Nature and Properties of Materials
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Lecture 9
The Role of Crystal Structure 2

Good morning students, today we are going to talk about the crystal structure in terms of a new light, which is known as Miller index.

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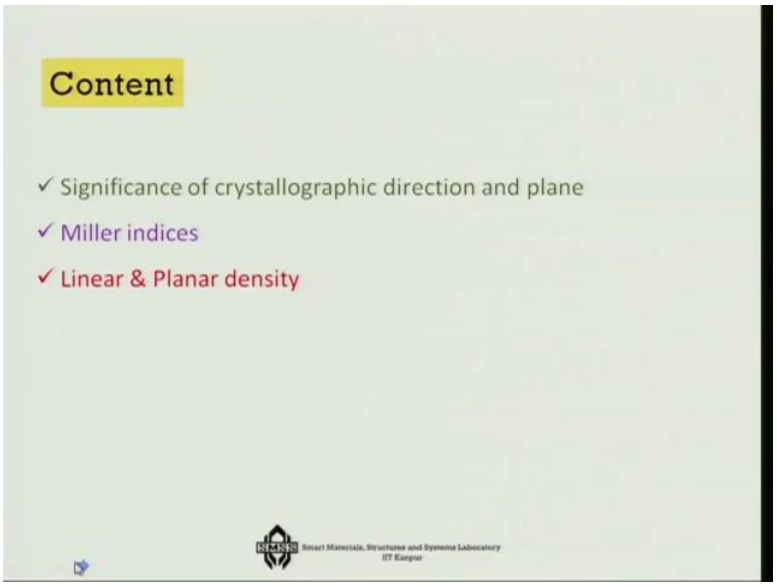

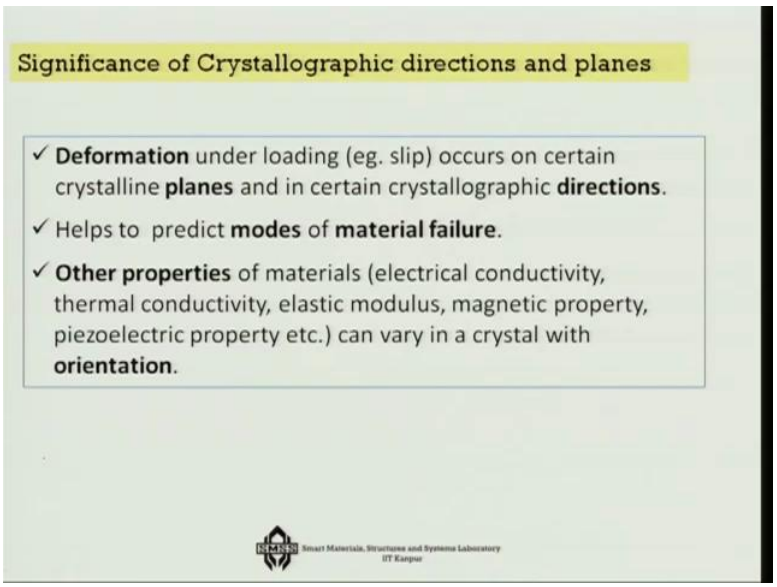

So we will talk about the significance of crystallographic direction and plane, Miller indices particularly. And then we will try to define the linear and planar density in terms of the Miller index. Now, the term Miller index is actually named after very famous British mineralogist

Miller. In around 1839 he coined this term and this has been used since then to define crystallographic planes in various types of crystals.

So various minerals which come out of crystalline forms, there also the same indices has been used, so from there the overall crystal community has taken this particular way of representing the plane and the direction of Crystals. Now, what is the significance of these crystallographic directions and the crystallographic planes? You know, why we are interested about it?

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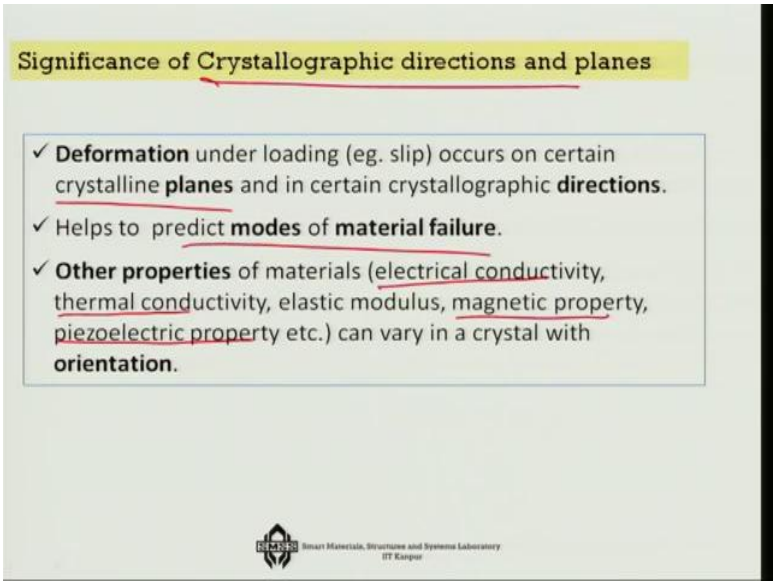

The important thing about this crystallographic direction and plane is that if the crystallographic directions, then the deformation under loading in the crystallographic directions you will be able to predict. And also you will be able to get the crystalline planes. Now, we will discuss about it later that there are certain planes for example, which has the highest densities of atoms, they are very important from the dislocation point of view.

It also helps once we know that what are these so called crystal planes, it also helps us to predict the modes of material failure, which we will talk about when we will talk about the failure of the various types of materials. And also there are other non mechanical but important material properties like electrical conductivity, thermal conductivity, okay magnetic property, piezoelectric property, and all these properties actually vary in a crystal with the orientation.

And hence, a quantitative way of defining the crystal direction helps us also to actually make it clear that these properties, what are the values of these properties and how is it varying

from one direction to the other direction. So let us go to the Miller index, there are couple of examples for example, the turbine blades which are these days this is being developed with the help of single crystal like nickel based single crystal that is used in some of the turbine blades.

