Basics of Materials Engineering
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Lecture – 06
Crystal Structure – 4 (Miller Indices for Crystallographic Points and Directions)

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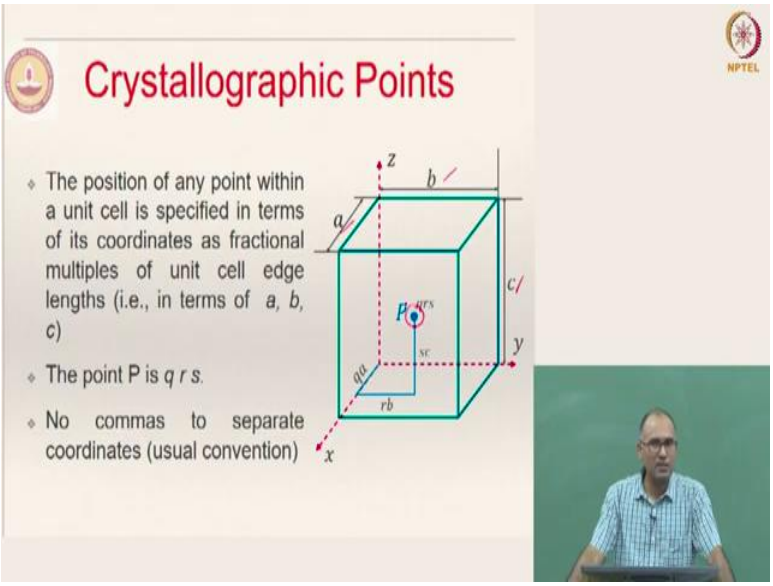

And then, once you have a unit cell, we will work with the unit cell. Now, each and every point or position in the unit cell needs to be represented. How do you represent that? So, these are called crystallographic points. How do you represent a crystallographic point? You have this unit cell *a*, *b* and *c* and *x*, *y*, *z* axes. So, let us say this edge length is *a*, this edge length is *b*, and this edge length is *c*.

So, now if you want to describe this point P, the way that you describe is you take the position and you find out the projections of this point on the coordinate axis and the fractions. For instance, this distance is *q* times *a*, where *q* is the fraction. This distance is *r* times *b*, and that distance is *s* times *c*. Then, you define your crystallographic point as *q r s*.

You do not write in an absolute value; you only write in terms of your lattice factor. That is important. And when you are representing a crystallographic point, you just simply write these three numbers besides each other. Let me see if I have an example.

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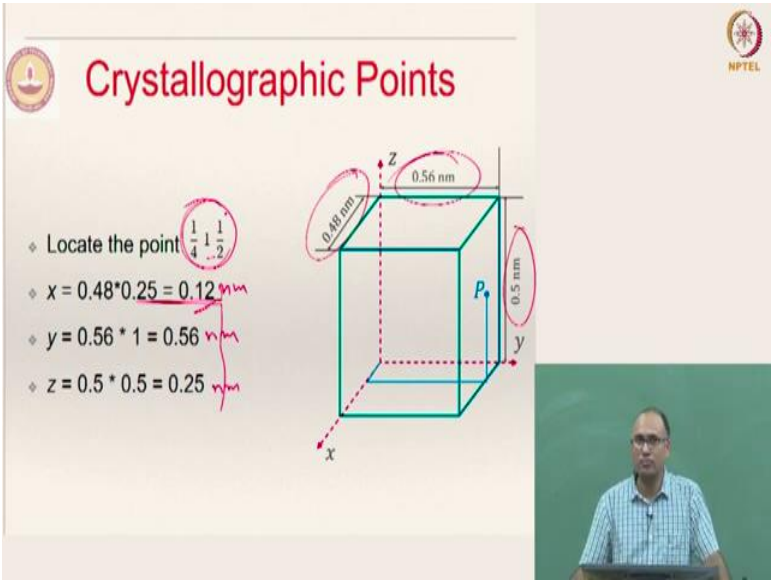

So, this is your point $\frac{1}{4}1\frac{1}{2}$. So, what I need to do? I need to move one-fourth in this direction. So, let us say this is 0.48, 0.56, 0.5. We actually do not need to do this calculation in principle; you know what is this distance. You move one-fourth of this distance and so on. So, if you do the calculation, this is 0.12; units are nanometers.

So, you move 0.12 in the *x* direction, 0.56 because this is 1; that will be full length, and then half of it 0.25, and that will be your point P. This is the way that we represent crystallographic points. It is pretty elementary, but it is important that we know how to represent them. Whenever you are reading a text book or a research article, if somebody is talking about crystallography, and they represent something like this, we should identify that they are actually talking about a crystallographic point.

