Introduction to Materials Science and Engineering
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Lecture - 18
Lattice And Motif Of A Hexagonal Close-Packed HCP Crystal

Hello and welcome we have in the last video we had discussed the structure of Hexagonal Close-Packed Crystal. We described the structure in terms of closed-packing of equal sized sphere and we saw that such close-packed layers are stacked in the sequence ab ab to give us hexagonal close-packed structure. In this sequence; we also saw that only the A centers of A atoms form the lattice; A and B atoms are not equivalent in the lattice sense and if we want to select lattice points we can select lattice points and if we select the lattice points at the at centers of A, then centers of B cannot be included in the same lattice.

So, B atom has to come as part of a motif. So, we stated that the hexagonal close-packed structure the HCP structure can be described as a lattice plus a motif consisting of two atoms, but this two atom motif description is not complete and we need to give more information; particularly the location of atoms in the motif to complete the description of our motif. So, that exercise we will do in this video.

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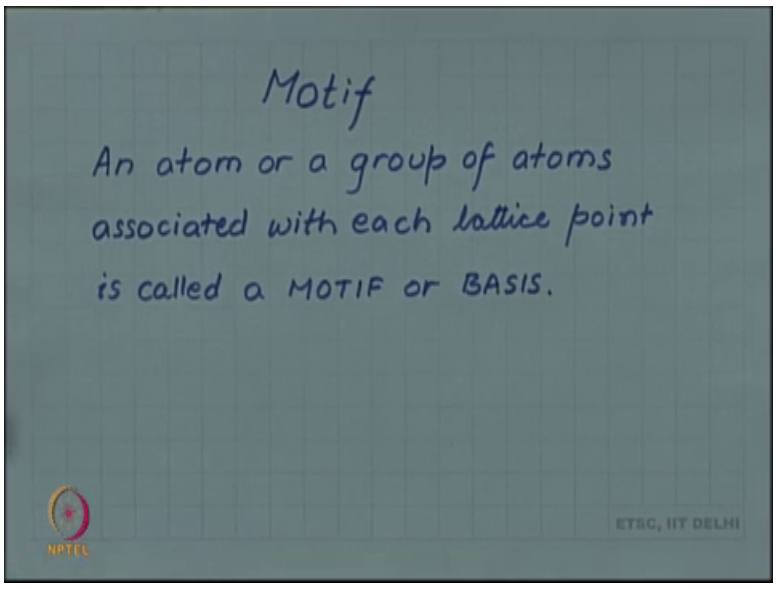

So recall the definition of motif which we had done in the past, that motif any atom an atom or a group of atom associated with each lattice point is called a motif or there is a synonym motif or basis; because we have seen that a lattice gives you only the skeleton of the entire structure its only a set of points and for crystal we need to provide atoms at those points.

So, that atom or group of atoms which by associating with each lattice point we can develop the entire crystal structure will be called motif. So, hexagonal close-packed structure provides a good example of motif.

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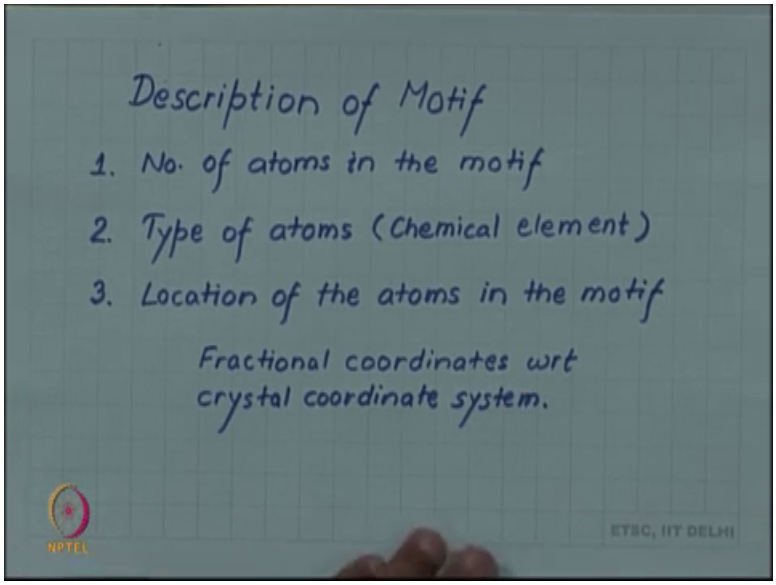

Now the description of the motif requires you need to give first of all the number of atoms; how many atoms are there in the motif? So, number of atoms in the motif; then you need to tell the identity the chemical identity of these atoms the elements. So, the type of atoms by which we mean chemical element and finally, and most importantly you are also have to give the location of the atoms in the motif. This for the HCP structure we have not yet done and this is the main goal of this video.

