Basics of Materials Engineering
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Lecture - 07
Crystal Structure – 5 (Miller-Bravais Indices, Linear and Planar Density)

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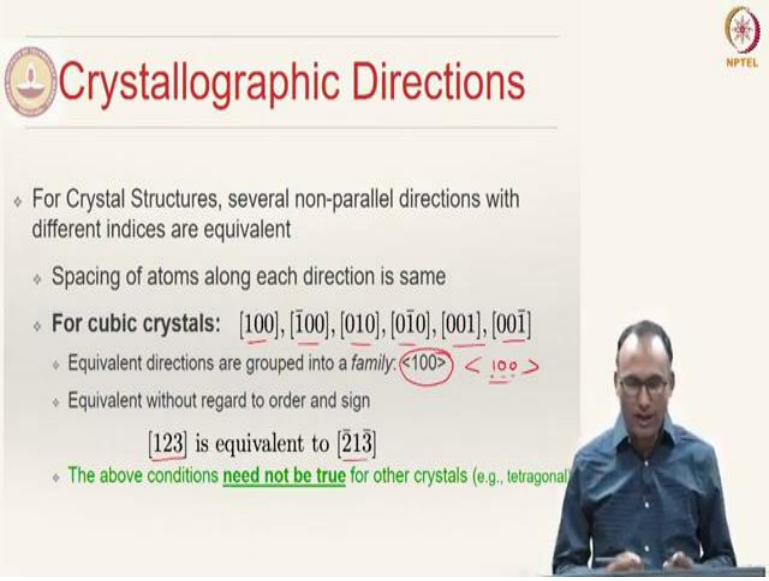

Welcome back. So, in the last class we have discussed the crystallographic directions particularly for cubic crystals. We have also introduced the concept of equivalent directions. For instance, in a cubic crystal you have: [100], [$\bar{1}$00], [010], [0$\bar{1}$0], [001], [00$\bar{1}$].

All these are equivalent directions and they are called a family of equivalent directions. The family of equivalent directions is represented this way; you have Macaulay sort of a bracket and then <100>, and all the permutations of these three indices will give you the equivalent directions for cubic crystals. And please note that this way of representing equivalent directions will only work for cubic crystals.

For other crystals, for instance tetragonal crystal, it does not work. This definition of equivalent crystals is only right for cubic crystals. By that definition, you can say that [123] direction in a cubic crystal must be equal to [$\bar{2}$1$\bar{3}$], [21$\bar{3}$], [213], and so on.

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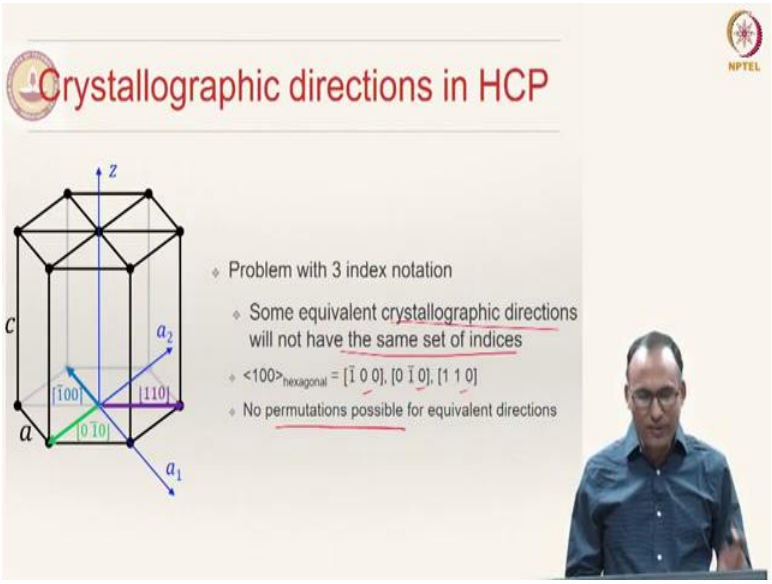

Having discussed how the crystallographic directions are shown in a cubic crystal, let us now look at hexagonal close-packed structure. Suppose you take a hexagonal crystal which has 3 lattice vectors a_1, a_2 and z. z is in the out-of-plane direction, and in the base plane or basal plane you have these two lattice vectors a_1, a_2.

This can also be one of the definitions of our unit cell for a hexagonal close-packed system. Let us now look at this particular direction; that is the projection of this line onto a_1 axis is 0. $\bar{1}$ because it is in the negative a_2 direction, and the projection of this line onto z axis is 0. So, that is why this direction is [0$\bar{1}$0].

If you take this line, it is given by [$\bar{1}$00]. But, if you take this direction then you have [110], right? But how do we say the equivalent directions? Basically, when you are moving from this position by same amount you should meet another atom right? By moving the same distance.

Here, this distance, this distance, and this distance are the same. So, by definition of our equivalent directions, these 3 should be equivalent directions. But, when we are talking about the definition of equivalent directions as we have discussed in the cubic crystal, the Miller Indices should be the same.

So, you have [100]. You should have two 0's and one 1 in any combination. But here you have two 1's and one 0. So, if you have this representation, for crystallographic directions

in hexagonal systems, you will not be able to use the permutation of same set of indices for representing equivalent directions. Just by looking at, you cannot say that these two are equivalent directions unless you actually draw and show that.

So, that is how the representation of that equivalent crystallographic directions is actually breaking down. This is the problem with 3-index notation. Because some of the equivalent crystallographic directions will not have same set of indices like these 3.