So, depending upon these lattice parameters, the actual values may differ, but this position is actually related to the fraction along the lattice directions.

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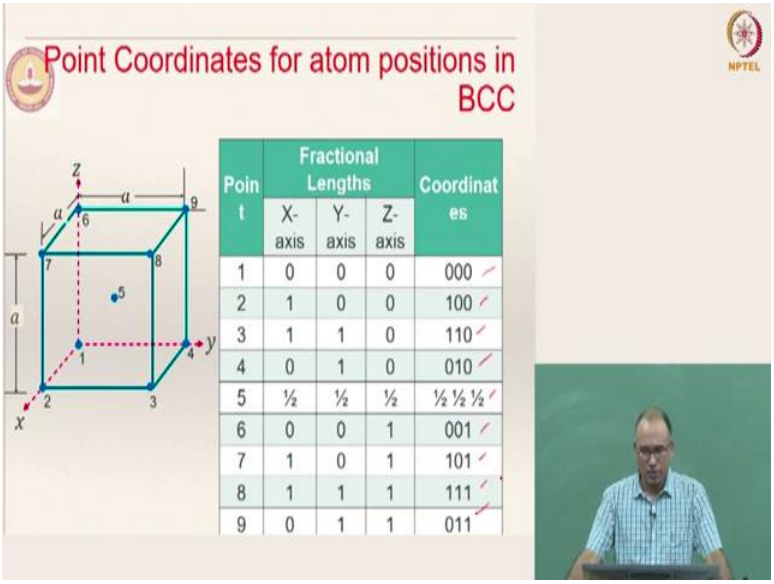

So, now if you have a body centered cubic structure, this is how a body centered cubic structure looks like. And I have only shown points at the appropriate locations, and now how do you represent the lattice points there?

So, 1 is at 000. So, you write the coordinates. This is how you represent all the lattice points, right? 1, 2, 3, 4 and the 5th one is the body center. So, $\frac{1}{2}\frac{1}{2}\frac{1}{2}$, and so on. Is this clear?

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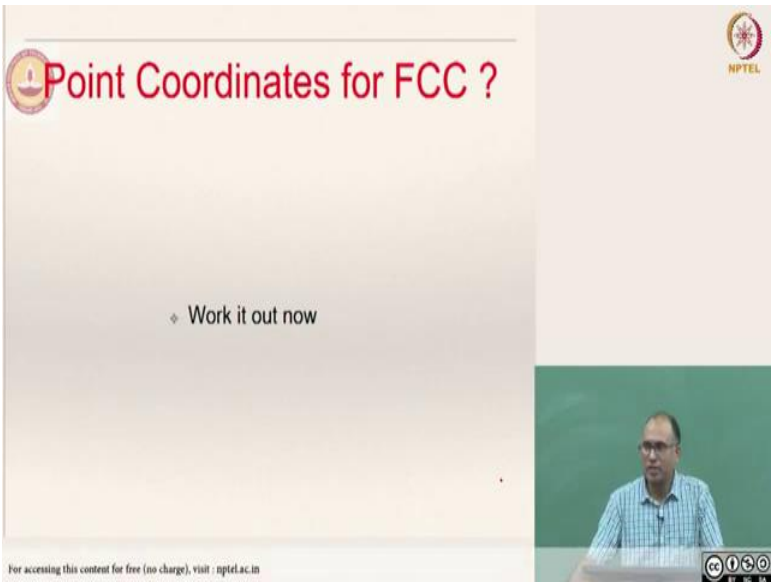

For FCC can you do that? For FCC; pretty straight forward, right? What will be the point on one of the faces?

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One half, half, why two halves?

Student: (Refer Time: 04:43).

Ok. You write it down. I will not think about it, you think about it ok.

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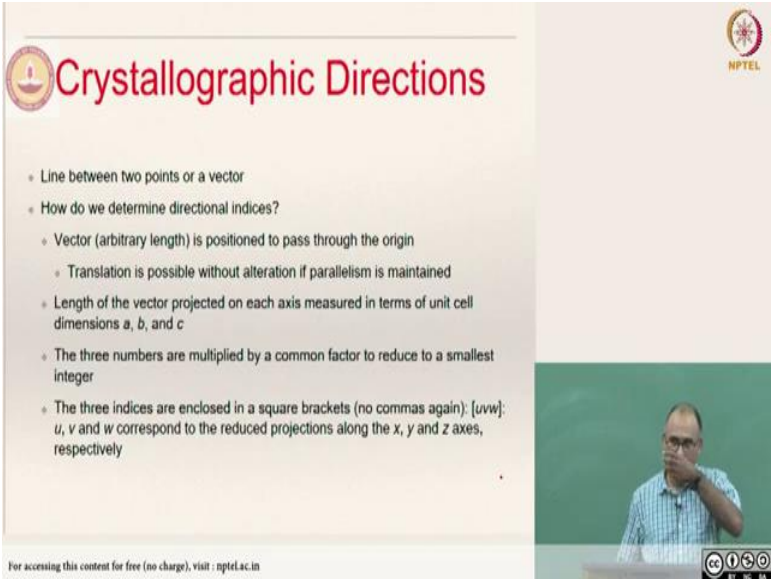

