Chemical Crystallography
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Understanding of Space Groups and Miller Indices
Lecture – 15
Miller Indices for Crystallographic Directions and Planes

Welcome back to the course of Chemical Crystallography. In last lecture, we were learning about how to do the space group representations in two-dimension and we discussed a large number of space groups starting from triclinic to monoclinic and then to orthorhombic and then to tetragonal and I would like you to practice some of those and some other space groups which are belonging to these 4 crystal systems.

So, now we would like you to this concentrate on a new aspect of crystals where we would like to know how to distinguish between different directions in crystals, how to identify them using some indices and then we will go ahead and learn how to identify the crystallographic planes using the 3 indices h, k and l. These 3 indices that I am talking about are called the Miller indices those are termed as h, k and l

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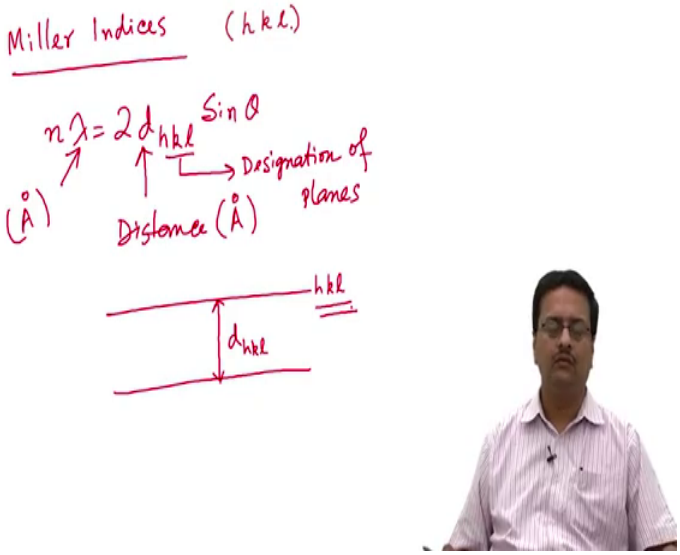

So, you might have seen in a new you may remember that the Bragg's law states n lambda equal to 2 d h, k, l sine theta. So, here that d is the distance in angstrom unit,

because we represent the lambda in angstrom unit and the indices h, k, l indicate the planes so, it is the designation of planes.

So, when we are talking about a set of parallel planes, suppose these are two set of parallel planes in a crystal lattice the distance between these two parallel planes are called as d and we designate these planes as h, k and l as a result, we identified this distance as d h k l. So, to do that; we need to know how to designate these hkls, what are the possible values of hkls and then we should know the significance of those planes with respect to the axis x, y and z.

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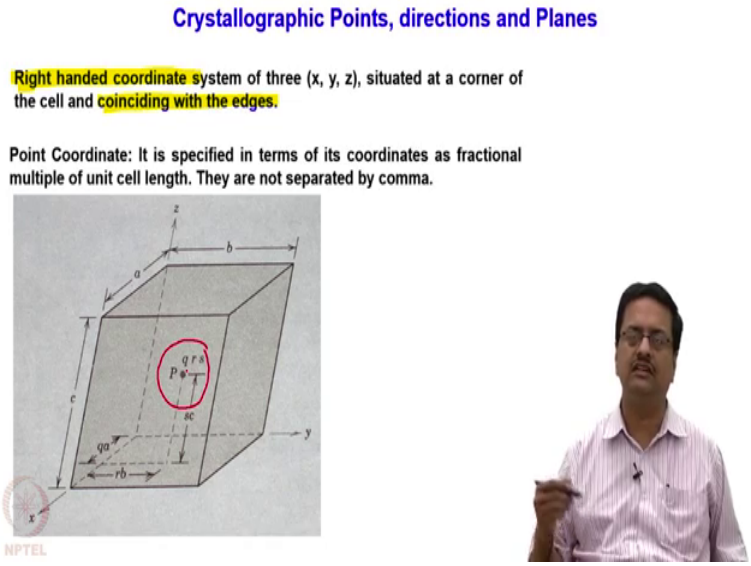

So, to know about that; we need to know about the crystallographic points directions and planes. So, in this subject; in the crystallography in while considering a lattice, we always use a right handed coordinate system as is indicated, here the right handed coordinate system of 3 axis x, y, z and going with the coinciding with the edges.