That means the permutations are not possible for equivalent directions, if you are using such a definition a_1, a_2 and a_3. How do we fix this problem?

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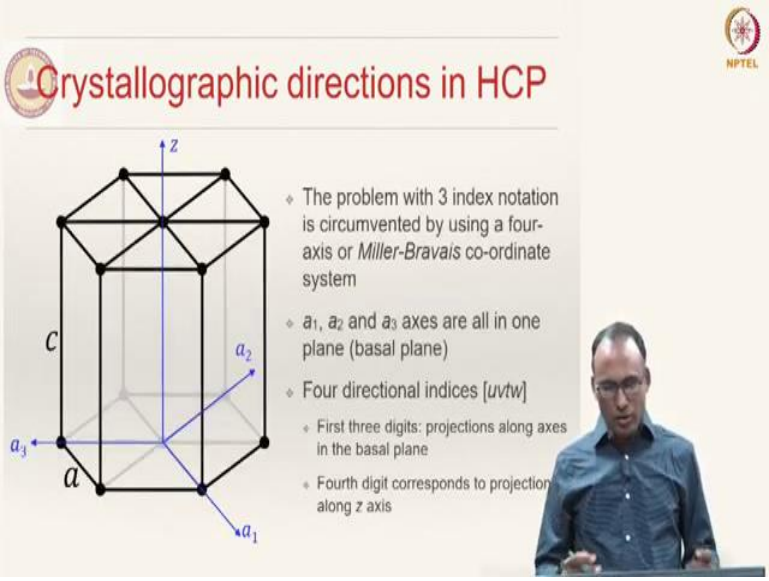

The problem with the 3-index notation is circumvented by a four-axis or Miller-Bravais co-ordinate system. So, you have to do some modifications to your coordinate system. Instead of having 3 indices now you can have four-axis system. Previously you had a_1, a_2 and z. We now introduce another axis a_1, a_2, a_3 and z.

So, now we have 4 indices representation. So, a_1, a_2, a_3 axes are all in the basal plane. And the fourth z axis is in the out-of-plane direction, i.e., the height direction. So, four directional indices notation is u v t and w. First 3 indices u, v, t are the projections along the axes on the basal plane. And the fourth index is the projection onto the z axis.

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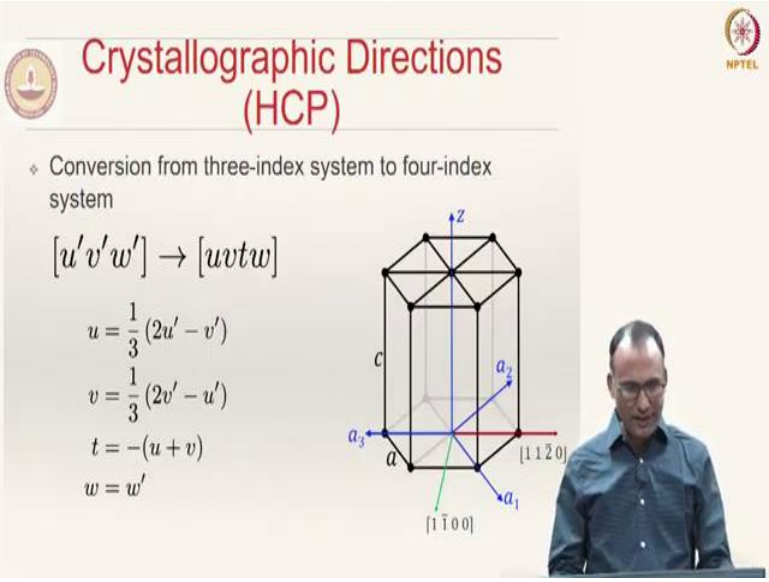

So now how do we actually convert three-axis notation to four-axis notation? Let us say our three-axis notation is represented by [$u'v'w'$]. How do we go from this notation to [$uvtw$]?

So, this is one of the prescriptions, but people can come up with different prescriptions if required. So, one of these prescriptions is that the u in four-index notation is related to the three indices notation as,

$$u = \frac{1}{3}(2u' - v')$$

$$v = \frac{1}{3}(2v' - u')$$

$$t = -(u + v)$$

$$w = w'$$

The third-index in a four-index notation should always be negative of sum of the first 2 indices; that is important. And w is directly w', ok? So, this is how one can transform a three-index notation to a four-index notation. Once you do that, all the equivalent directions will be having same set of indices.

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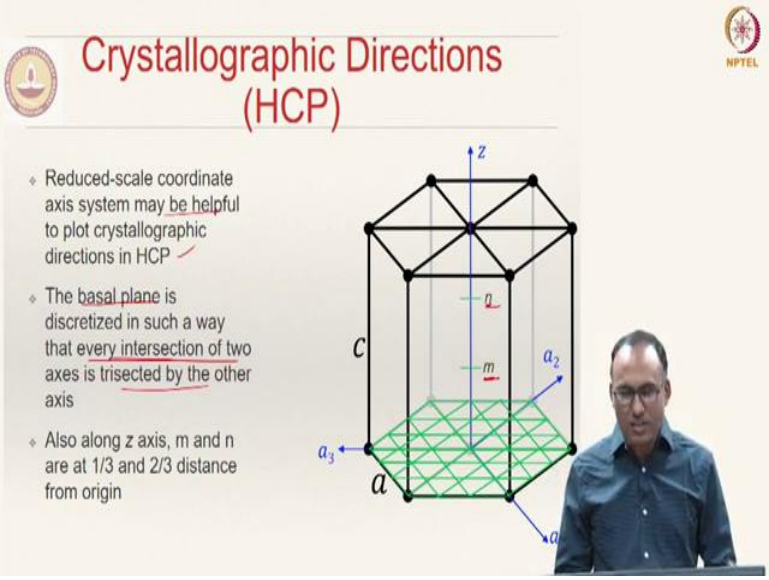

So, how do we talk about this reduced coordinate system? The reduced-scale coordinate system may be helpful instead of using the full-scale coordinate system to plot the crystallographic directions in HCP.