So, location of the atoms is traditionally given as fractional coordinates with respect to crystal coordinate system. The meaning of fraction coordinate will become play when we look at this HCP example in details.

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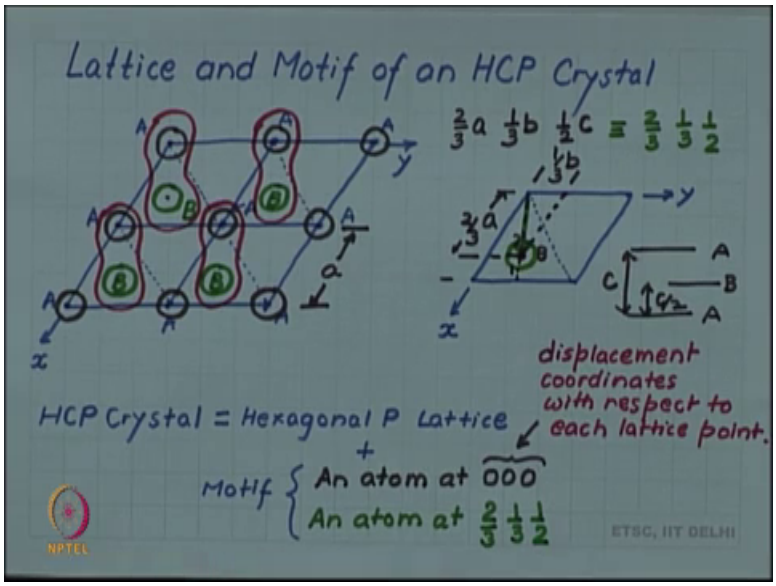

So, let us build up the HCP crystal. So, we again start with the lattice. So, let me draw a few lattice points. So, the these are the lattice points in one layer. So, these are the centers of atoms of A layer let us say and I am drawing it in projection. So, all the A layers projection on this A plane. So, all A layer atoms will project exactly at these locations. So, these are my lattice points. So, let me draw the line joining them to outline the unit cell.

The crystal coordinate system for hexagonal as we know is along the edges of these rhombus unit cell. The unit cell is of a shape of a rhombus the two sides are equal the angle between them is 120 degree. So, that is my x and y axis. So, that's why we are calling this as a crystal coordinate system and not a Cartesian coordinate system which always has to be orthogonal. So, in hexagonal the crystal coordinate system the axis x and y are at an angle 120 degree. This we have discussed in the previous videos also. Now these centers these corners of the lattice points are what is deciding the A location in the structure. So, this is where the centers of A atoms will be placed. These are all A locations I mark them as A.

So, what we have now? Is the projection of all the lattice points in the crystal on one of the planes; the basal plane of the crystal structure. Of course, not all we have we are showing you 2 by 2; 4 unit cells. So, all the lattice points within this 4 unit cell, but of course, by repetition you can fill the two dimensional plane and get other points and also

you know that in the third direction perpendicular to these planes the repetition distance is C. So, such A layers will again repeat at each C distance. So, after a height of C there is another A layer, but those locations will also project exactly at these points. And then a two C there is A third layer which will also project at these points. So, in terms of projection all A sites will project at these locations shown here.

Now, but this is only the lattice. This is the simple hexagonal lattice. So, we have our hexagon also let us write our equation remember, we said that any crystal structure and thus HCP crystal structure can be described as A lattice plus motif. So, we write HCP crystal as a lattice and we recognize that the lattice is simple hexagonal. So, I write this as hexagonal P; hexagonal P or simple hexagonal or primitive hexagonal all are equivalent phrases. So, I write this as hexagonal P lattice. So, lattice is hexagonal P, but lattice alone is not the crystal structure I don't have the atoms as yet.

So, all I have is the skeleton of the structure where I should place the atoms. So, that's what the lattice tells? Lattice gives us the periodicity of the structure; atoms are repeated with this kind of periodicity, but what are the atoms which are being repeated? And where they are placed with respect to this lattice point that description comes in motif? So, to complete the structure we have to give the description of the motif.

So, hexagonal P lattice plus a motif and what is that motif. So, to build up our structure let us first place an atom at one of the lattice points one atom at a give at this lattice point at the origin let us say. As soon as I do this; since all lattice points are translationally equivalent, they should have identical surroundings. So, if this lattice point gets an atom all such A lattice point get an atom. So, my structure starts building up by provide an A atom at all the lattice point.