So, now if we have a point inside a lattice which is designated here as p, then what should be the coordinate q r s of that point P, this point q r s has the coordinates which are the fractional coordinates with respect to the unit cell parameters a, b and c.

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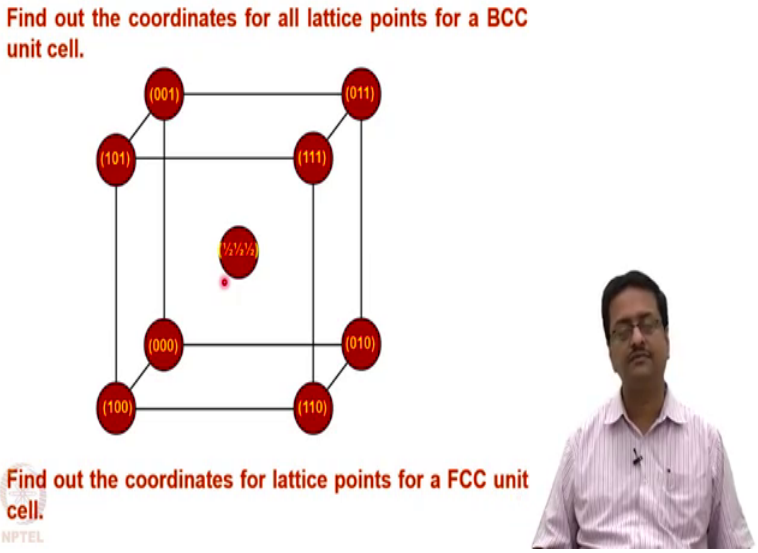

So, in case of a body centered lattice, we have atoms at the 8 corners as you can see the atoms 8 corners and the atom at the center of the lattice.

What are the coordinates of those corners with respect to a given origin which is 0 0 0, the ones which are 1 unit along x 1 unit along y and 1 unit along z are designated as 1 0 0, 0 1 0 and 0 0 1 set of coordinates, set of points because those are at 1 unit away from the origin, then the other corners which are now here 1, 2 and 3, they are first 1 unit away along x 1 unit above along z and 0 along y so, this point is 1 0 1.

Similarly, from here you go 1 unit along y, you go 1 unit along z and not going anything anywhere along x means it is 0 1 1. So, like that the opposite corner of origin becomes 1 1 1, we travel 1 along x, 1 along y, and 1 along z. So, it becomes 1 1 1 the point at the center of the lattice which is a body centered unit cell then is half half half; that means, from the origin we traveled half along x half along y and then gone half way along z and reach the center of the lattice and designated it as half and half half half

So, for your homework you find out the coordinates for lattice points for the FCC unit cell.

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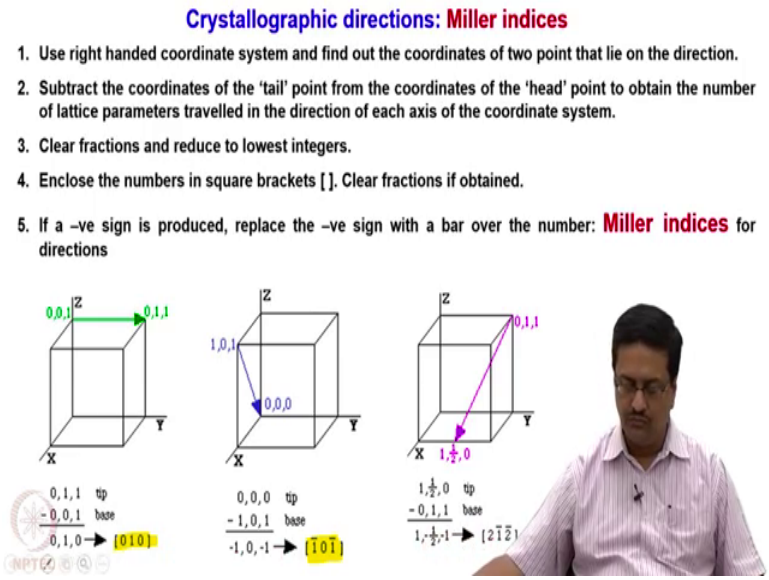

So, now let us try to identify the crystallographic directions and the corresponding Miller indices for that; once again, we use the right handed coordinate system to find out the coordinates of the two points that lie on the direction. Suppose, if this is the direction, I want to find out the two points the bottom point and the top point and determine the corresponding coordinates.