How do we go about doing that? You discretize the basal plane in such a way that every intersection of two axes is trisected by the other axis. You basically trisect each of the coordinate axis. And along with *z* axis also you trisect at *m* and *n*; *m* is at a distance one-third to *z*, *n* is at two-third, and this point is at 1 in the one-third of the lattice vector dimension there.

So, here this is how we do the trisection. This is the trisection of coordinate axis along a_2, and that is a_1, and a_3, right? Now, we can actually see how do we use this to represent the coordinate directions for hexagonal close-packed structure.

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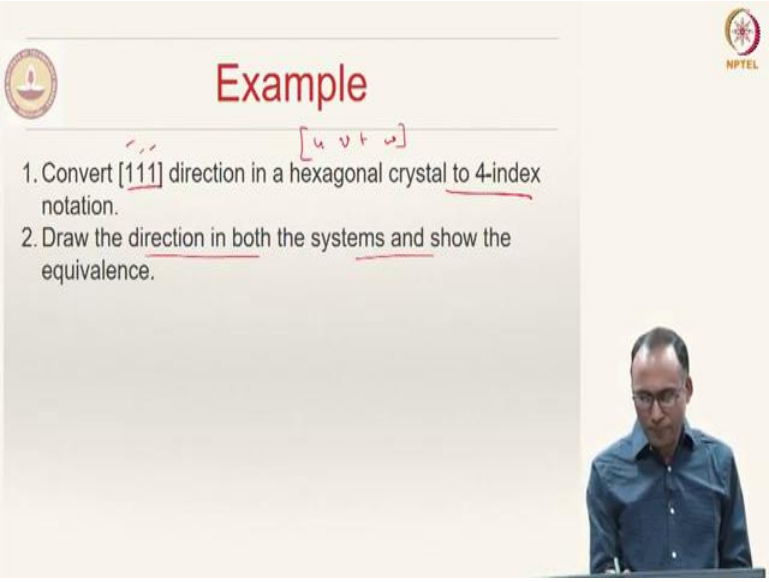

Let us see how do we convert [111] direction in a hexagonal crystal to 4-index notation, and then draw the direction in both the systems and show the equivalence. That is the problem that we have to do. So, this is [*u′v′w′*] and that you have to convert it into [*uvtw*].

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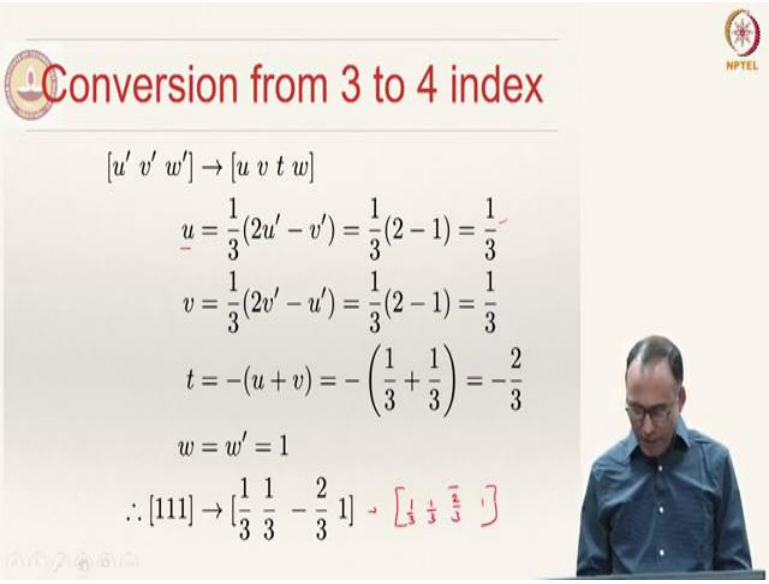

The transformation from u dash to u is given by this formula. So, it will become $[\frac{1}{3}\frac{1}{3} - \frac{2}{3}1]$. So, that should be written as $[\frac{1}{3}\frac{1}{3}\frac{\bar{2}}{3}1]$. But, of course, again the minus should not be written

as minus. You do not have to calculate *t*, you just have to calculate *u* and *v*, then *t* will be negative of sum of these two.

And then you need to show that on the hexagonal unit cell; let us show that.

