Introduction to Materials Science and Engineering
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Lecture - 17
Hexagonal Close-Packed (HCP) structure

Hello, in this video, we will look at one of the important classes of Close-Packed Structure, the Hexagonal Close-Packed Structure also known as HCP. In the last video, we introduced the concept of close packing of hard spheres.

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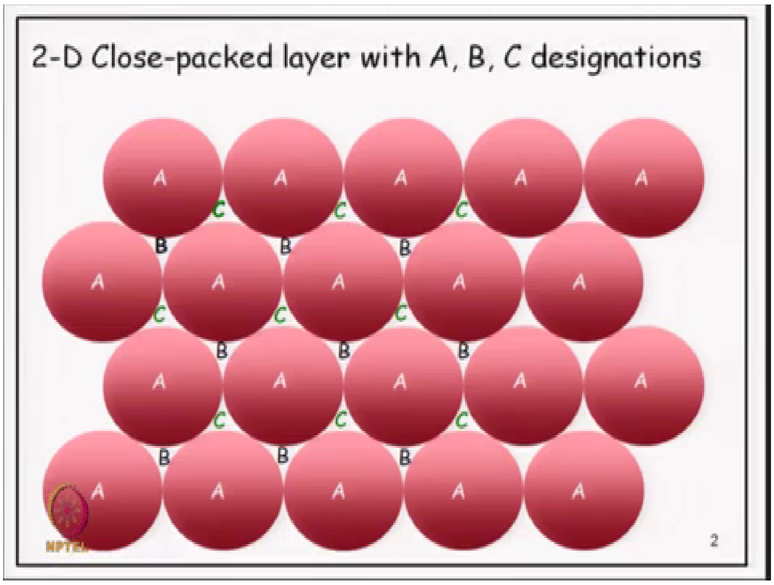

2-D Close-packed layer with A, B, C designations

We looked at a 2 dimensional close-packed layer, a hexagonal layer which is shown here and introduced the designations A, B and C for different layers. In a single layer which is shown here all is spheres are known as the A spheres or the entire layer is known as the A layer. In this is in this one we have two kinds of crevices the B crevice centered on a triangle an upward pointing triangle of A or a C crevice centered on downward pointing triangle of A. And we have seen that these spheres the next layer spheres can be placed either on B or on C, but not on both.

So, when we build up the stacking in three dimensions we can after an A layer we can have a choice of either B or C and then on B layer we again have a choice of either A or C.

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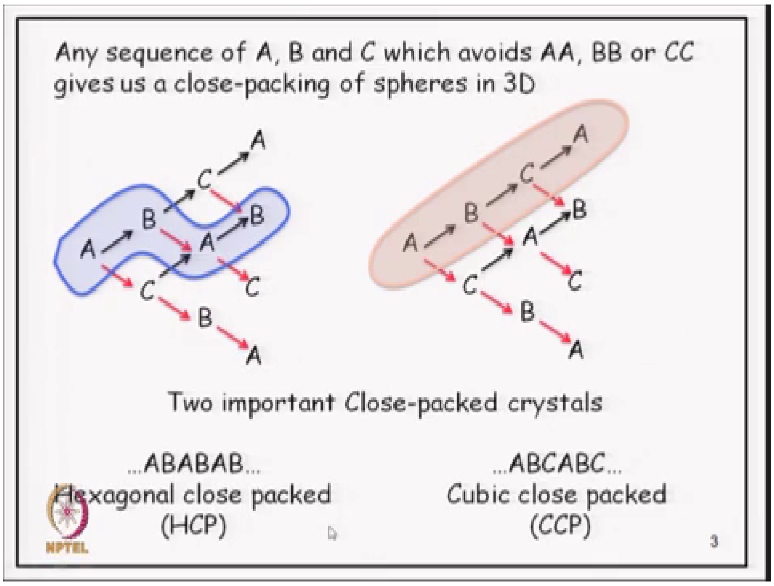
Any sequence of A, B and C which avoids AA, BB or CC gives us a close-packing of spheres in 3D

Two important Close-packed crystals

...ABABAB...
Hexagonal close packed
(HCP)

...ABCABC...
Cubic close packed
(CCP)

So, we have seen this diagram and we stated that any sequence of A, B and C which avoids two identical layers coming together like AA, BB or CC. If we avoid this kind of identical layers coming one on top of the other, because they will not give close packing then any sequence of A, B and C will give me a close-packed structure. So, I have shown you that we can begin with A and then we can go to B on B again have a choice of C or A on C I have a choice of B and a and so on.