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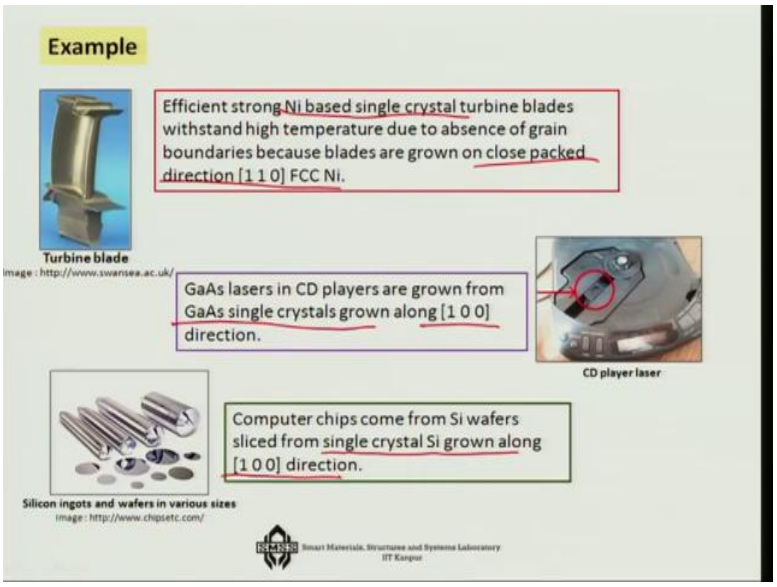

Now, they can withstand very high temperature due to the absence of green boundaries it is because the blades are grown on close packed direction 1 1 0 in a FCC structure of nickel. What is this 1 1 0 structure, this is what we will be discussing about, a similar couple of other applications like Gallium arsenide lasers which is used in CD players, they are grown from Gallium arsenide single crystals along 1 0 0 direction.

And silicon itself as it is the single most important thing in the meme's industry, in computer industry, they are grown from single crystal of silicon along 1 0 0 direction, so that the direction plays a very important role in the mechanical and other material properties and hence, we need to define a system of direction, a system of plane that is the motivation of us for discussing about the Miller index.

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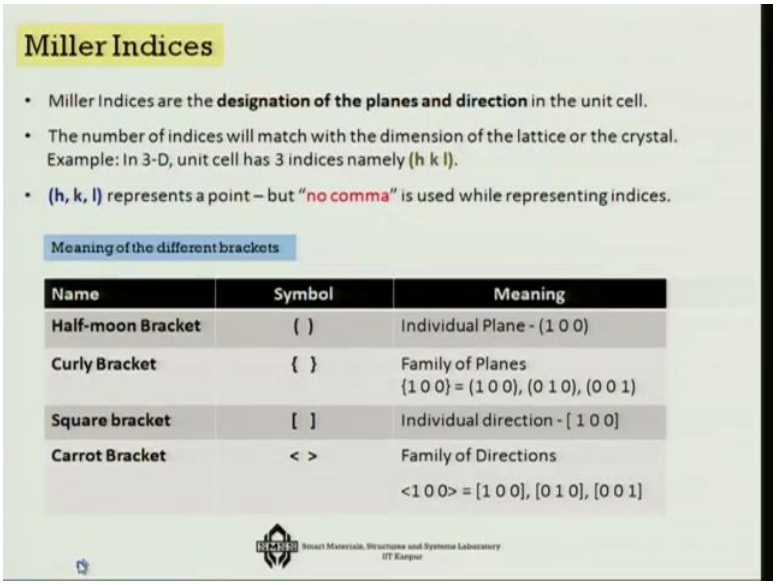

Now Miller indices they use know they are the designation of the planes and directions okay, so the number of indices actually matched with the dimension of the lattice of the crystal. For example, if it is 3D then it is, there are 3 of the indices that are used H, K, L. And other important thing here is that if there is a comma between h, k and l, then that would be in that we are actually referring to a particular point.

But if there is no comma, then it would mean that we are actually referring to an individual plane, so this comma plays a very important role. Now there are 4 types of actually symbols that are used in the Miller indices. The 1st one, which is known as the half moon bracket okay. So that is used for denoting the individual planes like in this case 1 0 0 is an individual plane. What exactly is this plane, we will see it soon.

Similarly, if there are there are other planes like 1 0 0, 0 1 0, 0 0 1, all of them together we show actually a curly bracket so that it shows a family of planes. Now, if we want to indicate just a direction, but not the plane then we use the square bracket that is the convention, so individual direction is actually a square bracket with 1 0 0. And when we want to say about a family of directions, then we use this carrot bracket okay that shows the family of the directions.

So we have to keep this sign convention in our mind that half moon bracket is for individual plane. Family of plane we are going to use curly bracket. Square bracket is for individual direction and family of direction you are going to use the carrot brackets. With these conventions in mind, let us see that how to find Miller indices of a given plane.

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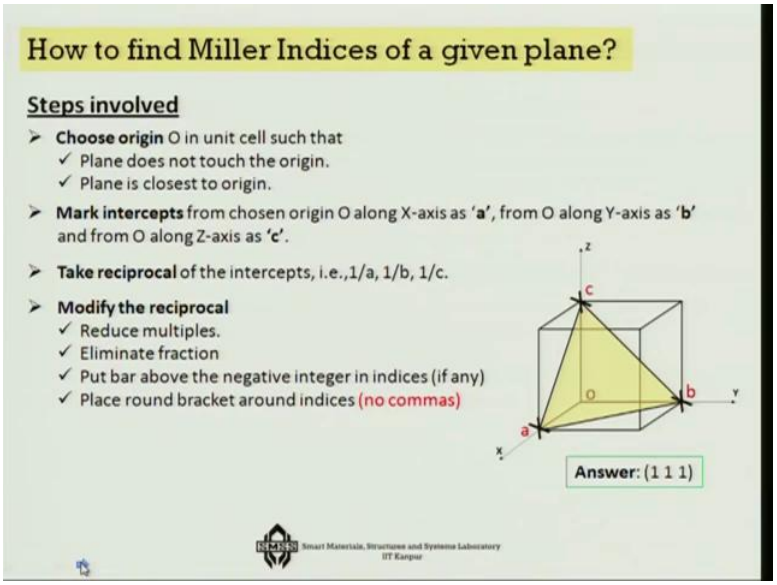

Okay, so here we have a particular lattice structure in which the plane ABC as you can see here that the plane ABC with yellow colour, we want to find out what will be the Miller index of the plane. So what should be the step that should be involved in it? 1st of all, choose the origin O in the unit cell okay such that plane does not touch the origin okay. That is very important that is why I cannot take any one of these corners because those corners will be touching.

If I take them as origin, then the plane will be touching, so plane can never touch the origin. And the plane should be closest to the origin that is also another point why between 2 points say O and this point at the other corner, we have chosen point O because most of the points are actually closer to this origin O, so that is how 1st you choose origin. Then you mark intercepts from the chosen origin O around X axis A, Y axis B and Z axis C.

Now take the reciprocal of them that is 1 over A, 1 over B, 1 over C. After taking the reciprocal, if you find that there are some multiples that are involved in this thing, and then you can actually reduce the multiple, this will simplify it. You can also eliminate the fractions by multiplying them suitably if that is needed and then if there is any negative integer, in this case it is all positive, but if there is any negative integer then put a bar above the negative integer in the indices.

And finally of course, you are going to indicate a plane, which means you have to place the moon bracket okay that round bracket is that moon bracket around the indices without any commas, because if you put a comma then it will become a point. So without any comma,

you just do this that means in this case if I follow that notation, so let us say A, B and C in this case are all 1, 1, 1, their reciprocal is also 1, 1 and 1 okay.

So there is no question of reduction of multiple of fraction here, so now we can directly write it with a moon bracket 1 1 1 without any comma. So that is how you can find the Miller index of a given plane in this particular case. Let us discuss about some other cases.

