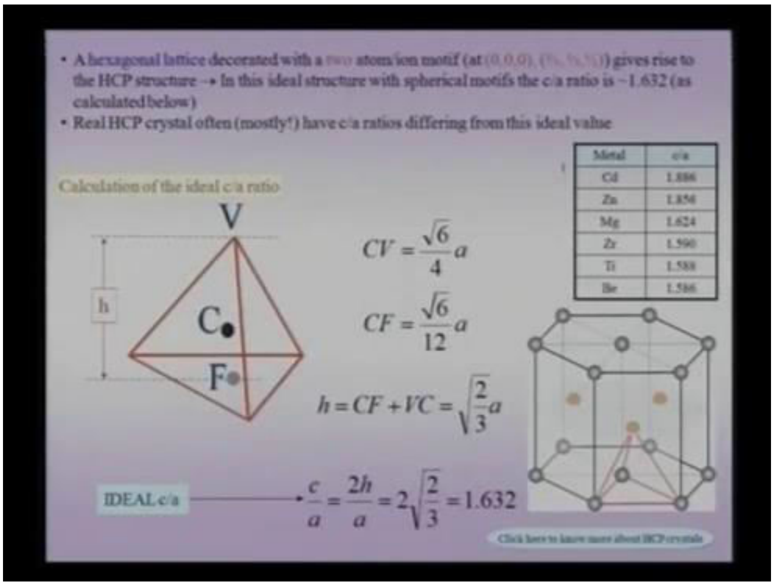

- A hexagonal lattice decorated with a two atom/ion motif (at (0,0,0), (⅔,⅓,½)) gives rise to the HCP structure → In this ideal structure with spherical motifs the c/a ratio is ~1.632 (as calculated below)
- Real HCP crystal often (mostly!) have c/a ratios differing from this ideal value

Metal	c/a
Cd	1.886
Zn	1.856
Mg	1.624
Zr	1.590
Ti	1.588
Be	1.586

Calculation of the ideal c/a ratio

$$CV = \frac{\sqrt{6}}{4}a$$

$$CF = \frac{\sqrt{6}}{12}a$$

$$h = CF + VC = \sqrt{\frac{2}{3}}a$$

IDEAL c/a $\longrightarrow$ $\frac{c}{a} = \frac{2h}{a} = 2\sqrt{\frac{2}{3}} = 1.632$

Click here to know more about HCP crystals

So, this is where the additional atoms located and next we will try to calculate, what is known as the ideal c by ratio for an hexagonal close pack crystal. Now, we have just put pack the layers along the C directions and therefore, if we have perfect sphere there is the mathematical values for this C based on the atomic diameters. So, now have the hexagonal lattice decorated to the 2 atom motif at 0 0 0 and at 2 3'rd 1 3'rd half, now we will see that the I ideal structure which spherical motifs as a C by ratio, which is 1.632

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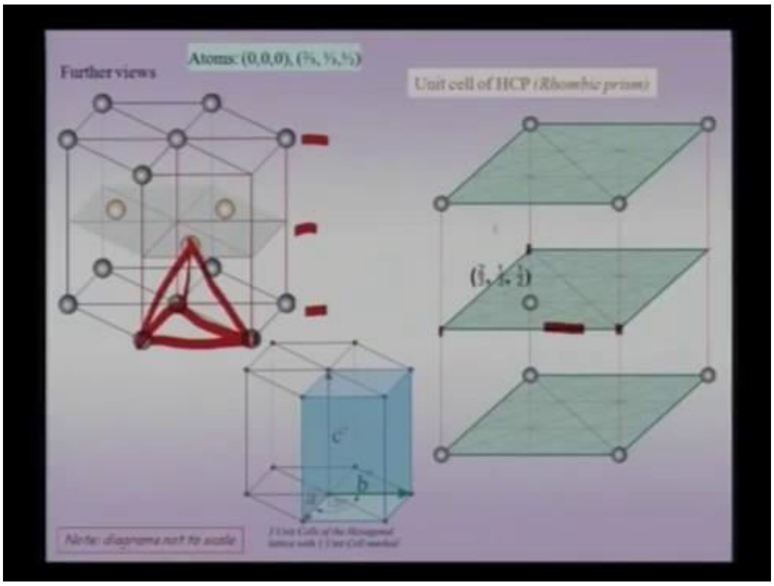

Further views

Atoms: (0,0,0), (⅔,⅓,½)

Unit cell of HCP (*Rhombic prism*)

Note: diagrams not to scale

So, let see how this 1.632 comes about now for to calculate that let me consider tetrahedron which is form by this atom, and the atoms which are located and this vertices. So, I am make a tetrahedron out of this atoms because, I join this atoms and base to form a tetrahedron.