So, a variety of or infinitely many different kinds of close-packed structures are mathematically or theoretically possible, but nature prefers especially two of them and these are two important classes of close-packed structure. One such sequence is shown here as AB, AB. So, if we place an A and then on that B layer, then again A and then on B always avoiding the C sides then we get a stacking sequence AB, AB, AB . This gives us a hexagonal close-packed structure or HCP structure. The other one other important one which occurs in nature is A, B, C, A. So, if we continue in this sequence ABC, ABC then we get a cubic close-packed structure. So, these two are particularly important and we will deal with them one by one.

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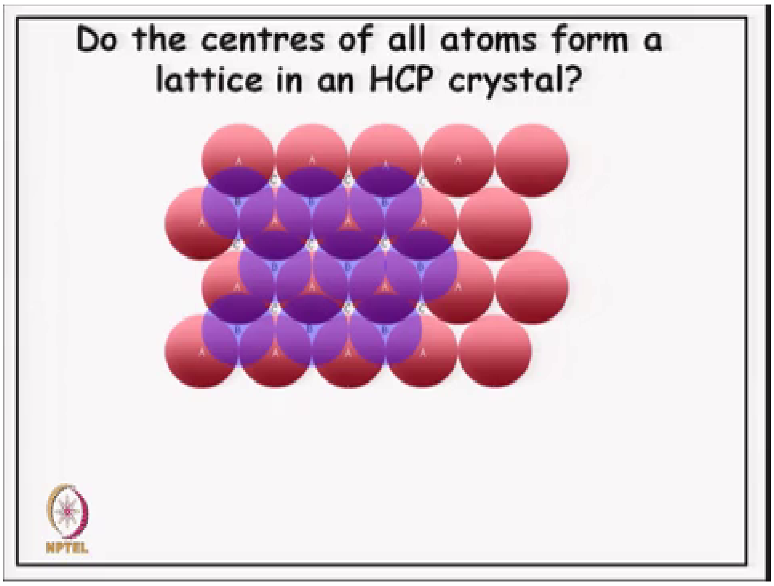

Do the centres of all atoms form a lattice in an HCP crystal?

In this video, I begin with the hexagonal close-packed or HCP structure. So, let us look at our closed-packed layer again: two layers A and B are shown. A in red and B in blue. So, all the B sides atoms of blue color are sitting. Of course, I am showing you in this in a projection, you have to imagine that in 3d the B will be sitting on top of A. Now important questions to ask are all these atoms equivalent in the lattice sense. Do they form a lattice? Do red and blue atoms or A or B atoms form a lattice. To look at this let us try to reduce the sizes of these spheres.

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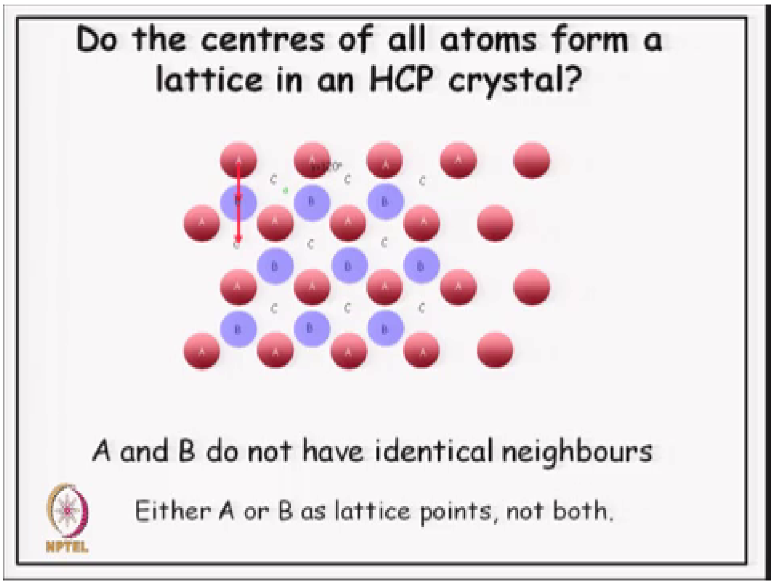

Do the centres of all atoms form a lattice in an HCP crystal?

A and B do not have identical neighbours

Either A or B as lattice points, not both.

So, that the positions are seen more with more clarity of course, we know that the red is spheres touch the nearby reddish spheres and the blue spheres touch the nearby bluish spheres, but the diagram becomes too cluttered as was our previous diagram.