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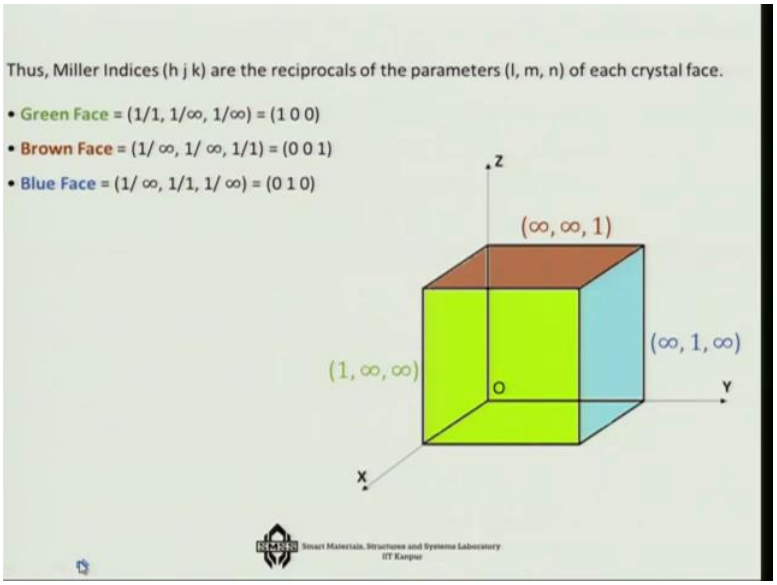

For example, the Miller index h j k, which are reciprocal of the parameters l, m, n of each of the crystal faces okay. So if you consider the green face, then green face if you look at the intercepts, so the green face has an intercept value which is finite in the X direction okay. And Y and Z direction they are infinite why because this green plain is parallel to the Y-Z plane.

So that is why the intercepts are 1, infinity, infinity, their reciprocal is 1 0 0 and that is what is the green face, the Green face here is 1 0 0. Now if you look at some other face okay for example, you look at the brown face is actually you can see here that it is a new no parallel to the X-Y plane, so in this case it is X-Y that is why it is 1 over infinity, 1 over infinity for X-Y, but for Z it is unity, so reciprocal of it is 0 0 1, so that means this brown face has a mill index of 0 0 1.

Let us look at the blue face then, the blue face is parallel to what, X and Z. So that is why X is infinity, Z is infinity, so the reciprocal of them is 0 1 0, so then the blue face will have a Miller index of 0 1 0. So all the basic faces of a crystal lattice thus you can very easily write down what are the Miller indices of them. Now let us say if this 1 0 0, 0 1 0, 0 0 1, all these

faces you want to put them together, then you have to have a curly bracket and you can write 1 0 0 because they qualitatively indicate all the same type of faces okay, so there are family of the faces.

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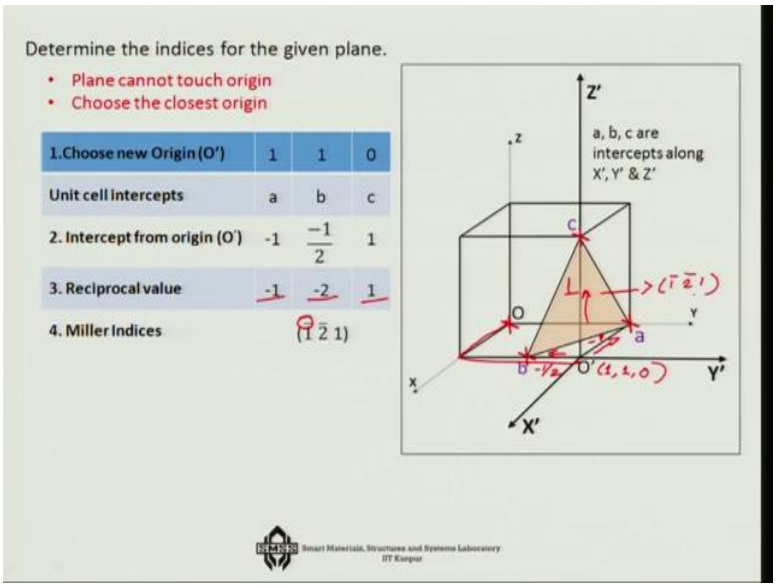

So let us go to the some other problem little more complicated. Suppose we now have a plane which is as has been shown in this particular case, okay. Now we have to 1st choose the origin okay. Now this again the plane cannot touch the origin, so that means we cannot take any of the vertices is the origin okay, we can't choose between O and O prime, now O prime is the closest in this case so we go for O prime here.

And then O prime has the if you look at the O prime's coordinates then it is 1, 1, 0 because X axis unity and then Y axis unity and then Z axis unity, so this is where we are that is what is our O prime point okay. Now with respect to the O prime point, let us look at the intercepts of the same okay. So X axis intercepts how much is it, it actually the X axis direction from O prime we are going the negative direction, this way, so that is why it is - 1 is the intercept okay.

Y axis what is the intercept? Here again I am going in the negative Y direction and this is - 1/2 and Z axis what is the intercept, this is in the positive direction and this is unity. So I can write that the interception - 1, - 1/2 and 1 okay. Now you cannot keep a fraction, so let us multiply this all these things um further, so okay before we do that of course we have to find out the reciprocal value of the system.

So if you take the reciprocal, then it is - 1, - 2 and 1. So any way the problem of fraction is not there because we are taking a reciprocal is this particular case okay. Now, we have taken the reciprocals, so and there is no further reduction possible, so we can the minus I already said you have to use a bar, so you can now write it as 1 bar, 2 bar and 1 that is the Miller index of this particular plane as 1 bar, 2 bar and 1.

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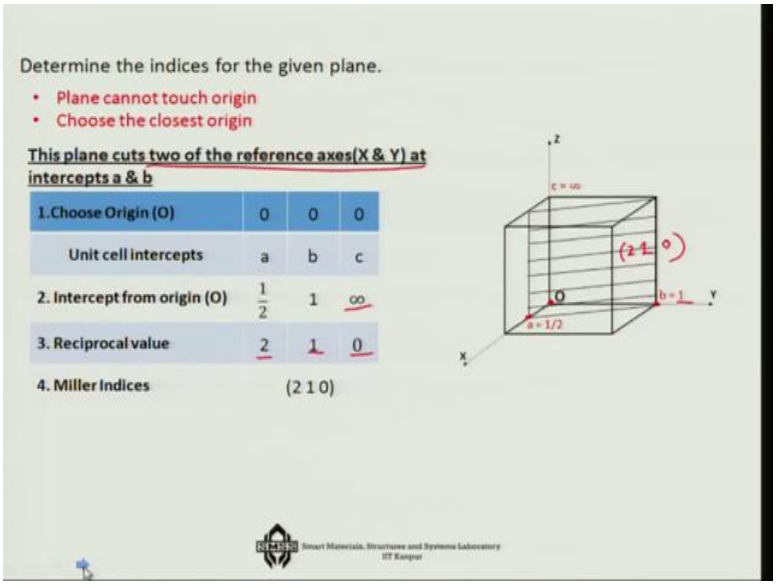

So that is how you can take on the basis of intercepts, the Miller index of a little more complicated case okay. Now let us look at the indices for a given plane okay. So for example, this particular plane that we can see, this plane has a specialty that it cuts 2 of the reference axis X and Y okay and intercepts them at A, A and B at these points they are intercepting.