Then you subtract the coordinates of the tail point from the coordinates of the head point to obtain the number of lattice parameters traveled in the direction of each axis of the coordinate system, then by doing the subtraction, if you end up getting fractions, you clear the fractions and reduce it the numbers to lowest integers enclose those numbers in square brackets clear fractions is obtained and if you have a negative sign produced, replace the negative sign with a bar and then that number the set of 3 numbers are called the Miller indices of that particular direction.

So, here are 3 examples at the bottom the extreme left one I want to know what is the direction from this point which is 0 0 1 to 0 1 1. So, the tip is 0 0 0 1 1 the base is 0 0 1. So, I am subtracting the base coordinates from the tip coordinates and I am getting the numbers 0 1 0. So, if 0 1 0 should be written in square bracket and the particular direction indicated here in green is the 0 1 0 direction.

So, these are the Miller indices of that particular direction let us see the second one here the direction is from this corner which has coordinates 1 0 1 from there if we are trying

to find out what is the direction towards the origin. So, the origin is the tip the base is 1 0 1. So, what we have on subtraction minus 1 0 minus 1.

So, when we represent it with in third bracket or the square bracket then the Miller indices for that direction is 1 bar 0 1 bar in the same manner in this case you have from 0 1 1 we are trying to find out the direction which is the middle point of this edge. So, this is one along x half along y and 0 along z. So, this half 0 is the tip and the base is 0 1 1. So, on subtraction it becomes 1 minus half minus 1.

So, now we have a fraction here. So, this fraction has to be cleared so, we multiply these 3 numbers by 2 to remove the fraction so, it becomes 2 1 bar 2 bar and that 2 1 bar 2; what is the Miller indices for that particular direction that we have seen now; now let us do a few more.

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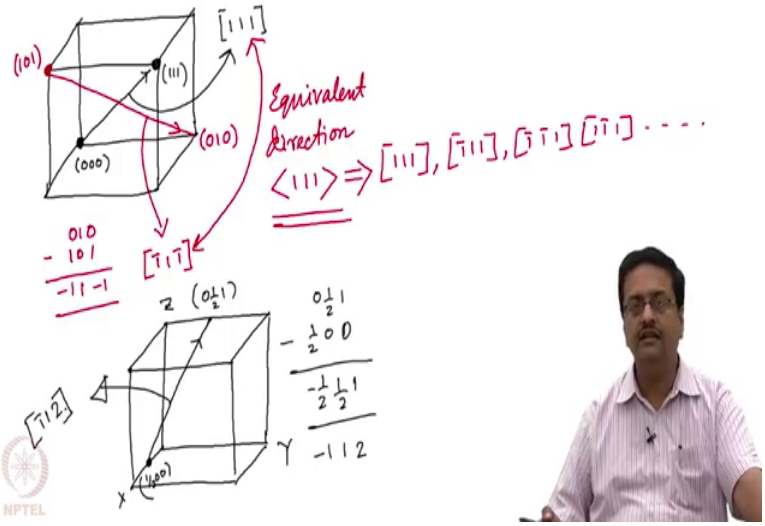

Because I would like you to learn this and do it yourself and we should do it from the scratch again because there are some aspects which I would like you to understand here.

So, I am drawing a cube and I want to know; what is the direction from this corner to the other corner. So, this is a body diagonal. So, the starting point origin is 0 0 0, the ending point coordinate is 1 1 1. So, if you subtract the coordinates of base from the tip you get 1 1 1 and hence the direction that we have got as Miller indices 1 1 1.

Now, if we try to see the direction from this corner to the other corner of the unit cell. So, what is the coordinate of this corner it is 1 0 1 and the tip is 0 1 0. So, if we subtract 1 0 1 from 0 1 0, what we get is minus 1 0 minus 1. So, immediately sorry 0 1 minus 1, I am sorry, 0 1 minus 1 which means the Miller indices for that plane that for that direction will be 1 bar 1 1 bar.

Now, you compare these two directions they have same indices 1 1 and 1 with a different sign minus on two cases and they are body diagonals. So, these body diagonals are equivalent directions and they are can be represent as 1 1 1 within this greater than and less than sign it means that you are referring to all the planes which can be formed by combination of 1 1 1 with plus and minus signs on each.