The ability to identify crystallographic directions is one of the most important activities in this course, because this is going to tell us a lot about the mechanical properties. So, we should be able to identify crystallographic directions properly, and if somebody gives you a crystallographic direction, you should be able to understand what direction they are talking about.

So, how do you represent the crystallographic directions? The crystallographic direction is basically a vector; a line between two points or a vector. How do you represent this direction using some indices? So, how do we determine the directional indices? First what we do is the vector is positioned to pass through the origin. You may have the vector anywhere, but then you can actually translate it such that it goes through the origin. That is the first thing that you will do.

Or you move the unit cell such that one of the ends of the vector meets the origin; both of them are possible, both of them are equivalent. And, the length of the vector projected on each axis is measured in terms of unit cell dimensions, similar to what we have done for crystallographic points.

The three numbers that you get are multiplied by a common factor. This is the difference between writing point coordinates and directional indices. Once you know the fractions, what you do is you multiply that with a common factor to reduce to a smallest integer. We will see what it means.

Let us say those numbers that you got are *u*, *v* and *w*, and then you enclose them in a square bracket i.e., [*uvw*]. That is how you represent a crystallographic direction.

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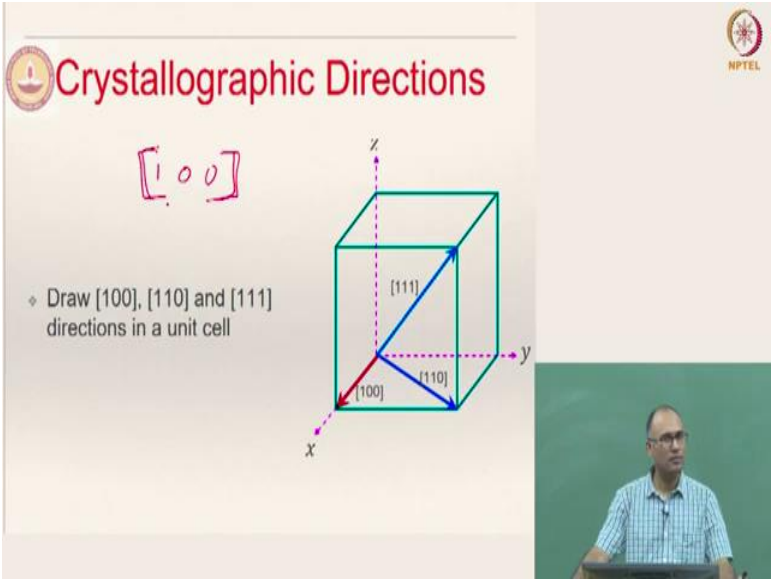

So now, when somebody tells you that [100], you should immediately understand that it is the representation of a crystallographic direction. We will not tell you. The fact that it is enclosed between square brackets tells you that it is a crystallographic direction. That is something that you should be aware of. And, now you need to draw these three crystallographic directions; the projection onto x-axis is 1 and y and z-axes are zeroes.

So, what should be that one? The unit vector; the vector along x-axis, and the length of the vector is equal to coordinate per unit cell lattice parameter in that direction, right? Similarly, [110] is that line, and [111] will be that line.

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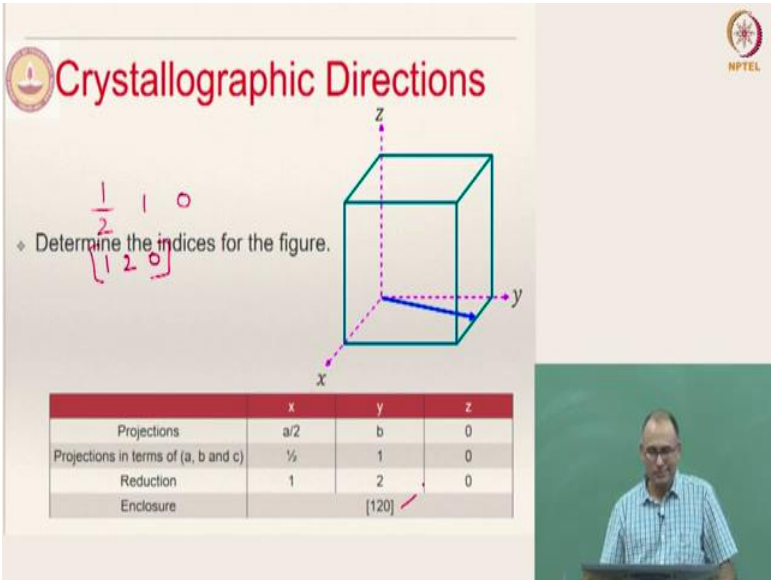