So 1st thing is of course choosing the origin, now in this case again we can choose O is the origin because O is not touching the plane and it is also very close, so in comparison to the other side, we can take O as the origin okay. Now, what are the intercepts in this case? 1/2 X direction, Y direction 1 and Z direction this whole thing is actually not cutting the Z axis, thus in Z direction it is infinity, so what is the reciprocal 2, 1 and 0. So the Miller index of this particular plane is 2 1 0 okay, so this is again another case that we have solved.

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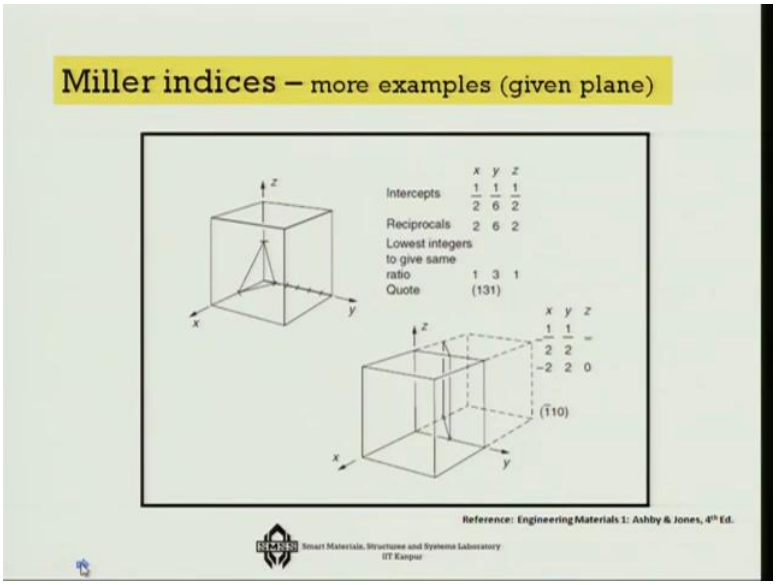

If suppose we have intercepts which are like fraction in this particular case the intercepts of the plain okay, so they are fraction 1/2, 1/6, 1/2, then the reciprocal will be what, 2, 6, 2. Now in this case you can reduce it okay because you have to try to simplify it as much as possible to keep everything inside the crystal structure, so by dividing it by 2 you get it as 1, 3, 1, so then you can write that this particular plane is 1 3 1.

Suppose I take some other plane this particular case for example okay, where it is - 1/2, 1/2 and infinity. Again I take the reciprocal, which is - 2, 2, 0 and I can simplify them dividing all of them by 2 first that means it will become - 1, 1, 0 and then I can denote it as 1 bar, negative is denoted as bar, so 1 bar, 1, 0, which is the Miller index of this particular plane. So thus we are trying to establish how under different cases you can consider the Miller index of the system.

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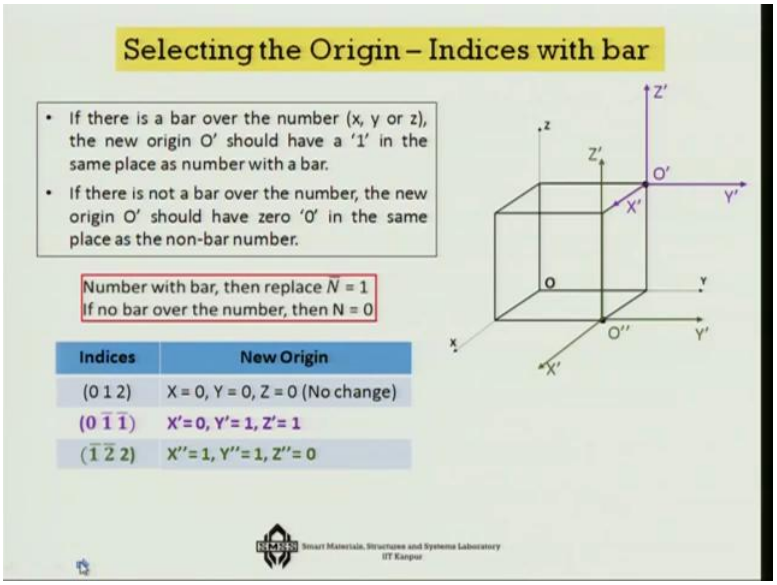

Now if there is a the other point is that there is a very simple way in terms of selecting the origin, when you have indices with a bar, so if there is a bar over a number that means which is a negative number, then the new origin O prime should have 1 in the same place as the number with a bar. And if there is not a bar over the number, the new origin O prime should have a 0 in the same place as the non-bar number.

So number with bar replace this by unity and if no number is there, then replace it by um 0. If if there is no bar, then replace it by 0. Some example suppose you have 0, 1 and 2, now there is no bar that means the new origin to define this can be 0, 0, 0. Suppose you have the indices 0, 1 bar, 1 bar, and then the origin will become 0, 1 and 1 because all the bars are substituted as 1 and 1.

1 bar, 2 bar, 2 that means, 1 bar is 1, 2 bar is 1 and 2 is 0, thus we can select the origin. This is important when if I give you Miller index and then if I tell you that find out the plane, find out the direction, then you need to define first the origin, so then this is the way we can define the origin of the system.

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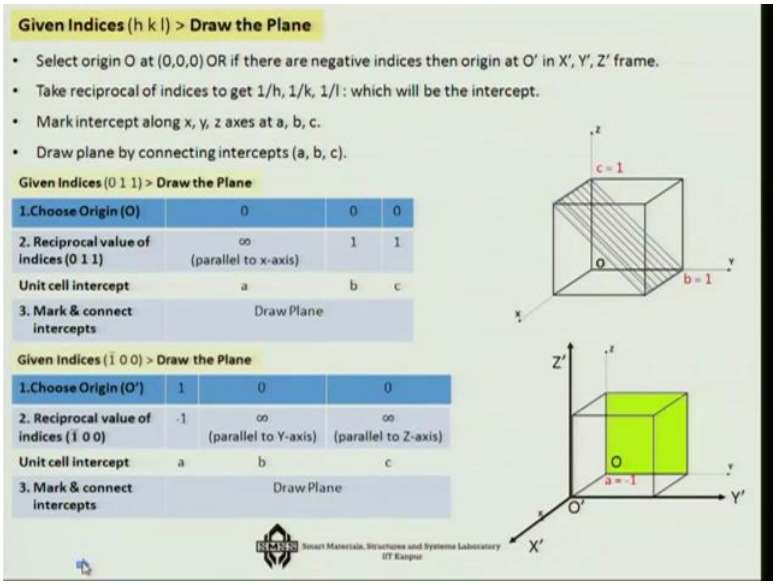

Now, given indices let us try to draw the plane okay, the other way round. So far we have seen that if I give you the plane, what is the index? Now if I give you the index, what is the plane? Okay. So select the original 0, 0, 0 or if there are negative indices, they will see that the origin at X bar, Y bar, Z bar as just now we have discussed. Now take the reciprocal of the indices and that will give you the intercepts, so you can take suppose H, K, L is that indices, then 1 by H, 1 by K, 1 by L will give you the intercepts.