So, 1 bar 1 1 1 bar 1 bar 1 1 1 bar 1 and so on; all possible combinations would represent 1 or the other body diagonal having different directions and they are called the equivalent directions, the next one that we would like to draw here a direction with fractional coordinates in it. So, we start from a point which is half 0 0 and we go to another point here which is 0 half 1.

So, we are trying to find out the Miller indices of that particular direction. So, we should do this 0 half 1 is the tip and half 0 1 is the base. So, we should subtract the base from the tip. So, we get minus half sorry; the base is 0 minus half 0 1.

So, now we have 2 fractions. So, we need to clear the fractions by multiplying by 2, we convert it to minus 1 1 2. So, the corresponding Miller index indices for that particular direction are going to be 1 bar 1; 2. So, this is how one should generate the Miller indices of the directions.

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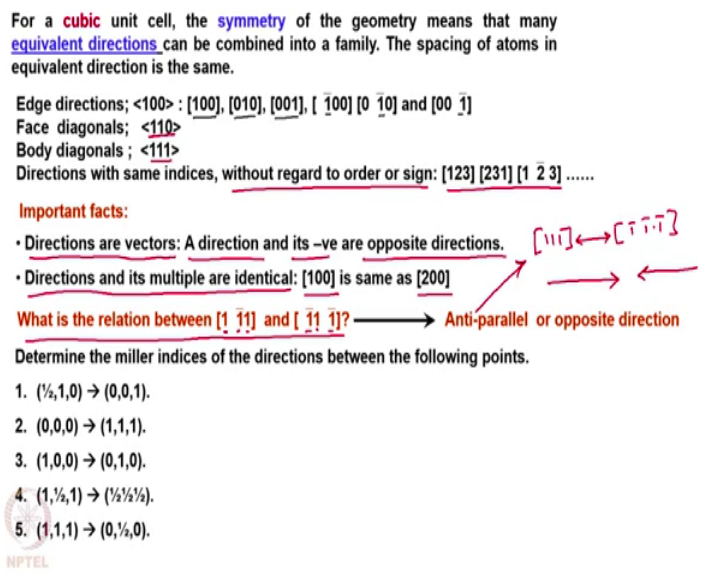

So, for a cubic unit cell, the symmetry of the geometry means that many equivalent directions can be combined into a family as we have indicated the spacing of atoms in those equivalent directions is the same.

So, when we say edge direction we are talking about the directions 1 0 0, 0 1 0, 0 0 1 and all combinations with negative signs of what these are the directions along the edge the face diagonals will mean they are of the family 1 1 0 and the body diagonals are of the family 1 1 1 that we already have seen and directions with same indices without regard to the order or sign are also can be classified as equivalent directions.

What are two things to be remembered directions are vectors. So, the direction and its negative are opposite directions; that means, if we write 1 1 1 and if we write 1 bar 1 bar 1 bar; that means, these two are opposite directions if 1 1 1 mean a direction left to right a direction 1 bar 1 bar 1 bar would mean right to left directions and its multiples are identical; that means, 1 0 0 is same as 2 0 0.

So, in case of directions one should always reduce the h k l indices to their minimum value and write that as it the correct Miller indices for those directions. So, what is the relation between these two point 2 2 directions 1 1 bar 1 and 1 bar 1 1 bar; the answer is anti parallel or opposite directions because here the one which was plus is now minus the one which was minus is now plus and the one again which was class is now minus.

So, in the same manner as we saw 1 1 1 and 1 1 1 bar 1 bar are opposite direction, it applies for other combinations also. So, I would like you to practice at home that determine the Miller indices for the direction between the following points there are 5 such examples, I would like you to do yourself.