So, in motif I call this as an atom at the lattice point which is an atom at o o o I write this as o o o. The meaning of this phrase is that at each lattice point there is an atom and that is my A atom. So, o o o really it does not indicate that there is only one lattice point at the origin; with respect to each lattice point; with each lattice point assumed as origin I place an atom. So, these coordinate which I have shown here are not some sort of absolute coordinate, but with respect to each lattice point. So, these are displacement let me write this as a displacement coordinate with respect to each lattice point. So, that's the idea of

the motif in when I say there is an atom at o o o this is an atom in one motif, but identical motif motifs are associated with each lattice point.

So, each lattice point get an atom an o o o says that the atom which the lattice point is getting is not displaced with respect to the lattice point. So, it is exactly at the lattice point. So, in simple language I could have called it an atom at the lattice point, but I wish to give the fractional coordinate of the atom. So, I write an atom at o o o. Now, but this has not completed our hexagonal close-packed structure; I have only got the A layers So, my stacking sequence currently is a, a, a, a this is not hexagonal structure as you already know we need to have the B layer. So, I have to provide atoms at the B layer also and that description should also come in this description of the motif.

So, where are this these B atoms. So, to get that to locate them it is better to divide my rhombus unit cells into triangles; and as in the last video you have seen that we have two kinds of triangle: one a triangle pointing up and another the triangle pointing down. And only one of these two triangles can be considered as a B side. So, I locate the centroid of the up triangles let us say as my B sides. So, I place an atom at one of these B sides let us say; this is my B atom. And mentally I associate this B atom with this lattice point at A. This is a mental association. So, atom b; obviously, cannot be sitting at the same lattice point, because that lattice point is already occupied by an atom A, but we are associating atom B with the same lattice point where the A atom is located.

So, in the motif description, I say that there is another atom at the B side. So, I have to complete the description I should give it's fractional coordinates. So, to work out the fractional coordinate of the B atom, let me redraw the unit cell, but before that since I have given a B atom to this A lattice point and since all lattice points are identical I should give identical B atoms to all the lattice points. So, I start filling all these B sides this A is little confusing. So, let us put an arrow this A is this one. So, just like this B atom is associated with this lattice point A corresponding B atom is associated with this lattice point all lattice points have to be identical.

So, all lattice points are now having not one atom, but a pair of atoms; and this pair of atom is what is our motifs? So, the motif description also includes both the atoms. So, one atom at the lattice point o o o; another atom at this displaced position and what is the displaced position is what we now have to work out. So, we I make another unit cell

because there it has got very crowded. So, we have a rhombus divided into equilateral triangles this is my x and y axis and I wish to locate the centroid of this up triangle that is the B location with respect to the crystal coordinate system that is with respect to x and y axis shown here.

So, to get the coordinate of this, I need to draw lines parallel to my coordinate axis. I will not draw perpendicular, but I will draw parallel to the axis not that in Cartesian coordinate system also you do the same; you draw lines which are parallel to the axis, but there since the axis themselves are orthogonal; it seems that we are dropping perpendicular to the axis, but for coordinates always we need to draw lines which are parallel to the axis. And since this B location in this B location is the centroid of this triangle. So, it divides the height into 2 is to 1 that is the property of the centroid. And thus a parallel line from this centroid to the x axis will also divide this side of the rhombus in 2 is to 3 ratio.

So, then this coordinate becomes two-third of the entire length and the entire length we are calling A; so, this becomes two-third A because our lattice parameter our lattice parameter in the plane is A; I draw it here. So, since the size of the rhombus the side of the rhombus is two A and this is two-thirds a. So, that is the x coordinate of this B point. So, the x coordinate we can write as two-thirds A. Similarly, if you work out I leave this as an exercise; if you work out this in terms of the entire side of the rhombus along y axis you will find that this is one third of this side and all the sides are equal I use the symbol B for the unit cell edge lengths along the y axis. So, this is one-third B. So, the second coordinate the y coordinate of the atom is one-third B.

Now, the question is what is that z coordinate? Remember z is orthogonal to the x y plane in the hexagonal crystal and the repeat distance or the unit cell edge length in this direction is equal to C, but the C is from A we have A stacking sequence A, B, A. So, the entire distance from A to A is what is called C. So, distance from A to B is half of that and that is C by 2. So, the third coordinate is half of C. Now when crystallographers want to give these coordinates they know that the first coordinate has to be in terms of A, the second coordinate has to be in terms of B and the third coordinate has to be in terms of C.