Mark the intercepts along X, Y, Z axis as A, B, C and then draw plane by connecting this intercepts. Suppose, I give you the indices as 0, 1, 1 okay, you have to draw the plane. There is no negative number here, so you can choose the origin as 0, 0, 0, so I have chosen the origin as 0, 0, 0 okay. Now what are the reciprocal values of 0, 1, 1 okay, that is infinity, 1 and 1. So already I get an idea that the plane should be such that it will not touch the X axis okay so it will you know.

Now let us find out this the intercepts okay. So if we find out the unit cell intercepts in this case, so we get the unit cell intercepts values and then you can draw the planes, so essentially each one of them will be lines parallel, so you can see each one of them they are not actually touching the X axis okay, so they are not intercepting with the X axis, so then and already that the intercepts are 1 and 1 okay, so 0, 1, 1.

And then you can easily draw the family of lines and you can easily get the plane that we are talking about which is nothing but 0, 1, 1. Suppose I give a negative Miller index 1 bar, 0, 0, then what do I have to do, I have to select origin now such that this one bar will be one, 0 is

0, this is 0. So that means with respect to my earlier case, I have to shift it now, so this is what is my new position where the O prime has this is one with respect to the earlier coordinate system this is one, then 0 along Y and Z along said.

So this is what O prime is because that is how I have given the comma for them. Now, what is the reciprocal of them? The reciprocal value of 1 bar, 0, 0 okay, so that if we find it out that means this is - 1, 0, 0 reciprocal, so this is - 1 as the 1st reciprocal, then infinity and infinity as the other 2. That clearly tells us that since there is it cannot cut either the Y or the Z axis that means it has to be parallel to this particular plane has to be parallel to the Y-Z plane itself.

So that is how and also we know that it has to be from O prime at the - 1 direction. So, at this point we draw a this parallel plane and this is the plane that we are talking about, which will have infinite intercept with respect to Y prime and Z prime and it is going to only cut this X axis at a distance of - 1. So that is how we show this line, we show this plane from the mirror index of the plane.

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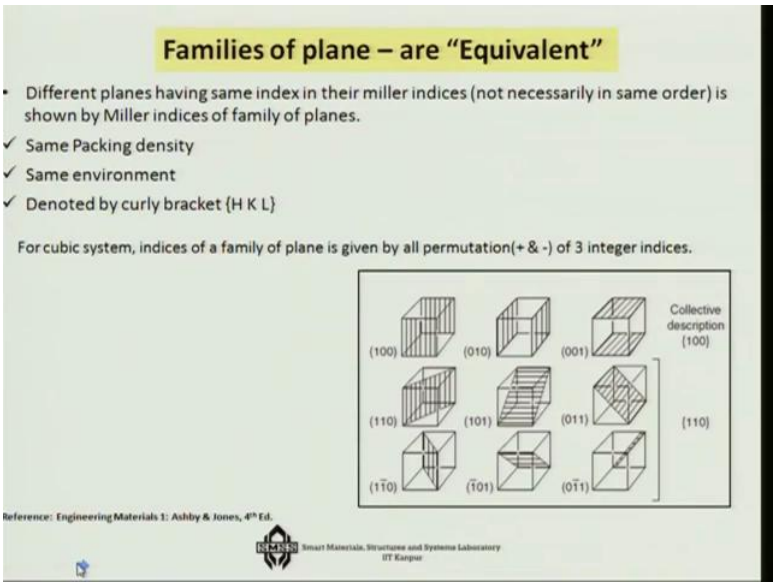

Now, there are families of planes which are actually equivalent okay. So different planes having same index in their mirror indices of course not necessary in the same order is actually shown by the family of planes that means you use a curly bracket okay you use curly brackets and essentially they indicate actually planes which may have same packing density or same environment okay.

For example, I look at all the edges of the cubic crystal structure okay. So then this edge, the 1st edge as has been shown 1, 0, 0, then the 0, 1, 0, these are 0, 0, 1. Now if all these edges,

vertical edges, this one this one okay this, this and this, this okay. So if all these edges I want to put them together collectively, I can call them as the family of 1, 0, 0 meaning thereby that you can have all the permutations and combinations inside.

So that means, the curly bracket 1, 0, 0 can actually generate 3 of the planes that is 1, 0, 0 plane and 0, 1, 0 plane, whatever are the combinations possible 0, 0, 1 okay, so that is what we have shown. Suppose, we consider this particular plane which contains the diagonal direction, so this is actually 1, 1, 0 plane. The other diagonal plane is 1, 0, 1 and the other one is 0, 1, 1.

Again the family is called 1, 1, 0, so the family is 1, 1, 0 that means I can get actually 1, 1, 0 of course and then 1, 0, 1 and 0, 1, 1 okay. So those are the 3 planes that we have shown. Similarly, in the negative direction we do the same thing and get another family of planes. So that is how the family of planes are actually defined with the help curly bracket.

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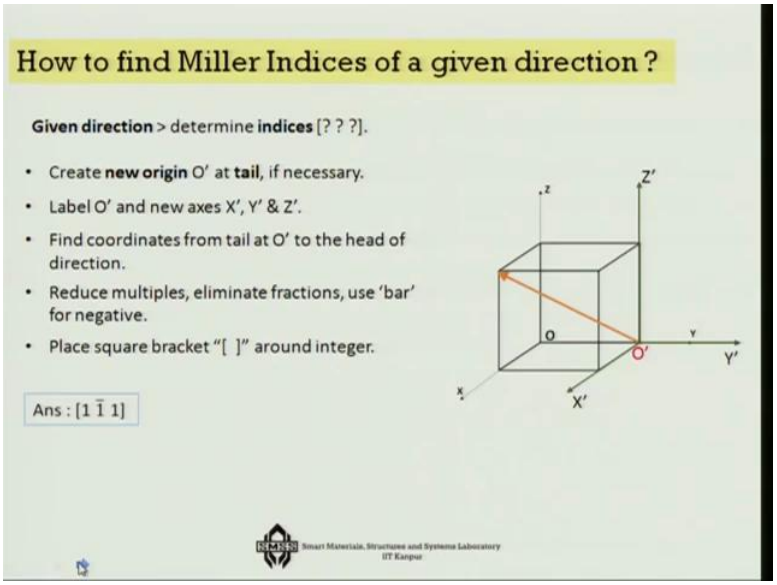

Now, how to find Miller indices of a given direction okay. So far we have discussed about the planes, for the direction how do we do it that is very simple. Here, you again given a direction, 1st create a new origin O prime at the tail okay and then level O prime okay a new access X prime, Y prime, Z prime, then find coordinates from the tail to the head of the direction okay and reduce multiples as usual, eliminate fractions and use bar for negative.