So, I have just shortened the radius of each sphere, only to indicate the locations. Now, if we begin our journey on an A atom and reach the nearest B atom; I have a translation shown in red here. Notice that again we are in a projection. So, this translation although appearing horizontal is not a horizontal translation, it has a horizontal component from an A atom to the centroid of the triangle of A atoms. So, this is the horizontal component of this red vector. It also has a vertical component from the centroid we have to lift ourselves up to the centre of B atom and B atom is the next layer and so it is above A atom so that particular vector going from A to B having both horizontal and vertical components as shown in red here in the projection.

So, A atom has a neighboring atom at this translation vector. What about B atom? If I translate myself by the same vector from B you can convince yourself that you will end up on a C side, but I have left the C side unoccupied. We decided that our stacking sequence is AB, AB. So, we are never placing any atom at the C. So, we see that although A has a neighboring atom at B on this red translational vector. An identical translation vector from B does not give me any atom in the neighborhood.

So, A and B have different neighborhood. So, what we conclude from this that A and B do not have identical neighbors, their neighborhoods are different; which means that they cannot be considered together they cannot be considered as forming lattice centers of both A and B atoms do not form lattice, because they don't they are not translationally equivalent. The translational neighborhood of A and translational neighborhood of B is different.

So, we can select the lattice points on either at A or at B, but not at both. Of course, all A atoms are equivalent this forms a 2d lattice in one layer and then the next layer is also equivalent to the previous layer. So, all A atoms are equivalent and they form a lattice. Similarly, all B atoms are also equivalent and they also form a lattice. So, we can select either A or B as a lattice points, but together if the combined set of A and B atoms or their centers cannot be considered as the lattice. So, this is a very very important a point to keep in mind. And this is where often confusion comes; that we have two kind although chemically we have the same kind of atoms A and B are chemically the same, but positionally or translationally they are not equivalent and they are not forming a lattice.

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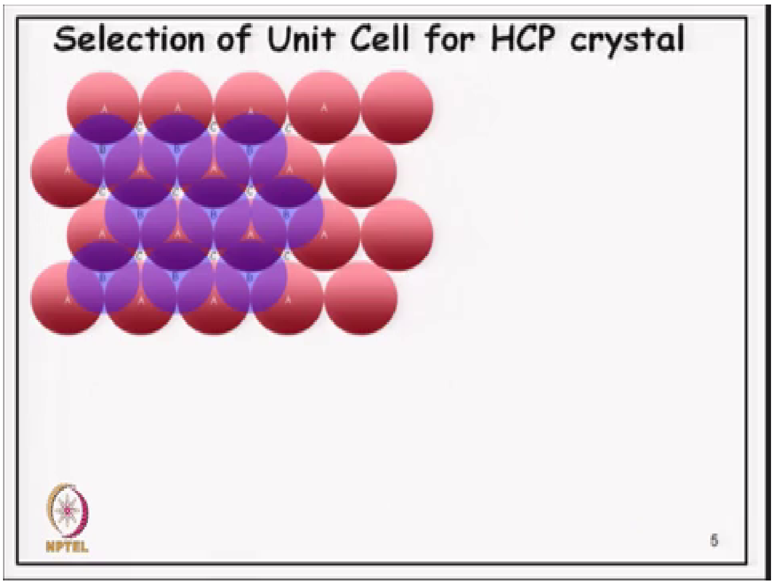
Selection of Unit Cell for HCP crystal

Now, let us select a unit cell for this HCP crystal. Do this again we reduce the sizes of the atom to look at the positions more clearly.

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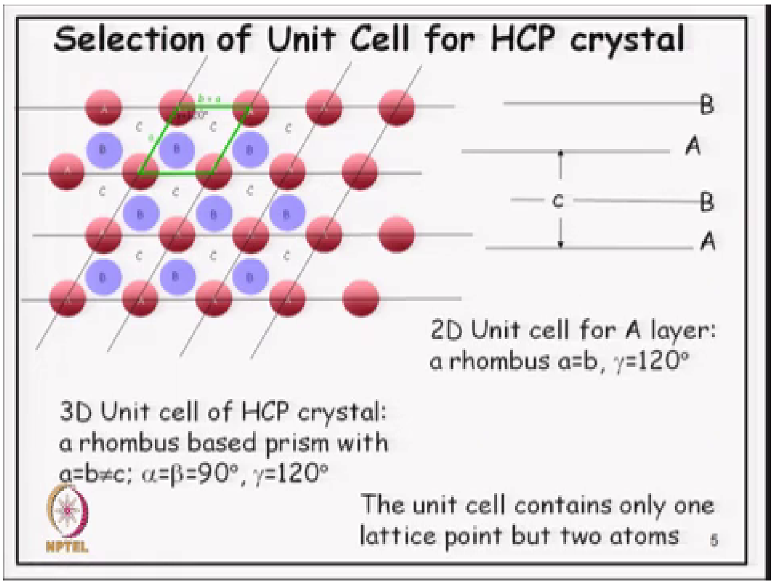
Selection of Unit Cell for HCP crystal