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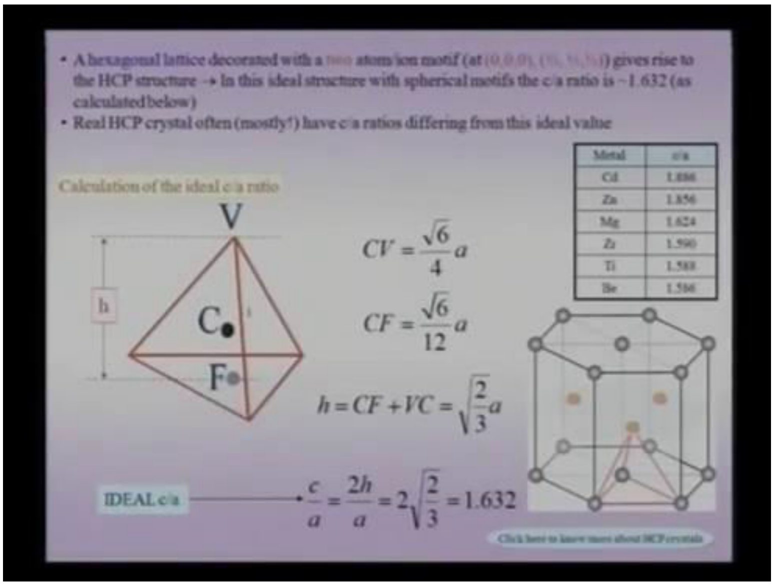

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Calculation of the ideal c/a ratio

$$CV = \frac{\sqrt{6}}{4}a$$

$$CF = \frac{\sqrt{6}}{12}a$$

$$h = CF + VC = \sqrt{\frac{2}{3}}a$$

IDEAL c/a

$$\frac{c}{a} = \frac{2h}{a} = 2\sqrt{\frac{2}{3}} = 1.632$$

Click here to know more about HCP crystals

So I have and tetrahedron and I can say that tetrahedron and the vortex of that tetrahedron call V. Now, because, as a regular tetrahedron C V, C is the center of this tetrahedron C V is root 6 by 4 a, where a is this edge cell edge cell length in this cell of edge length is a, C F is root 16 by 12 a in other words 1 3'rd of that value, and h is nothing, but half the C value; ((Refer Time: 37:32))that means, the by C length is length from this my C value and this h is half that, so it is the middle plan, so it is a distance of mid plan. So, my edge mark here is half which is nothing, but F V is half the C value.

And h is equal to C F plus V C which is root of 3 by a and the c by a value you can calculate is nothing, but 2 h as I said h is half of the value of c. So, h 2 by h by a just twice root of 2 by 3 which is 1.632, so this calculation of course, simple a geometry calculation, which you can perform independently. But, the important pointed we noted here is the value we have calculated that is the ideal c by ratio is 1.632.

Now, if I look at this ideal c by ratio some other common metals which cyst lies in the hexagonal close pack, structure like cadmium, zinc, magician, zirconium, titanium and prelim. You notice that in the even in this less there is just one which comes even close which is magnesium, which has got an c by a ratio of 1.624 in other words most of the matters which have the hexagonal close factors structure do not have an ideal c by a ratio.

In other words how did I get this ideal c by ratio assuming that all atoms are hard sphere and I get an packing which is A B, A B kind of packing. So, in nature this kind of assumption is not true, in other is not valid 100 percent and therefore, I can get an non ideal c by ratio for most of the metals, some of the c by ratios are larger like for instance cadmium has 1.886 zinc has a larger value.

But, some of the materials like beryllium have smaller c by ratio, and what is smaller c by ratio mean, it means that and quashing the hexagonal down word a largest c by ratio means I am expanding the hexagonal. So, let me take up the model to show you what is hexagonal close pack structure, so I have a model here which show the hexagonal close pack structure.

So, I have atoms in the A layer, the B layer which is the middle layer and the layer which is above which is about A layer right about the vessel layer. And this as you can see nothing, but 0 0 0 1 plane of the hexagonal close pack structure, and my bases vectors are the vectors along say for instance this is my A 1 this would be my A 2. So, this is in my A 1 this my A 2 and the vertical vector this is C vector which is above, this as we said this part of the motif.