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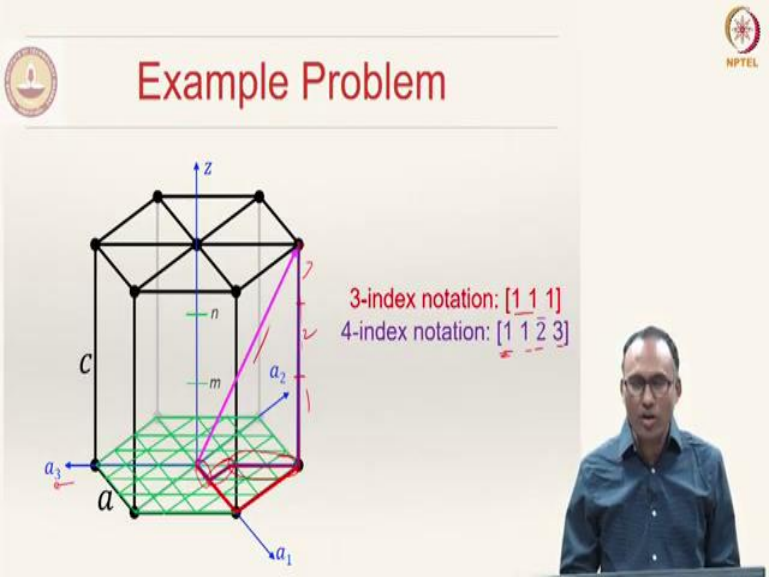

So, this is 1/3rd distance. So, we have to move 1/3rd along a_1. That is your 3-index notation: [111]. In 4-index notation you have to move 1/3rd so, that means, from there to there and so on. This is our 1/3rd along a_1 axis, 1/3rd along a_2 axis, -2/3rd, because a_3 is shown in this direction. So, minus -2/3rd is this and then this is 1.

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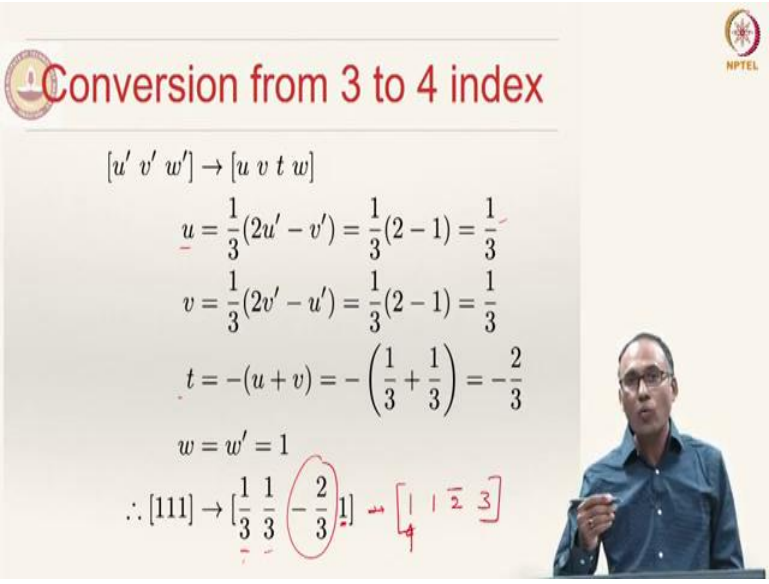

When we are representing the crystallographic directions, you do not work with fractions; you try to convert into smallest integer. So, multiply everything with 3; that means, [11$\bar{2}$3]. Here 1 actually means one-third distance on your crystallographic plane.

So, that is why your [11$\bar{2}$3] means -- 1 means one-third along that line in 4-index notation. Again one-third and 2 times -- 1, 2 that is two-third. And 3 means one- third two-third and 3. So, that means, this is 1 2 3. So, one-third is 1 unit when you are talking about 4-index notation. And both of them are showing the same crystallographic direction alright.

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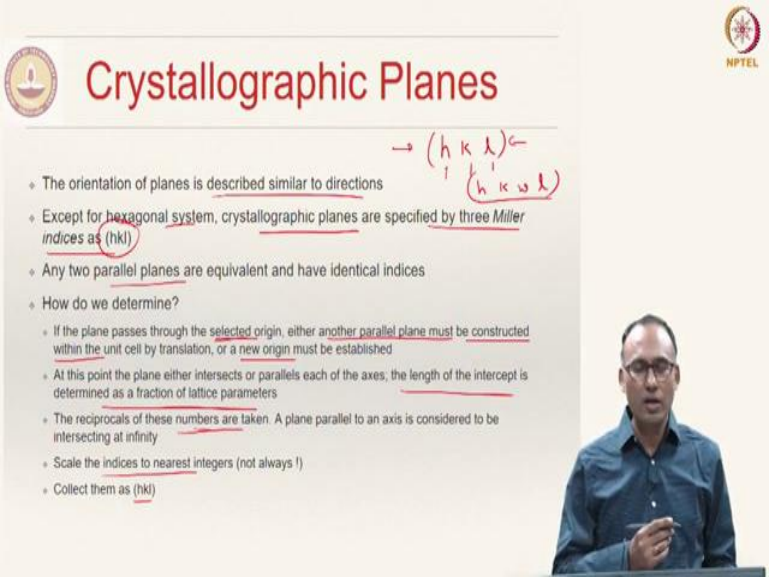

Having discussed how do we represent the directions, the next important aspect that we need to define is the crystallographic plane. So, the orientation of planes is described similar to directions, except for hexagonal system, crystallographic planes are specified by three Miller indices *h, k, l* and they are enclosed with parenthesis. So, (*hkl*) represents the representation of crystallographic plane and we will see what *h*, *k* and *l* are.

So, this is for 3-index notation. For 4-index notation you need to have *h*, *k* maybe *w* and *l*. But first, we are going to discuss about 3-index notation, and then, for 4-index notation the same philosophy that we have used for directions can be applied to planes as well. Note that any two parallel planes are equivalent and have identical indices. If two parallel planes are equivalent, they have identical indices.

So, how do we determine the Miller indices for crystallographic planes? Firstly, you need to check whether the plane for which you want to write the Miller indices is passing through the origin of the unit cell that you have chosen.