Finally, you actually place the square bracket, so in this case this is a square bracket that we are using in order to denote that this is a direction and this is not a plane okay. So in this

particular case for example, for this direction okay, so we have O prime as the centre origin okay.

From here this is the point which is connected and then if I try to look at it that this point how do I reach, I go one unit here positive okay, I go again one unit here, but this is negative and then I go one unit here that is positive okay. So that is why I can write this to be with the square bracket that 1 then 1 bar for this negative and then 1. That is how I am denoting Miller index of A direction.

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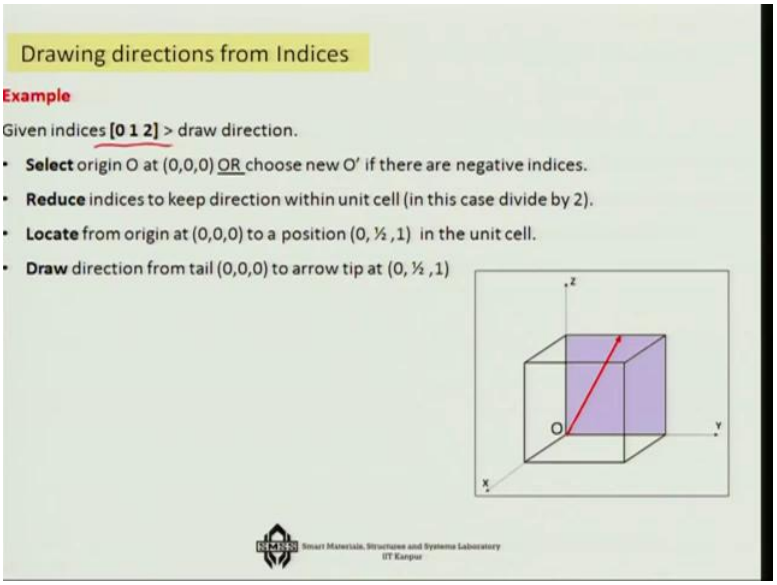

Let us practice more okay driving directions from the indices. Suppose 0, 1, 2 is given to us and we have to draw the direction, so we have to select origin. Select the origin in this case has there are no negative indices, so it is 0, 0, 0, so I have select it as 0, 0, 0 okay. Now from here, reduce indices to keep the direction within unit cell, so divide this whole thing by 2, so that means this should become 0, 1, 1/2 and 1 okay.

So now look at from origin 0, 0, 0 okay, so you have to go 0 and then you have to go 1/2 X axis 0, Y axis 1/2 and then you have to go 1 full unit to reach this particular point. So once I reach it, I put an arrow okay draw direction from tail 0, 0, 0 to the tip and that is how we are giving the direction corresponding to this Miller index. So we can read it, see a Miller index you can read what direction we are talking about.

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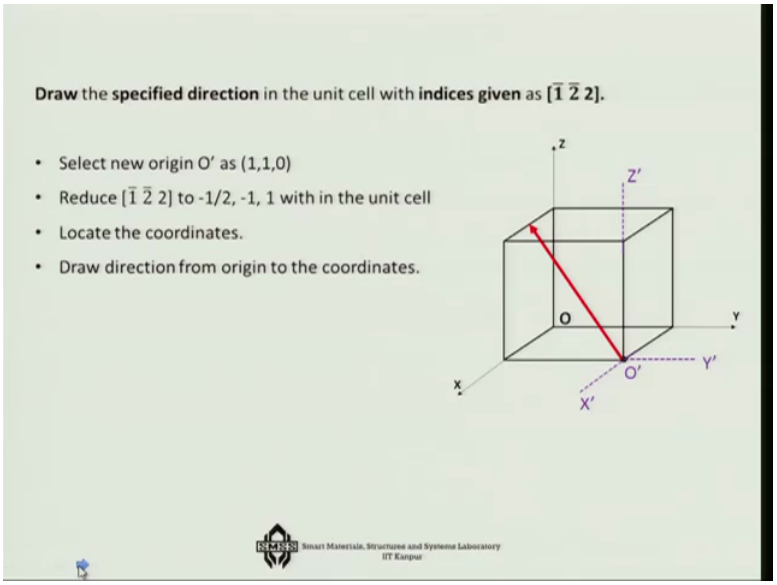

Suppose I give a negative one now, 1 bar, 2 bar and 2, so now I have to select the new origin. And we say that if there is a bar, then we put 1, 1 and there is no bar means 0 that is what is my new origin. So from the old origin, let us first go to X axis 1 okay and then Y axis 1 and Z axis 0, this is the new origin. Now from the new origin, let us try to define this 1 bar, 2 bar, 2 okay.

So one bar, 2 bar, 2 is actually - 1, - 2, 2, so the intercepts will be - 1/2, - 1, 1, so let us try to show where is this - 1/2, - 1, 1 is. So this is where is my new axis now, we have to keep in our mind that this is our new axis system. So from here I have to choose the particular point from the origin in such a manner that I have to go - 1/2 along the X axis okay.

So this way I am going - 1/2 and then I have to go - 1 along the Y axis, negative - 1 I am going and then I am going I am going 1 on the top positive that is how we are getting this point and join it by arrow that is how we are specifying the direction corresponding to 1 bar, 2 bar and 2.

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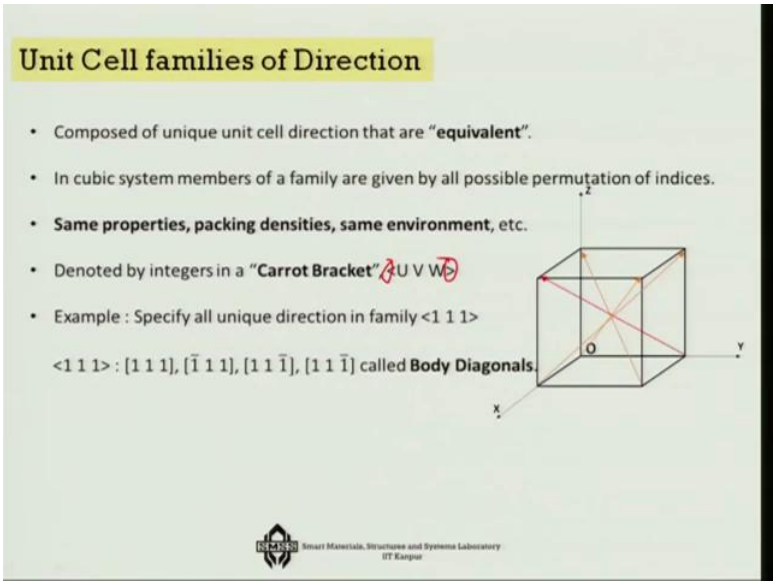

Now similar to just very similar to the other case, unit cell families which are the equivalent families in this case they are shown with the help of the carrot bracket. Just like we have used curly bracket for the planes are here we are using carrot brackets for the family. So if you are talking about 1 1 1 carrot bracket, it means 1 1 1, 1 bar 1 1, 1 1 1 bar, 1 1 1. These are actually if you look at it these are all Body Diagonals of the system. So that is what the equivalent family is in this case.