And therefore, my two atom would be sphere here and sphere here, which goes on to decorate every lattice point. So, I would put a two atom sphere here and here and, so forth and some of them would set within this rhombic units cell and some of them would not set within the rhombic unit cell. Now, as I mention this kind of structure is what is got let me show on the side has got a proximately the ideal c by ratio, but as I told you the real hexagonal close pack crystals can have a c by a ratio which is stranded that could be larger or smaller.

And; that means, that my spheres cannot be assume to be the hard sphere model of atoms is no longer valid. Now, the tetrahedron which I consider can also be seen nicely in this model of the hexagonal close packed structure, wherein of course, there are more than one units cell here. But, you can clearly see the tetrahedron which was mentioning to calculate my ideal c by a ratio or this 4 atoms, which form the tetrahedron from which I made my ideal c by ratio calculation.

We will return to this model, when we talk about wide in hexagonal close packed crystals. The next important crystal we would consider and before that I have question from Hari.

STUDENT: What will the effect of deviation from the ideal c by ratio 1.63 to the close packing of the hexagonal.

Very good question very, very good question; obviously if we have deviation from there are two important question we can ask here, one is the question if you ask is what is the packing fraction how is affected by a non ideal c by ratio. And number two suppose question what is the consequence and the properties of the crystal, the first one; obviously, it is divertive from the ideal packing fraction.

So, ideal packing fraction is assumed using hard sphere and if there is non ideal c by ratio. Obviously, this number would be affected this packing fraction affected, the second question is the impart properties now we will see typically, if the these vessel planes are the slip plane in another when we are talking about plasticity because, slip plane and if you have this vessel plane separate out, then we vessel slip would be promote, if you have this plane squash together then bases plane would be other normally that much easy to take place.

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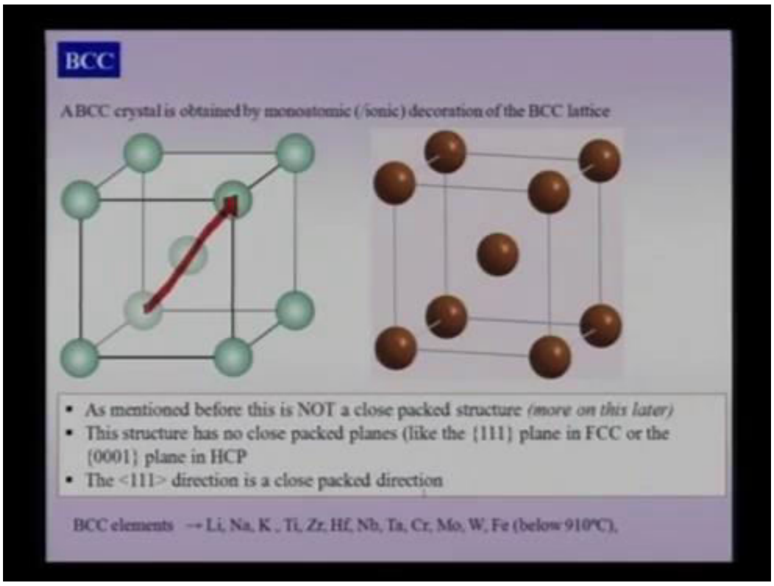

BCC

A BCC crystal is obtained by monoatomic (/ionic) decoration of the BCC lattice

- As mentioned before this is NOT a close packed structure *(more on this later)*
- This structure has no close packed planes (like the {111} plane in FCC or the {0001} plane in HCP
- The <111> direction is a close packed direction

BCC elements → Li, Na, K , Ti, Zr, Hf, Nb, Ta, Cr, Mo, W, Fe (below 910°C), So, the next structure we take up is what is known as the BCC crystal which we know is the mono atomic or mono ironic decoration of the BCC lattice. So, we have seen this structure before and there are two views of structure right here, and you can see that there is two atoms per unit cell. That means, it a double non primitive crystal structure, and the important point we already noted, and we will reemphasize that this is not the close pack structure.

And we will see little more about this later, and more importantly it has got no close pack planes. In the case of HCC and HCP we start off with close pack planes, and those plane assuming of course, an ideal c by ratio in the case of hexagonal, that this plane remains close pack planes, when you continue to make the crystal out of close pack planes. But, in the case of BCC crystal the construction not done the wave we have done the FCC or the CCP on the ACP crystal.