So, they simplify they don't write A, B and C. The coordinates are just given as two-third, one-third half this is what is called the fractional coordinate. So, which means my the location of the B atom in the unit cell or the location of B atoms with respect to the crystal coordinate system, the displacement vector this is the displacement vector with respect to the lattice point I can reach there by A two-thirds displacement along A, one-third displacement along B and half displacement along C. So, that becomes the two-third, one-third half becomes the fractional coordinate of the second atom. So, we have now worked out in full detail in the motif of hexagonal structure.

So, we conclude by stating that the phrase hexagonal HCP lattice or hexagonal close packed lattice these are very common phrases, but these are wrong phrase.

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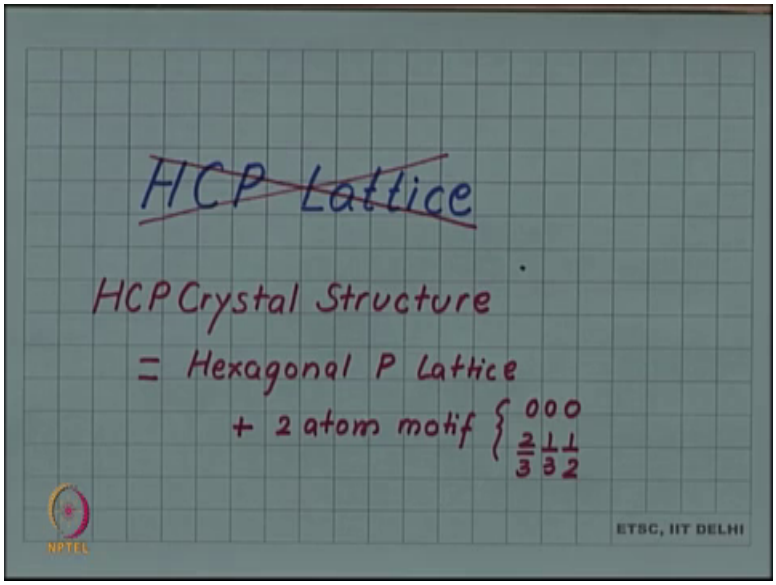

If you have followed this video you should not use HCP lattice; it's always HCP crystal structure, because if you have HCP lattice remember we already have 14 Bravais lattice with only one hexagonal lattice the simple hexagonal; if you have another hexagonal lattice hexagonal close-packed lattice. So, you are going for 15 lattice; this is something which we don't want to have. So, HCP crystal structure is the correct phrase and this crystal structure is described in terms of a hexagonal p lattice as we saw that and a 2 atom motif at o o o an two-third, one-third half, but this phrase HCP lattice is quite widespread in literature on the web in textbooks and so on.

I will just show you an example on my computer. So, let us try to look at, what the Google gives us for this phrase so this is a Google is celebrating Persian newyear. So, happy (Refer Time: 26:45) to all of you and let us now do an exact phrase search for hexagonal close-packed lattice. We just discussed this is a wrong phrase should not be used, but let us look at.

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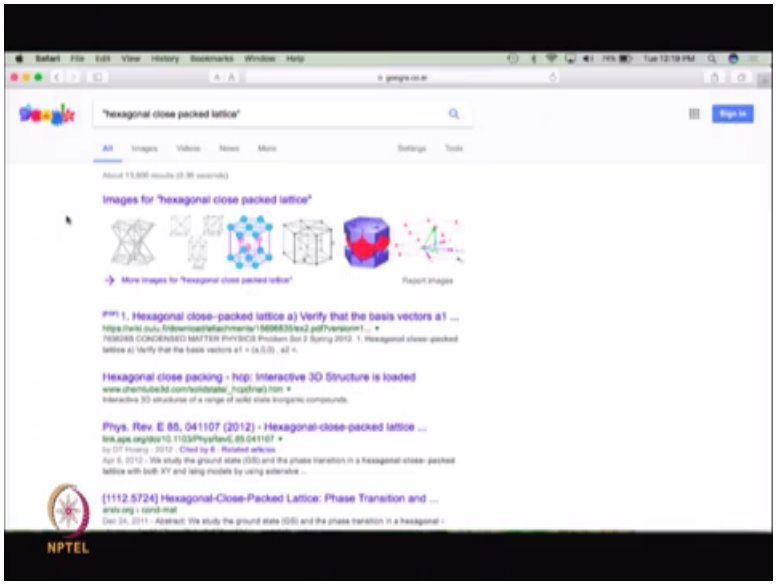

What the search engine gives and we can see that in just point 36 seconds we have 13600 websites which are using this phrase hexagonal close-packed lattice. So, this is an incorrect phrase and after this video you should not be using this phrase always use hexagonal close-packed crystal; there is nothing like hexagonal close packed lattice.