So, can you tell me how do you write the directional indices for this guy? So, normally what will you do? First you have to write the projections on to each coordinate axis. What is the projection onto x-axis? $\frac{1}{2}$. What is the projection onto y-axis? What is the projection onto z?

Then what you need to do? You need to multiply these numbers with a common factor, so that you will bring it to a smallest possible integer except 0 sorry, smallest possible number. So, that means you multiplied with 2; then this becomes [120]. And then what will you do? You put a bracket.

You should not stop there. Unless you put the bracket, you are not telling the world that it is actually a crystallographic direction; it is very important. You should not write the projection as $\frac{1}{2}$. It is actually $\frac{a}{2}$, b, 0, then you will only write the fractions, projections onto the fractions.

So $\frac{1}{2}$, 1, 0 and multiply it with 2; [120] and then that will be your crystallographic direction. So, like that you should be able to write crystallographic directions for anything.

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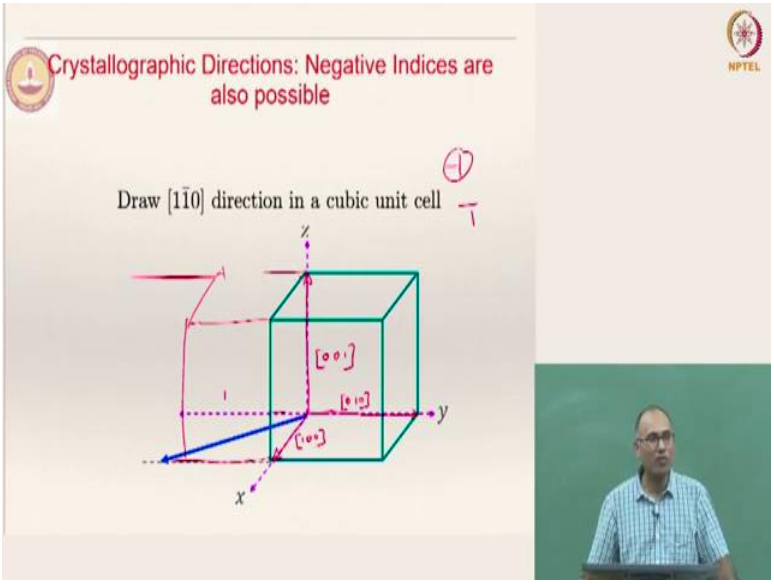

Now, what is this direction 1$\bar{1}$0? So far, we have talked positive directions, but you can also have negative direction, right? So, you do not write -1 when you are talking about crystallographic directions. The -1 is represented as $\bar{1}$. So, let us say this is your unit cell, and now you need draw this particular direction.

So, how will you do? This is your *x*, *y*, *z* axes. You can actually move this guy, this way, right? So, you can actually draw something like that, and then that will be your new axis. Sorry, this is your new axis, not that one, and then 1 is this line, and -1 will be in this direction.

So, that will be your 1$\bar{1}$0. Now, you will be able to draw and identify any crystallographic direction.

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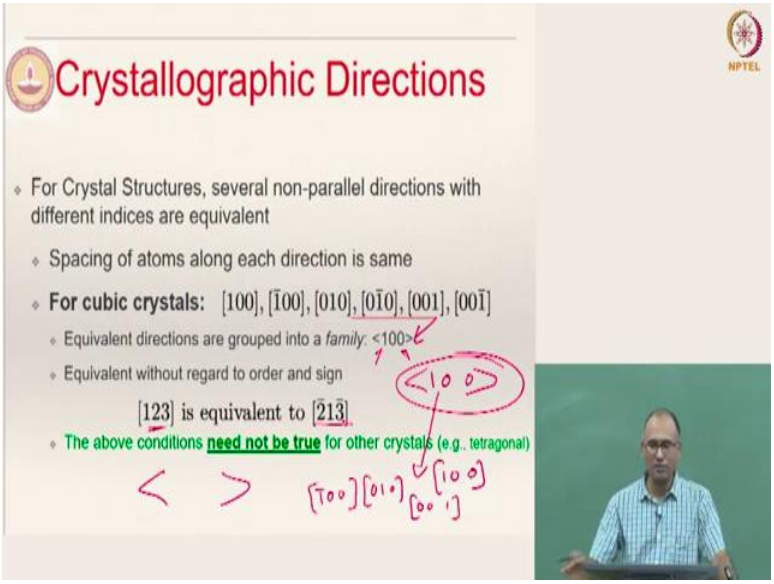