And therefore, this crystal structure has no close pack planes, however the 1 1 1 direction is a close pack direction. That means, the atoms touch along the 1 1 1 direction this is origin for instance, and this is the other vortex, so may 1 1 1 direction with the direction connecting this, and the atom touch along the 1 1 1 directions. And therefore, that is a close pack direction in the BCC crystal.

So, when I mention BCC crystal without any other qualification, and we will see later of examples that we should careful in this regard, when I say BCC crystal what I mean is a mono atomic decoration of the or mono ionic decoration of the BCC lattice. And such structure very emphasize has is not close pack structure, has no close pack planes, but still continues to have a close pack directions.

Some of the common metals which are elements which show define this is the crystal structure are tungsten, ion below 910 degree Celsius, which is called alpha ion and some important element like sodium and potassium.

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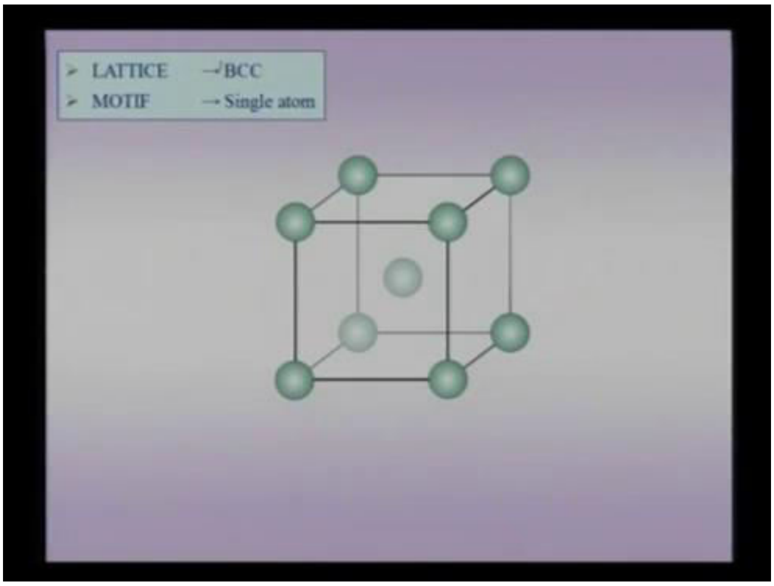

- LATTICE → BCC
- MOTIF → Single atom

This is in this case of course, which obvious the lattice PCC and all have a single atom degrading the BCC lattice.

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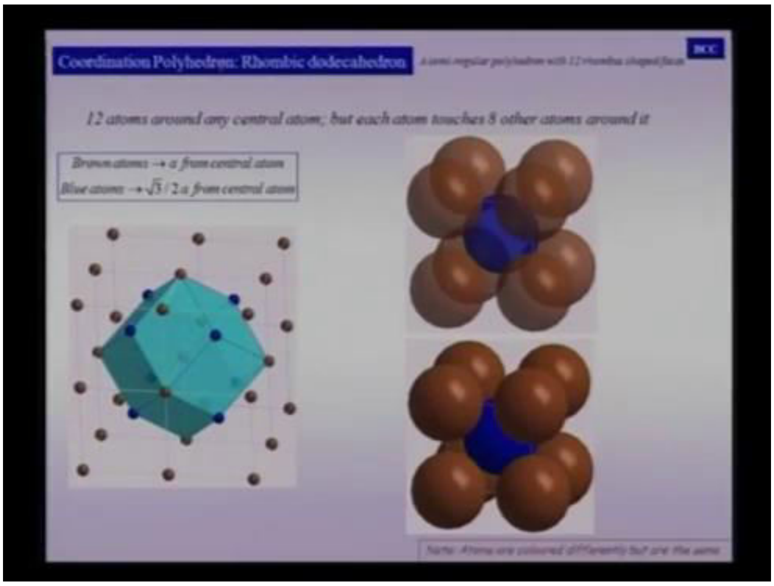

Coordination Polyhedron: Rhombic dodecahedron

A semi regular polyhedron with 12 rhombus shaped faces

BCC

12 atoms around any central atom; but each atom touches 8 other atoms around it

Brown atoms → a from central atom

Blue atoms → $\sqrt{3}/2$ a from central atom

Note: Atoms are coloured differently but are the same

Now, the coordination polyhedron for BCC is different kind of polyhedron, and we already deal with this polyhedron or we have encounter this polyhedron in the context of the space fill. We saw that cube is the regular solid which is as got space filling properties, we saw that there are two non regular solids or two important non regular solid which are space filling property, one is detract hedron, other one is rhombic head ran, and this rhombic hadrons is the solid you see here or the which is the coordination polyhedron for the BBC structure.