2D Unit cell for A layer:
a rhombus $a=b$, $\gamma=120°$

3D Unit cell of HCP crystal:
a rhombus based prism with
$a=b\neq c$; $\alpha=\beta=90°$, $\gamma=120°$

The unit cell contains only one lattice point but two atoms

And then we have seen that we all A’s are equivalent and let us decide to select our lattice points at A and we leave out B. Now, I superimpose a grid of lines on this on the A layer joining all the A atoms. We can select a two dimensional unit cell shown in green here a two dimensional unit cell for the A layer. So, this is a rhombus. This is a 2d unit cell which is a rhombus with A equal B the two sides are equal two sides are equal. In fact, remember that this is close-packed structure and the two atoms along this length along A or along B are touching. So, both of them are equal to twice the radius or diameter of this sphere.

So, A and B; A equal B equal to the diameter of the atom. And the angle gamma between them is 120 degree. So, this becomes the two dimensional unit cell of a given layer, but of course, the crystal structure is three dimensional. So, we have to extend this unit cell in the third direction to complete our 3d unit cell. In the third direction you can see the stacking sequence we have decided is A B, A B which is shown in profile here. So, each line is representing the entire layer. So, A layer and above that we have a B layer then again A layer and then again B layer and so on.

Now, we have already seen that the B atoms are not equivalent to A. So, since we have selected our corners as lattice points in the plane A. The next set of lattice points will form the other corners of the unit cell. Recall in our previous discussion in the very beginning, when we defined the unit cell we said the unit cell the corners should be the lattice points. So, we have the lattice points at A; B does not have any lattice point. So, our unit cell cannot end on B in the third direction. So, it has to go all the way to the next layer A to find the lattice point. And of course, A is exactly above the A below it. So, I can go vertically from an atom in A layer to the next A layer to find another equivalent lattice point there.

So, the third direction is perpendicular to the A layer and goes from one A layer to the neighboring A layer crossing the B layer. So, the C distance is actually twice the interplanar spacing. This is important to keep in mind. So, the C distance is not from an A layer to a B layer, but from A layer to the next A layer. So, and the interplanar is spacing is from A to B, so C is two times the distance interplanar is spacing of these close-packed planes. So, with this we complete our 3d unit cell which is a rhombus based prism where A equals B of course, this is not equal to C and alpha and beta are 90 degree, because the C axis we have selected perpendicular to the layer plane. So, alpha beta 90 degree and gamma is equal to 120 degrees.

So, this as we know is conventional unit cell of a hexagonal lattice and that is what we have selected for our hexagonal close-packed structure. But it's important to keep in mind that this unit cell contains only one lattice point, but two atoms. We will look at this in little bit more detail in the next slide.

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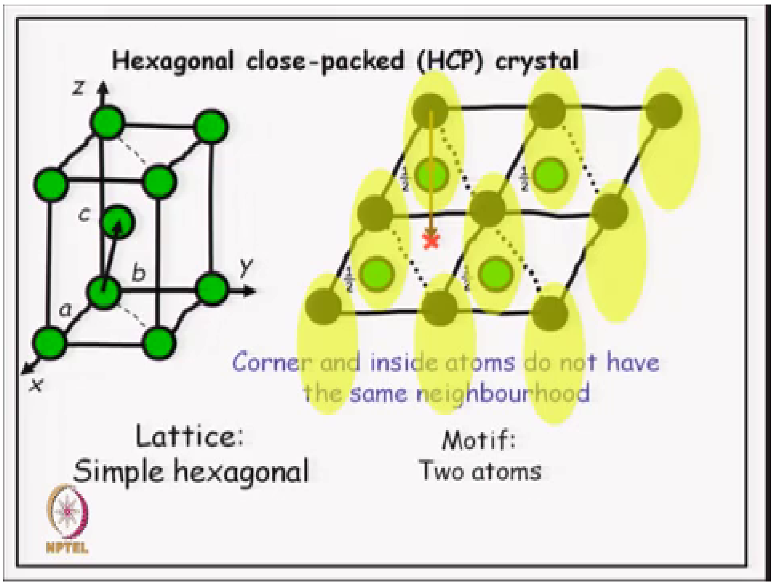