If the plane passes through the select origin, then what you need to do? Either another parallel plane must be chosen within the unit cell i.e., another parallel plane must be constructed within the unit cell by translation, or you have to choose a new origin. The basic guideline is that the plane should not be passing through the origin.

Because we said all parallel planes are equivalent and have exactly same indices, you just have to translate the plane such that it is parallel to the original plane, and then it is not passing through the origin. All that that we need to do is ensure that the plane is not passing through the origin.

And at this point what happens? The plane is going to either intersect the coordinate axis or it will be parallel to the coordinate axis. Because originally, if it is parallel to one of the coordinate axes, by translation it will not become non-parallel, it will still remain parallel to the coordinate axis.

And you know at what length it is intercepting. So, the length of the intercept is determined as a fraction of the lattice parameter. And then, you have to take the reciprocals of those numbers. So, first you have to identify the intercepts and write them as fractions of the lattice parameters.

If it is intercepting at a distance $\frac{a}{2}$, then you have to write $\frac{1}{2}$. And then, you take the reciprocals of them. So, the reciprocals of the numbers are taken and if a plane is parallel to *x* axis; that means, it is intersecting x axis at infinity. If it is parallel, then the reciprocal of that will be 0.

Now, scale the indices to the nearest integers. Sometimes you do not actually do the scaling. But, usually in this class we will do the scaling to the nearest integers and then collect the numbers and put them under parenthesis. That is how you will identify Miller indices for crystallographic planes.

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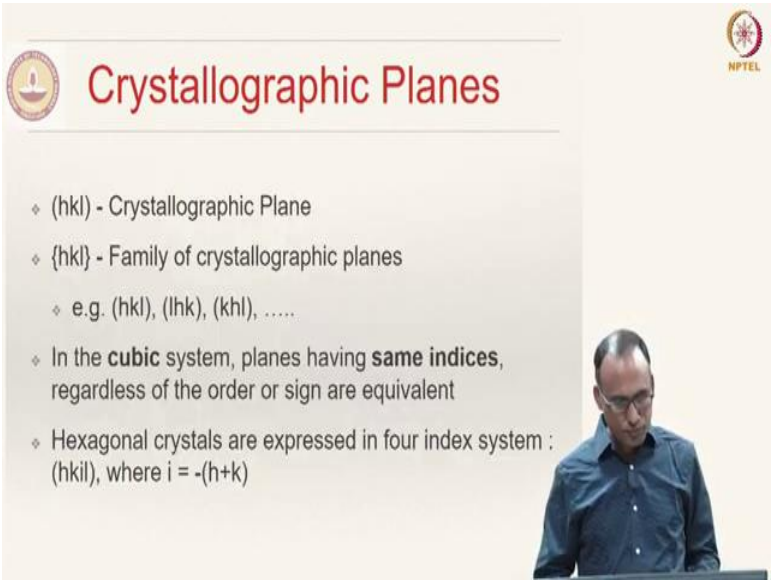

So, this is the representation for crystallographic plane. And the family of crystallographic planes are represented or designated with curly braces. In a cubic, the planes having same indices, regardless of the order or sign, are equivalent.

They need not be parallel, but they can be equivalent planes. And hexagonal crystals are expressed in four-index system: wherein they are represented (*hkil*), where

$$i = -(h + k)$$

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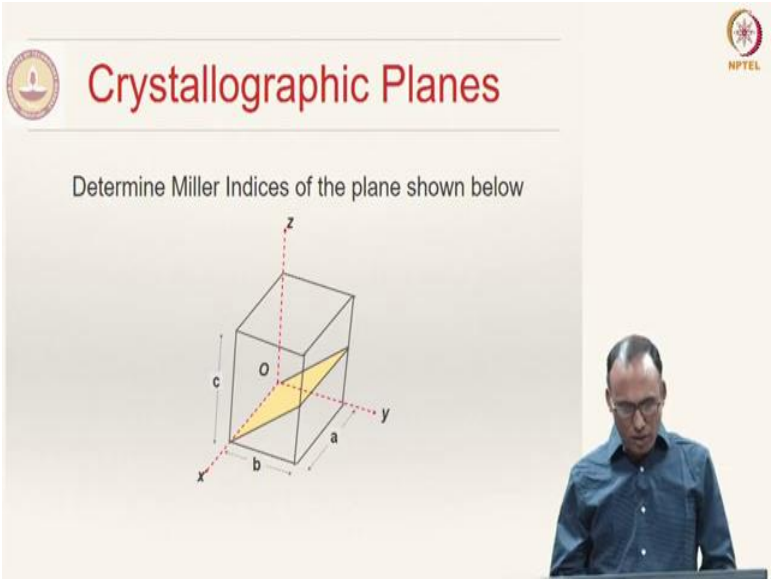

Let us now look at this particular system, try to see whether we can identify the Miller indices for this plane. You can see that this plane is actually passing through the origin; this is our origin. So, the first check to be made is to see whether the plane is passing through the origin. If a plane is passing through the origin, what is that we need to do? Either change the origin or translate the plane.