So, I take any atom it could be one which is shaded blue or the one shaded in red both of them are identical atoms and I if I construct the polyhedron around it could be a rhombic hadrons. But, the important point we noted here is that even though the rhombic hedron is made up of single kind of phase, which are rhombus the effective as a central atom which is here of course this is my central atom. Then all the atoms are not located at the same distance from the central atom.

This is the important point note for instance the atoms which are shown in the blue are located at the distance of root 3 by 2 a from the central atom. And one shown in the brown are located at the distance a; that means, the coordination polyhedron is known not only made up of nearest neighbors, but also next nearest neighbors. So; that means, there are two kind of distance which I need to encounter a and root 3 by 2 a, so this is what, so of course, a is root 3 by 2 as a bracket here, so therefore, is root 3 by 2 into a.

So, let me look at the model of the rhombic hedron, so that we can understand how does shape look like, and then we will proceed to the other further picture of the BCC crystal. So, I have here the model of the rhombic Doric hedron, and as you can see this is not one of the regular solid, it is not a mechanical solid and this is got identical faces, the solid consist all the faces of the rhombus. But, the kind of vertices it got two types, there are vertices which are three connecting you can see these vertices three connecting vertices which is in green.

And there are red vertices which are four connecting vertices, so there are four connecting from this vertices. So, the rhombic Doric hedron is very special kind of solid, which is a space filling solid it is not a regular solid, it is got identical kind of phase of solid, but two kind of vertices, the three kind of vertices and the four connecting vertices. So, this is a important solid as for as geometric goes which is the rhombic Doric hedron.

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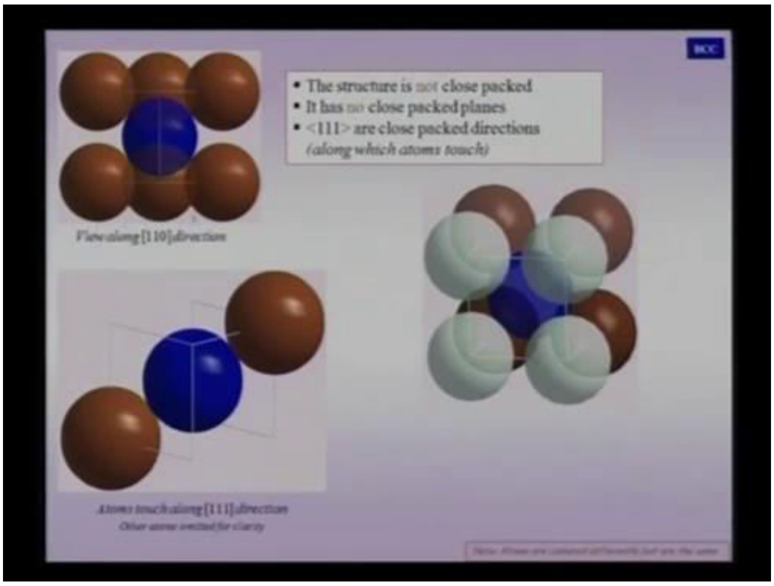

- The structure is not close packed
- It has no close packed planes
- <111> are close packed directions
  (along which atoms touch)

And it is called the do Doric hedron because, it is called 12 phases which you can see from this diagram 12 faces 4 above, 4 in the mid plane and 4 below. So, this is got a is a rhombic hedron, now this diagram below for distance shows as the touching direction which is 1 1 direction along which atoms touch. Again you should node that all atoms are identical and they have just been shaded for clarity.

And this is a slide transfer model to show that were the central atoms sets and how the atoms touch one another. Suppose I look along the 1 1 0 direction, then you will see and of course I remove the atoms which we are front of blue serial then I can see the relative position of this blue serial, which is the body centering position, with respect to other spheres. Of course, like in many other cases, if I would not chosen any origin here, I would have chosen the origin blue spheres, the structure would be total an alter.

And in the other this atoms which are in the vertices of the cube all becoming body centering position atoms. Now, we should know that whenever we deal with the new structure it is very, very important that we actually look at the structure from various point of view, try to understand some of this concept out line in again and again, the direction close packing. The direction of touching and which are the atoms touch and which are do not touch each other, and also the concept of the coordination of polyhedron, so that is a very important concept.