Hexagonal close-packed (HCP) crystal

Corner and inside atoms do not have the same neighbourhood

Lattice:
Simple hexagonal

Motif:
Two atoms

So, this is our hexagonal; hexagonal prism. Now we have selected our one of the corners of the prism as origin and the X and Y axis in the plane forming this rhombus base and the c axis is going the Z axis is going perpendicular to this plane and the height of the prism is c, but there is a b layer atom which is inside this unit cell.

The corner atoms the 8 corner atoms will effectively contribute to one atom in the unit cell and the inside atom the b atom will also contribute to one atom. So, that's why in this unit cell we have two atoms, but if you look at lattice points only the corners only the 8 corners are lattice points. So, effectively there is only one lattice point that's why I made a statement that the unit cell contains only one lattice point, but two atoms and hence this unit cell despite containing two atoms is a primitive unit cell. Recall, the definition of primitive unit cell. A primitive unit cell is one which has effectively only one lattice point per cell and this is a kind of unit cell which has in our current example also we have a unit cell which has only one lattice point.

So, despite having two atoms, since the second item is not a lattice point, the centre of the second item is not a lattice point this unit cell is not a non primitive unit cell; it is a still a primitive unit cell. This is an important point to keep in mind something which often creates some confusion. Let us now look at the projection of this unit cell here. And I am seeing the projection of 4 unit cells. So, I have the rhombus base which is shown here and then on at the centroid of one of the triangle, this atom will project that is my b side, on the centroid of the other triangles since that is a C side there is no atom. And I have given a coordinate a fractional coordinate half to indicate that the position of this atom the internal atom is a half the unit cell high it is half c; c by 2. So, the indication of that is given here by this fractional coordinate half.

So, these are the these four are internal atoms to the respective unit cells and the other corner atoms are seen here. Again repeating that's exercise with the arrows which we had done. We see that a corner atom has this internal atom as its neighbor, but internal atom in the say if we move from the internal atom in the same direction the same distance we do not find a neighbor. So, the corner atoms and the central atom are not equivalent. The atom inside the unit cell is distinct from being a lattice. So, we can select lattice points only at the corners. So, the corner ones are the lattice point and lattice its simple hexagonal. I just stated that the unit cell is primitive and it has hexagonal symmetry. So, the lattice is simple hexagonal.

However, if I want to build up the structure from the lattice if I want to get the crystal structure I have to place all the atom. If I decide to place atoms only at the lattice point, I will miss out these internal atoms. Thus, just placing one atom at each lattice point will not give me the crystal structure that is why we say that the lattice the structure cannot be built up by a motif of one atom a two atom motif is required. So, if I place only one atom and I don't place any other atom, then these four atoms the internal atoms will be missing and this gives me a simple hexagonal structure, but this is not a hexagonal close-packed structure.

So, for hexagonal close-packed structure, I do need these additional atoms inside the unit cell. Now, how do I do that in the description of motif? So, what we decide that with each lattice point, I will place not only one atom at the lattice point, but also and another atom this green atom displaced by this vector with respect to the lattice point. So, in our in our mental imagination in our thinking we are now associating a pair of atoms with each lattice point. So, we are saying yes corners are lattice point, but we are not placing only one atom at each corner, we are placing a pair of atoms and of course, the pair of atoms cannot be placed at the same point. So, they are displayed with the respect to this translational vector and such a pair is then since all lattice points are identical such a pair is placed at each lattice point. And this is the reason why we are calling that the motif consists of two atoms.

If I place such a pair of atoms at each lattice point I will get all these other three missing atoms in my diagram and of course, these corner atoms which don't appear to have their a pairing atom will of course, have the pairing atom because the structure does not consist of only those these four unit cell, but continues in all the directions. So, when I draw the next unit cell here an atom here will exactly be the one which will pair with this atom. So, each lattice point have exactly identical pair of atoms and this pair of atom consist the motif. So, motif consists of two atoms. Just see just giving the number of atoms in the motif is not a complete description of the motif.

So, in the next video we will see that we should to complete the description of the motif we should also give their position with respect to the lattice point. So, we will calculate this position for this particular example in the next video.