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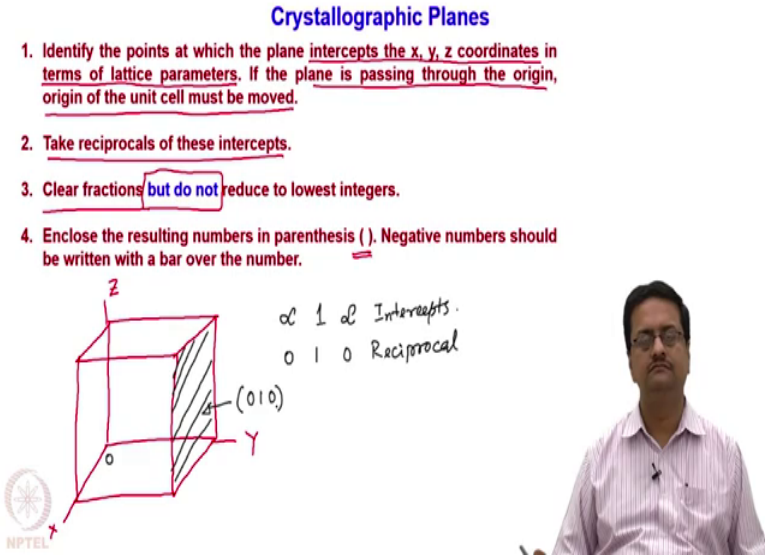

Now, I would like move to the crystallographic planes we would like to designate the planes in the same manner as the directions using 3 indices h, k and l and we try to determine those Miller indices by using a procedure which I am going to describe now.

So, what we need to do is we have to identify the plane in the lattice we need to find out the intercept of x, y, z coordinates in terms of lattice parameters, if the plane is passing through the origin, the origin of the unit cell must be moved to a suitable position such that the origin does not coincide with the plane anymore then one should take the reciprocal of these intercepts clear the fractions, but do not reduce to lowest integer which is different from what we saw in case of directions.

And then enclose the resulting numbers in first bracket and negative numbers as usual should be written with a bar. So, let us see the case of a few examples. So, I have drawn a cube and in that as usual this is my x direction this is y and that one is z here I want to designate a plane which is like that this is one face. So, what are the intercepts of this face on x, y and z you see the space is parallel to both x and z. So, this face is not going to have an intercept on x and z; that means the intercept of this plane with x and z are

infinity and this plane meets the y axis from the origin at a distance one. So, these are the intercepts.

So, if I take reciprocal of these intercepts I end up getting 0 1 0, there is no fraction to be clear there is no nothing to be reduced or anything. So, the Miller indices for that plane is 0 1 0.

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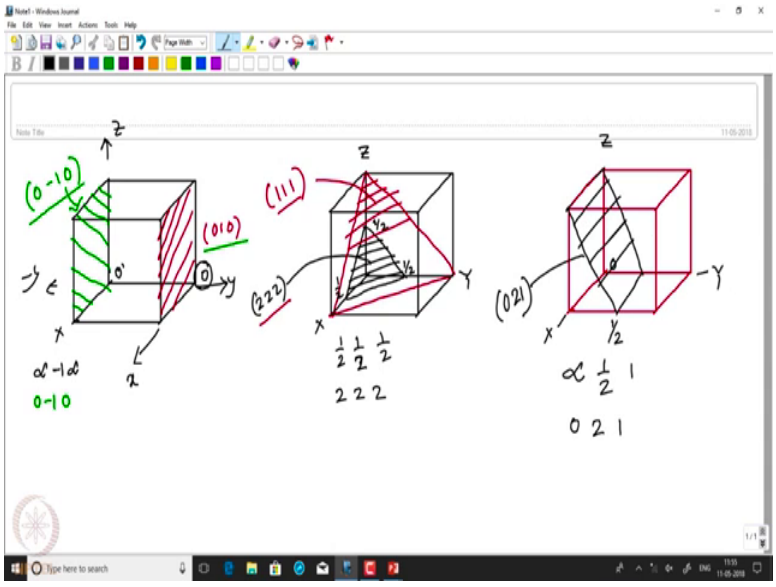

Now, let us see a different plane the plane which is here. So, the intercepts are 1 1 and 1 the reciprocal is again 1 1 1. So, the plane is simply 1 1 1.

Let me draw a few cubes here. So, that we can continue drawing the Miller indices for a few set of different planes, we have seen that the plane which is here is designated as 0 1 0 what should be the designation of that particular plane; you see that this particular plane is passing through the origin. So, we need to shift the origin to a suitable location such that the origin is no longer on the plane.

So, instead of having x, y, z like that I would shift this origin here. So, that this direction is plus x plus y this direction is plus x the backward direction is minus y and so on. So, now, with respect to this new origin this plane is parallel to x parallel to z and has y intercept minus 1. So, the intercepts are my infinity minus 1 infinity. So, on taking reciprocal it becomes 0 minus 1 0.