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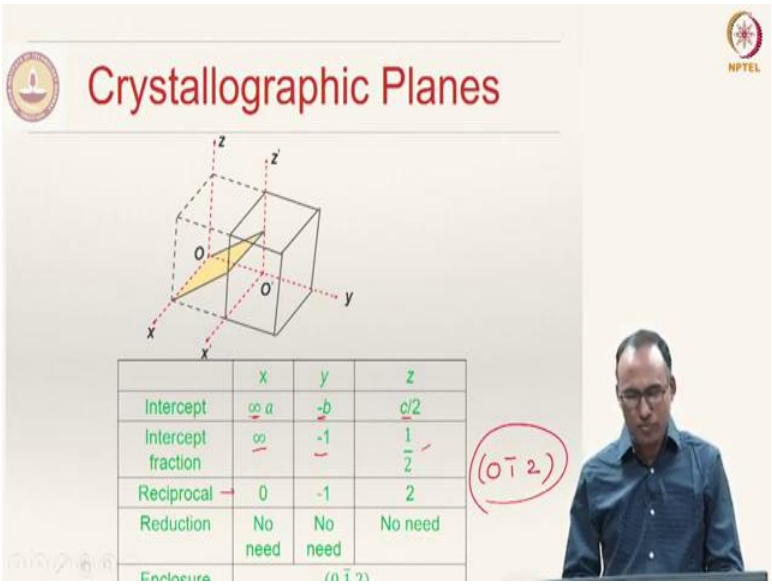

So, what we have done is we have actually moved our coordinate system from this point to this point; so, that means, you have moved the origin, but keeping the plane the same.

So, now, O' is your origin, and $x'y'z'$ is our new coordinate system. Now, the plane is not passing through origin. Let us look at, where this plane is intersecting *x* axis, *y* axis and *z* axis. Is this plane intersecting *x* axis anywhere? It is actually parallel to *x* axis. So, it not intersecting *x* axis.

Where is this intersecting *y* axis? So, this is intersecting *y* axis at this point. So, that means negative *a*. So, let us say this is *a*, *a*, *a*; it is intersecting at -*a*. And *z* axis it is intersecting at $\frac{a}{2}$. So, *x* intercept is ∞; parallel, that is why ∞ times a. And it is intersecting *y* axis at -*b*, and *z* axis at $\frac{c}{2}$. *a*, *b*, *c* are your lattice parameters.

Then, you write that intercept as a fraction of your lattice parameter. So, that is why I am writing ∞, -1, and $\frac{1}{2}$. Their reciprocals are 0, -1, 2. Do we need to do any reduction?

Because there are no fractions, there is no need for reduction. And hence, the enclosure will be $(0\bar{1}2)$. That is the representation of that plane.

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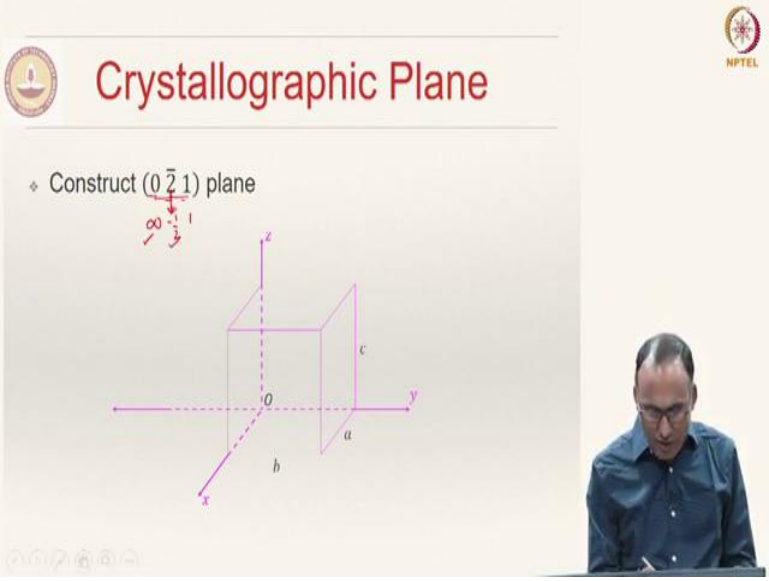

And now let us construct another plane $(0\bar{2}1)$. So, in order to construct what we need to do is first we need to find the intercepts. What are the intercepts? The intercepts will be the reciprocals of the Miller indices, right? When we are constructing, we have taken the intercepts and then taken the reciprocals of them to represent the Miller indices.

Now, in order to find the intercept, you need to find the reciprocals. So, that is ∞, $-\frac{1}{2}$ and 1; that means, this plane is parallel to *x* axis, intersects *y* axis at $-\frac{1}{2}$, and *z* axis at 1, right?

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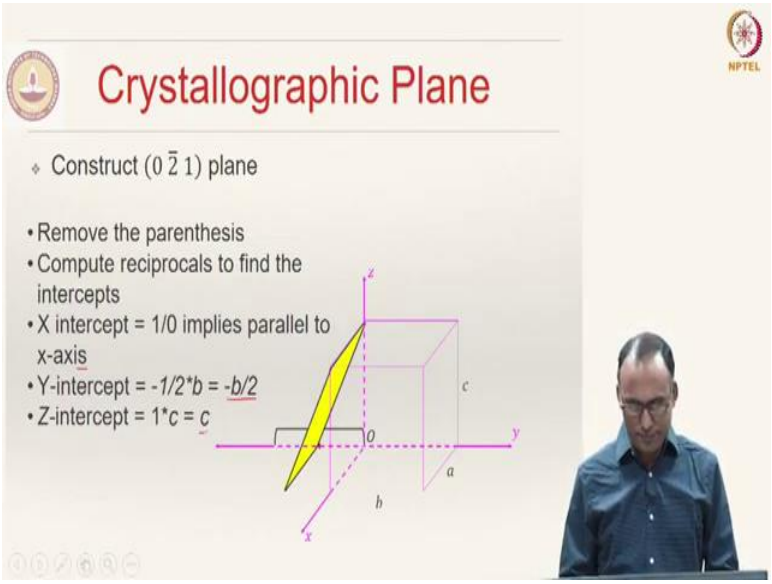

So, that is our plane (0$\bar{2}$1). All these parallel planes are equivalent, and they will have same set of indices.