So, another important concept and extremely useful concept; for crystal structures, what do you mean by an equivalent crystallographic direction? You can have several non-parallel directions; they need not be parallel, that is the key here.

You can have several non-parallel directions with different indices, but they can be equivalent here. What is the meaning of that? That means, the spacing of atoms along each direction should be the same. So, in the previous one, what is [100]?

Student: (Refer Time: 11:35).

In a cubic crystal, *a* equal *b* equal to *c*. So, if I draw this direction that is [100], and this direction [001], and this direction [010]. Now if I am here, by moving a distance of *a*, I am finding my next point. Similarly, here as well, by moving the same amount of distance, I am finding my next point. Here also, I am able to find the next point.

That means the distance between points in all these crystallographic directions are the same, and if that is so, then they are called equivalent directions. They are not parallel, but they are similar; they are equivalent. Because this need not be true for other unit cells. For cubic unit cell it will definitely hold good. So, for cubic crystals [100], [$\bar{1}$00], [010], [0$\bar{1}$0], [001], [00$\bar{1}$]: all are them are equivalent.

So, this set of directions are called equivalent directions, and because all of them are equivalent, we can group them into a family, and that is what you call a family of

equivalent crystallographic directions. And, if you want to represent a family, the family of these crystallographic directions are represented by these brackets, and when you write <100>, this actually means all permutations and combinations of 1, 0, 0.

So, 1, 0, 0 can be [100]; you need to have only two 0's and one 1. Other such combinations include [100], [010], [001], [$\bar{1}$00], and so on. That is what that is why this is called a family of <100> directions; all these directions are equal equivalent. To represent a family of crystallographic directions, the enclosure is < >.

So, by that argument, if you have a crystallographic direction [123] in a cubic crystal, that must be equivalent to [$\bar{2}1\bar{3}$] or [$\bar{2}\bar{1}\bar{3}$] or [$21\bar{3}$] and any combination of 1, 2, 3; all of them are equivalent. If you know one direction, you do not have to worry about other combinations because all of them will behave the same.

This is important because then we will see when we are talking about mechanical properties, certain properties of the materials or certain deformation mechanisms in the materials are governed by how atoms are arranged on the crystallographic directions. And, please note that this condition of representation of equivalent directions that we have just now discussed, need not be true for other crystals.

For instance, it is not true for tetragonal. In a tetragonal crystal, when you are moving in [100] direction and [010] direction, you will have to move by a different absolute amount, to actually reach to the lattice point.

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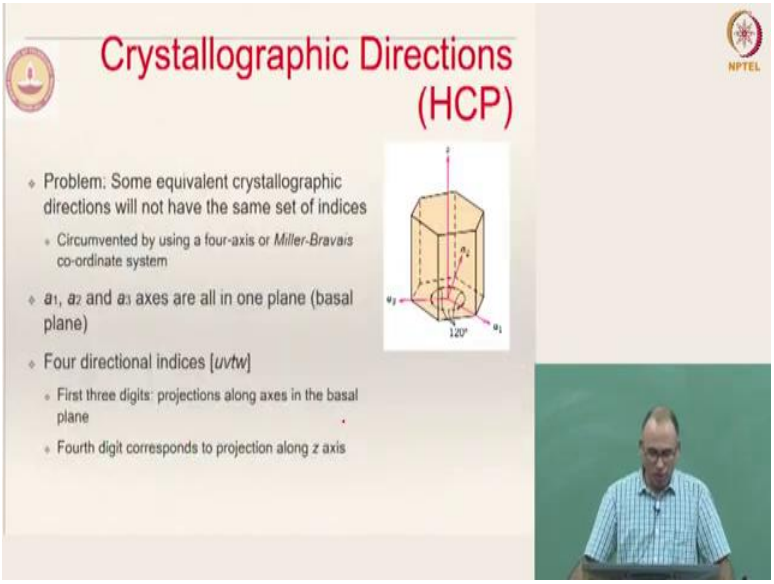

So, I think we will stop here.