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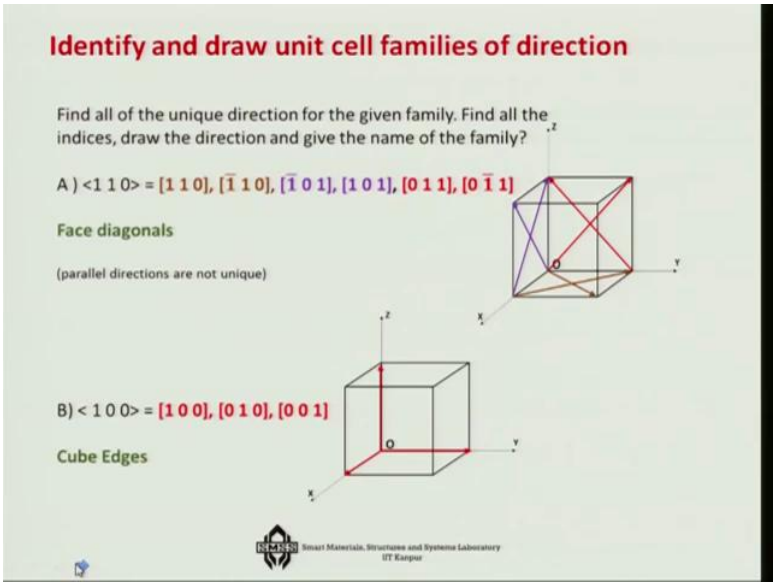

Now, there are very similar such families like face diagonals. All face diagonals are shown by 1 1 0s okay. Cube edges all cube edges are actually shown by 1 0 0 so these are directions for family of the directions.

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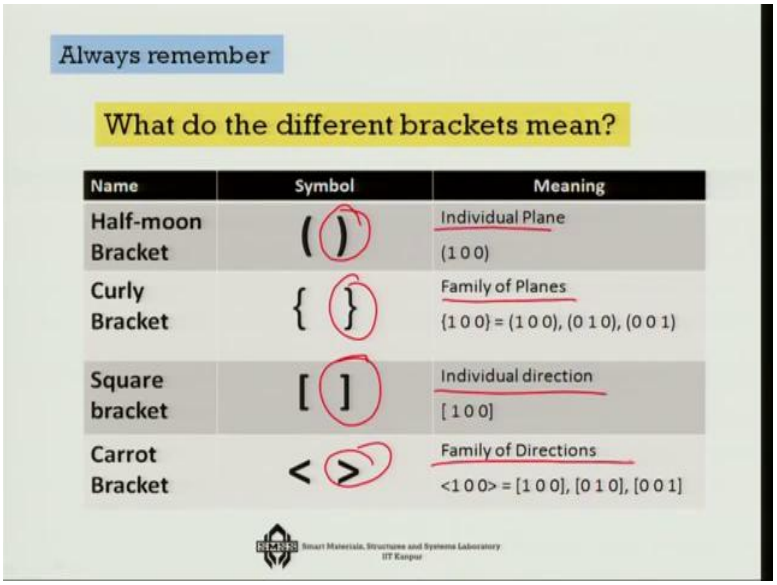

So keep in mind once again, half moon bracket individual plane okay. And curly bracket family of planes, square bracket individual direction, carrot bracket family of directions, so let keep this and practice. What are the other properties of the Miller indices that we can define?

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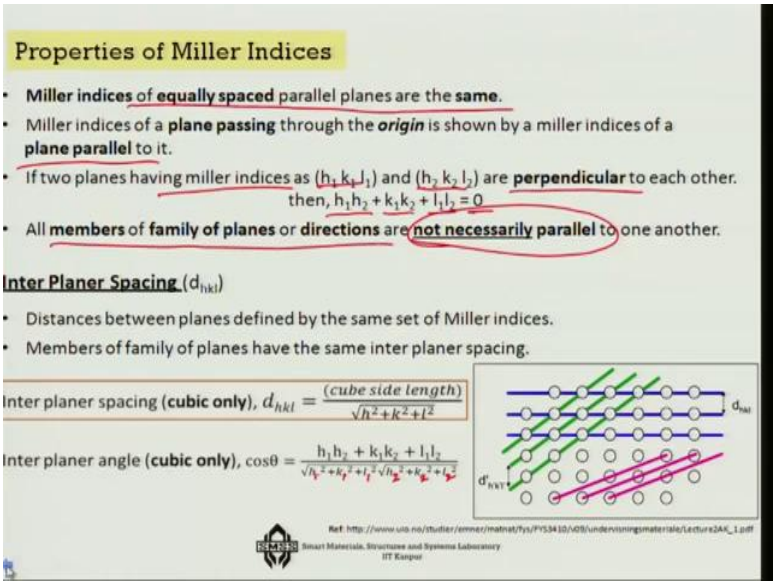

Miller indices of equally spaced parallel planes are the same. In fact, that is why we have shown that all the parallel planes can be actually represent with the help of say Miller index itself. Miller index of a plane passing through the origin is actually shown by a Miller index of a plane parallel to it because it cannot contain the origin, so it is shown as a plane parallel to it.

If 2 planes having Miller indices as H 1, K 1, L 1 and H 2, K 2, L 2 and they are claimed to be perpendicular to each other, so that means it is like their dot product H 1 H 2 + K 1 K 2 + L 1 L 2 = 0. So that is one condition of 2 perpendicular planes from the Miller indices you can say. All members of family of planes or direction are not necessarily parallel to each other, this you have to keep in your mind; I am just going back to ones to 2 slides.