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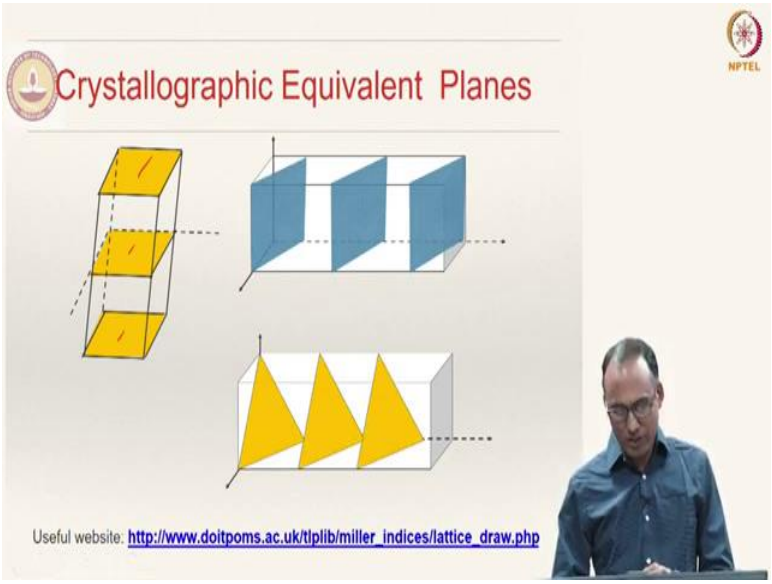

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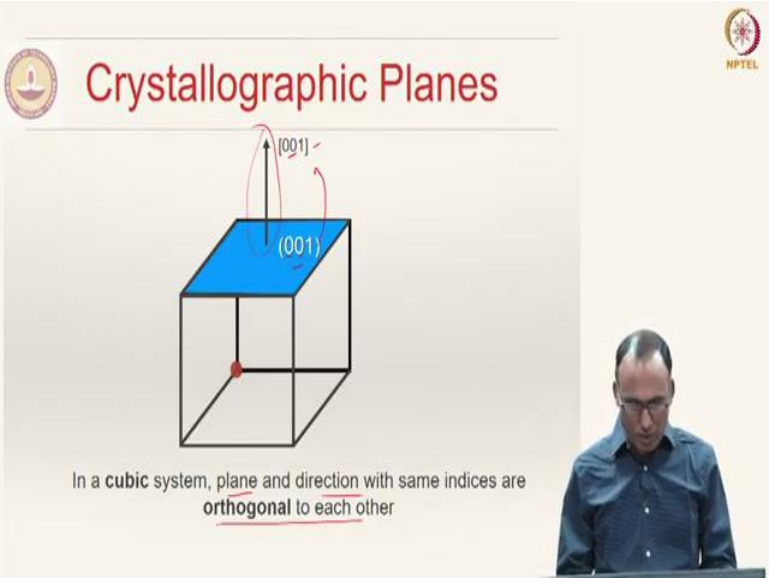

In a cubic system, for instance, a plane and a direction with same indices are orthogonal to each other. That means, if you take a plane (001). This plane is intersecting *z* axis at 1, but it is parallel to *x* and y axis. So, that is why these the indices are (001).

The crystallographic direction that is actually normal to the plane will have exactly the same indices as the indices of the plane itself. But the normal direction should be shown with different brackets. So, in a cubic system, the plane and the direction with the same indices are orthogonal to each other. If some direction is orthogonal, that is what is called normal to the plane.

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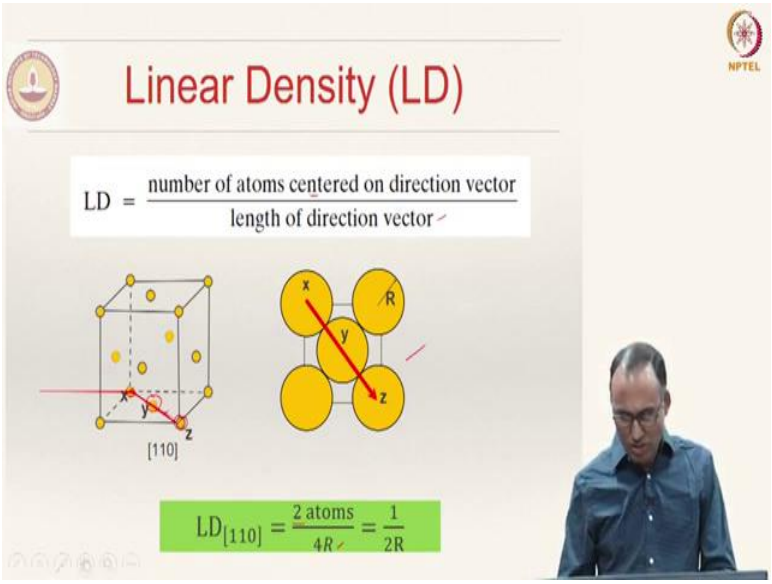

Let us now define something called linear density. What do we mean by linear density? The linear density is defined as the number of atoms centered on a direction vector. So, we have defined a crystallographic direction. On that direction vector how many number of atoms are centered divided by the length of the direction vector; that is what is called linear density.