So, the Miller indices of that particular plane is 0 minus 1 0; what do we see these two planes are parallel planes they have been the same, but the sign opposite. Now let us see a situation where we are trying to draw a plane which intercepts at half on both all the 3 x, y and z. So, the intercepts are half half half so, the reciprocals are 2 2 2 nothing to clear so, that particular plane should be designated as 2 2 2 plane.

Now if you remember the plane which was like this combining connecting the 3 diagonals 3 3 corners that plane we designated as 1 1 1, you see now the 1 1 1 and 2 2 2 are set of parallel planes and, but they are different the plane 2 2 2 covers a smaller area inside the unit cell compared to the area covered by 1 1 1 plane.

So, now on the third box here, I would like to draw a plane like this the intercept here is half so; that means, along x, y and z, we have this plane which is parallel to x axis; that means, x intercept is infinity along y it has intercept half along z, it means z at 1 unit away from the origin so, z is 1. So, now, take reciprocal so, it becomes 0 2 1 which means the Miller indices for that would be nothing, but 0 2 1.

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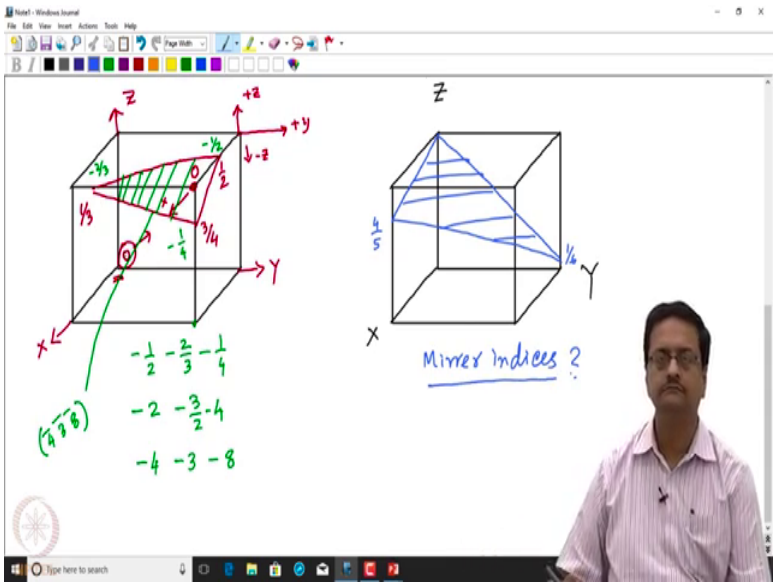

Now, let us see a different situation; suppose, we want to identify the Miller indices of this particular plane, this has intercept one-third with respect to that origin this intercept here is half and here this intercept is three-fourth. So, now, with respect to the origin located here it is difficult to find out where this plane would go and meet x, y and z and also this origin is not said sitting on this particular plane.

But still we can move the origin to a suitable position such that we can easily determine the intercepts. So, what we you do is we move this origin from here to the other body diagonal point which is here, then we move write it as any origin. So, with respect to that this is the plus x, this is the plus y anything above this plus z and anything below is minus z. So, now, with respect to this new origin what are the intercepts the intercept along x along this direction which is here is minus half with respect to the origin.

On y; earlier it was plus one third from that origin now this origin, this becomes minus 2 third and the z intercept which was three-fourth with respect to dot already means it is measured from the bottom most position here to that point there. So, this was three-fourth; that means now it has become one-fourth with the negative sign because it is downwards.

So, the new intercepts with the new origin are minus half minus two-third and minus one-fourth. So, now, we would like to clear the fractions. So, when we try to clear up the fractions. So, first we need to do take the reciprocals. So, when we take the reciprocal it becomes 2 minus 3 by 2 and 4. So, now, we need to clear the fractions. So, when we try to clear the fractions, we multiply by 2. So, it is minus 4 minus 3 minus 8.

So, the Miller indices for that particular plane become 4 bar 3 bar 8 bar. Now I would like to give a homework for you to do and come back in the next class and we will see how this can be solved. So, in this particular cube that I have drawn here x, y and z as usual, I am drawing a plane which is having an intercept on z axis here as 4 by 5 and it has again an intercept on z axis at 1 by 6th and this is the plane what would be the Miller indices for that plane is an assignment for you.