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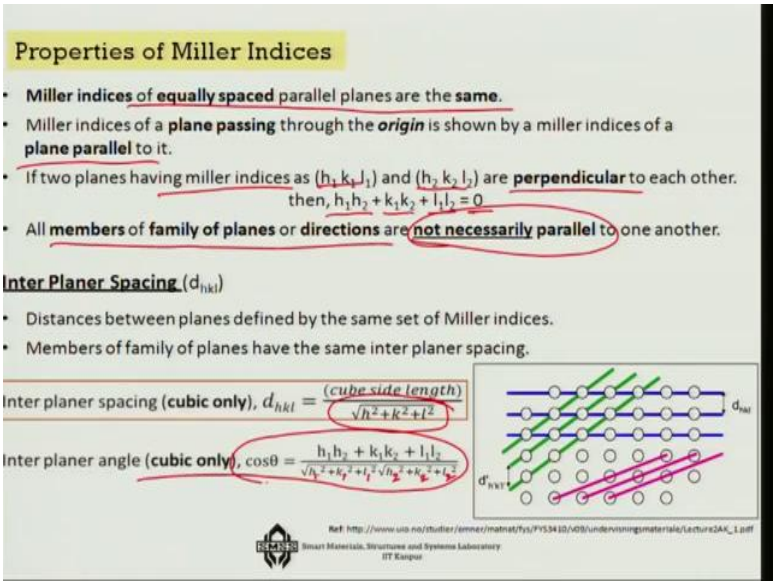

Look at this face diagonals okay. So they are all belonging to the same family but they are not parallel to each other, so that is the point that we are actually telling here. Inter planner Spacing is very important one, so the Inter planner spacing is defined in such a manner that this D H K L that is like the for a cube, cube side length over the square root of H squares + K square + L square that is the Miller index okay.

So if the side length of a cube, then square root of the square of the Miller indices will give you the Inter planner spacing. And Inter planner Angle you can also similarly find out by using this formulation, you can find out what is the inter planner Angle. So you can find out the inter planner spacing and inter planner Angle with the help of the Miller index.

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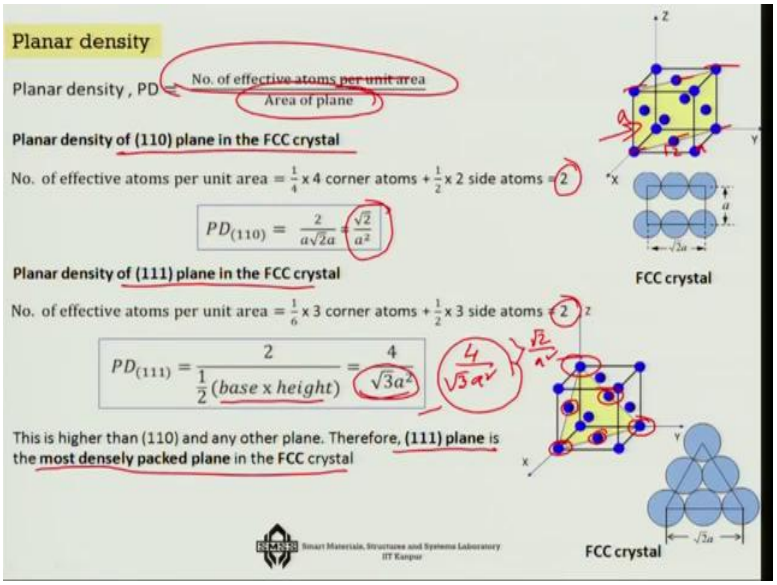

There are 2 more important things that you can find out with the help of the Miller index. These are planner density, so that is number of effective atoms per unit area divided by the area of the plane okay. Suppose we are considering planner density of 1 1 0 plane in the FCC Crystal, then if you look at the FCC structure okay, so you see that you have 1 fourth into 4 corner atoms all corners atoms okay + 1/2 into 2 side atoms.

So there are 2 sides atoms that is also having 1/2 into 2, then total number of effective atoms per unit area so that is 2 in this case and that divided by the total number of effective atoms actually that is it okay, so you can consider on that area basically total number of effective atoms divided by the area of that plane and the area of that plane is A times, so this is A and this side is root 2 A.

So A times root 2 A, so that is root 2 so that means it is A to over A times A times root 2 A that is root 2 by A square. Similarly, if you consider the 1 1 1 plane in the FCC Crystal, let us look at the 1 1 1 plane okay so that is thus containing the diagonals, so here you are having one sixth of 3 corner atoms okay and 1/2 of 3 side atoms. So there are these side atoms there you are getting 1/2 of this.

So total you are again going to get a number 2, but the area is different here. What is the area here? 1/2 times base into height that is if you work it out, you will see it will be root 3 A square, so the total number here is 4 over root 3 square. And this is actually larger than root 2 over A square.

As a result, you can say that 1 1 1 plane, this diagonal plane is actually most densely packed more densely packed definitely from 1 1 0 and you can check all other planes and you will see this is actually the most densely packed system. Similarly, this you have done for one case similarly; you can do it for the other cases.

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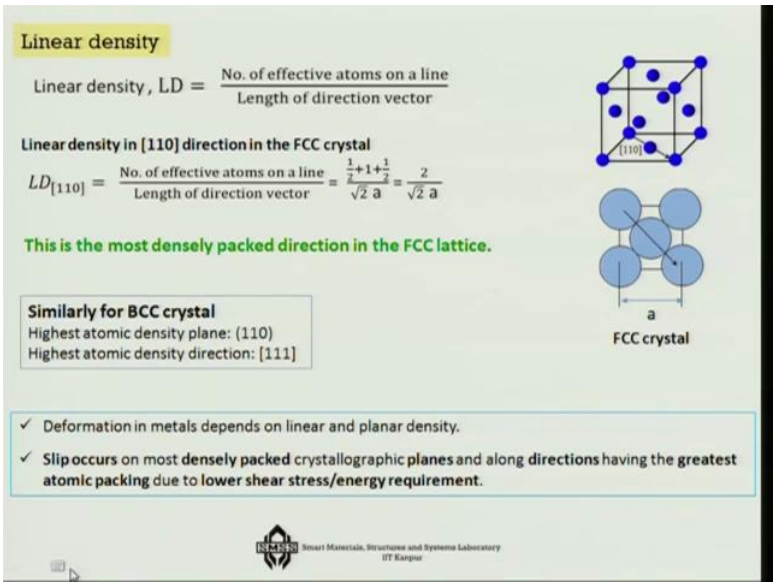

Now the linear density also you can find out in that case it is number of effective atoms in a line and the length of the direction vector. So in the direction like 1 1 0 you can find out that it will become 2 over root 2 A. In fact, 1 1 0 direction is again one of the most densely packed direction in the FCC lattice. For the BCC also it is similar then like highest atomic density direction is 1 1 1 and highest atomic density plane is actually 1 1 0.

Now deformation why this is important bescause deformation in metals actually depends on this linear and planner density okay. It is like this that if you have more number of atoms in a particular plane, then it will be much easier to push actually a dislocation over that plane comparison to any other planes that is why most of the time the dislocation travel over the highest density plane, okay their equivalency is something like you consider that as if you have a small piece of paper or clothes and you have some balls below that okay and you are trying to pull that cloth.

Now the direction where you are getting more number of rollers, it will be much easier to pull that cloth along that direction. So that is why the slip occurs on most densely packed crystallographic planes and directions and that is very important for us to know before and because then how to actually so to say (())(36:46).

So this is where we will stop and in the next lecture crystal defects and its effects like point defects, line defects and plain defects. Now that the Miller indices, it will be very easy for us to actually discover the defects and its effects. Thank you.