If you take the [110] direction in an FCC material, how many atoms are there on [110]? There is 1 full atom and this atom is part of another atom.

This atom is also part of another unit cell. So, half of this guy is present here and half of this guy is present here, and effectively you have 2 atoms lying on that direction. So, 2 atoms divided by the total length. If it is R, then this face centered atoms are touching each other.

So, this will be 2R and this is 2R. So, that total length is 4R. So, the linear density

$$\text{LD}_{[110]} = \frac{2 \text{ atoms}}{4R} = \frac{1}{2R}$$

So, that is how this looks like.

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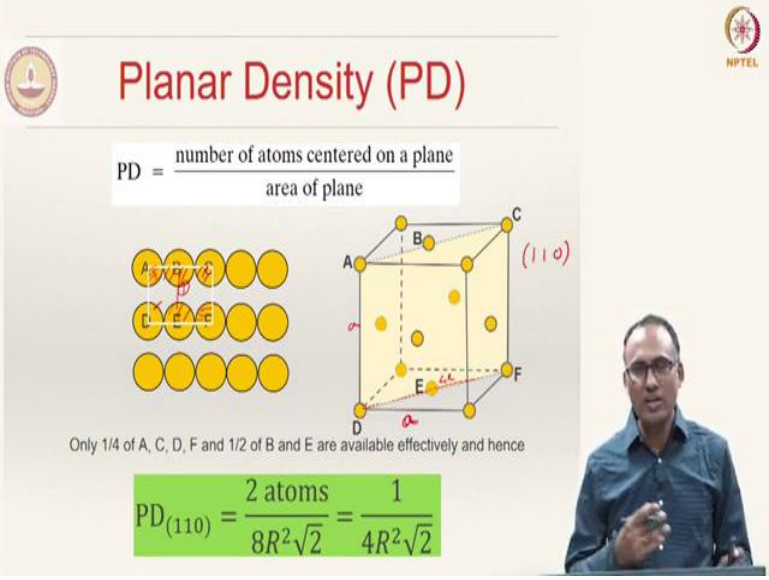

So, this is about linear density. Now we have defined crystallographic planes as well, and hence we also have to talk about planar density. What do we mean by planar density? Number of atoms centered on a plane divided by the area of the plane. So, if you take this particular plane, what is this plane by the way? It is intersecting *x* axis at 1, *y* axis at 1, and is parallel to *z* axis, and hence this should be (110).

This is what you call (110) plane in a face centered cubic (FCC) structure, and then let us look at the planar density. So, this is how the atoms are arranged, and you can see that in this plane, this part of the atom is available, this part of the atom is available, this part and that part. So, effectively these 2 together 1 atom, these 4 together another atom, right? There are effectively 2 atoms available divided by the area of the plane.

So, you know if this is *a*, you can find out the what is this distance. This distance is 4R. You need to find out this area.

$$\text{Area of plane} = 8R^2\sqrt{2}$$

$$\text{PD}_{(110)} = \frac{2 \text{ atoms}}{8R^2\sqrt{2}} = \frac{1}{4R^2\sqrt{2}}$$

The knowledge about linear density and planar density is one of the important aspects to be known because they give us some information about the deformation mechanism when we are talking about plastic deformation in materials. And hence, it is extremely important

to know what are the planes for a given unit cell which are most densely packed; that means, which are having highest planar density or lowest planar density.

What is the direction in which you have maximum linear density; that means that is the most closely packed direction. So, it is important that you need to know what are the most closely packed planes and most closely packed directions in a crystal structure.

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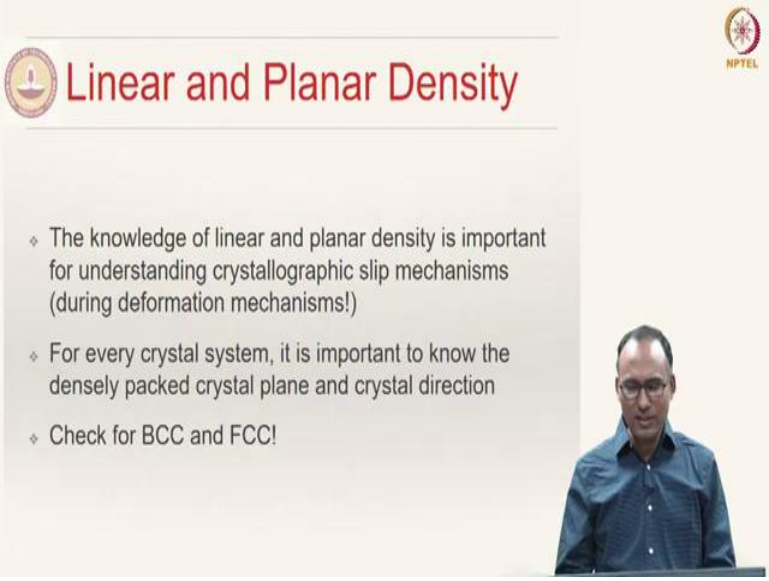

The knowledge of the linear and planar density is important for understanding crystallographic slip mechanisms during plastic deformation. For every crystal system like BCC, FCC and HCP, it is important to know the densely packed crystal plane and the crystal direction.

Please check that for BCC and FCC. What will be those closed packed directions and closed packed planes. With that I will close here and in the next class we will see some of the other most densely packed planes, and other details about crystal structure.

Thank you very much.