An Introduction to Materials: Nature and Properties
(Part 1: Structure of Materials)
Prof. Ashish Garg
Department of Materials Science and Engineering
Indian Institute of Technology, Kanpur

Lecture – 12
Miller Indices (contd)

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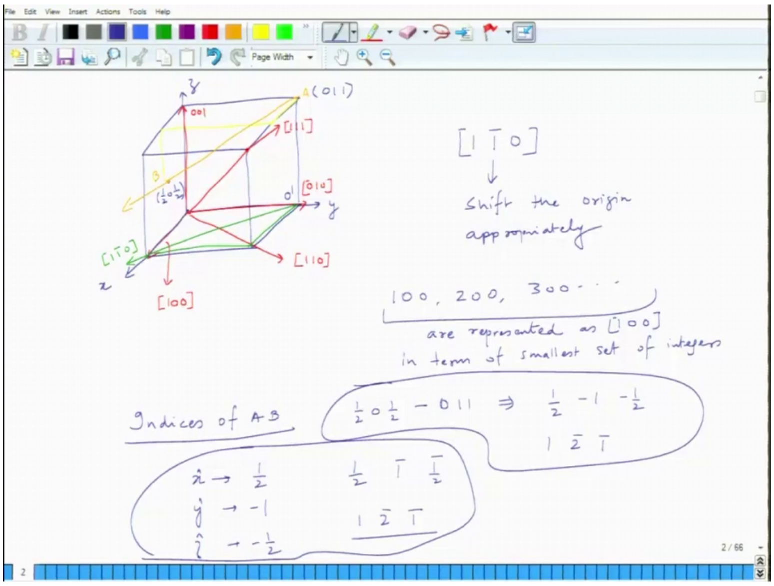

Ok; so in the last class last lecture we talked about we introduced, we finished off the planes family of planes in different systems and how the inter planer spacing is we will move on to hexagonal system. So, in case of cube you can see here now I just consider it as a unit cell; we will come back to cube and distinction with other systems a little later.

So, you can see that in this system if this is x, y and z this direction is depicted as what would this direction be if I take this as origin? This would be this direction would be?

Student: 1 0 0.

1 0 0 because you have intercept of 1 along 1; so, this is 1 0 0. So, this is 1 0 0 this is?

Student: 0 1.

0 1 0 and this is?

Student: (Refer Time: 01:27).

0 0 1; what is this direction?

Student: (Refer Time: 01:32).

Passing between these two this is?

Student: 1 1.

1 1 1 because it is one of this; one of that and one of that if you consider this direction.

Student: 1 (Refer Time: 01:47).

1 1 0 now in direction also you have a concept of negative; so, just like you have. So, let us say if I want to draw 1 bar 1 0 and again I need to shift the origin, shift the origin appropriately. So, I can see that my one translation along y axis requires me to shift the origin in such a fashion. So, that I am able to move along negative y axis.

So, I can now put my origin here. So, this is my new origin o prime and if I go. So, if I I need to go one along x which is this and one along minus y and if I connect these two points this would be?

Student: (Refer Time: 02:49).

1 1 bar 0 and in direction you can see that you know 1 0 0, 2 0 0, 3 0 0 all are same directions. So, in case of directions in case of planes we write 2 0 0 plane, 3 0 0 plane because they have different spacing. In case of directions when it is 3 0 0 direction, 4 0 0 direction you do not write it is 4 0 0 direction, you write it as 1 0 0 direction because it is a vector.

So, they are all represented as 1 0 0; basically smallest set of integer, in terms of smallest set of integers alright. So, I will just do one more example and before I; so, let me now draw one direction for. So, let us say this is A B direction what is the indices of A B direction? I mean one thing of course, is that you can do, you can determine the indices of you can determine the; this point this point is nothing, but?

Student: (Refer Time: 04:43).

Coordinates of this point are 0 1 1 right coordinates of this point are 0 1 1

Student: With respect to origin (Refer Time: 04:57).

This origin I mean this when you work out the coordinates of a point you always work out with respect to the main origin which is the this common origin this is o. So, this is 0 0 0 1 1 and what is the origin of this point?

Student: (Refer Time: 05:16).

This point; the one in the center this is half of x and half of z; so, this is half 0 half. So, one way to determine the direction is this is half 0 half minus 0 1 1. So, what do you get at the end?

Student: Half.

So, basically half minus 1, minus half; so, this is nothing, but 1 bar 2.

Student: Bar 1.

Bar 1 another way to determine is you just move along the xy directions. So, I can see that I need to go if I take this as a half of x in negative x direction in positive x direction. So, I have moved x intercept as half.

Now, I go along y. So, along y I have moved minus 1 and then along z I have gone I have gone.

Student: Minus.

Minus.

Student: Half.

Half; So, my u v w my direction is half minus 1 and if I multiply this by 2 it will be 1 bar 2 I get the same answer right. So, we can do it by this fashion, you can do it in this fashion both are fine. So, this is how you determine the indices of any direction which is nothing, but a vector alright.

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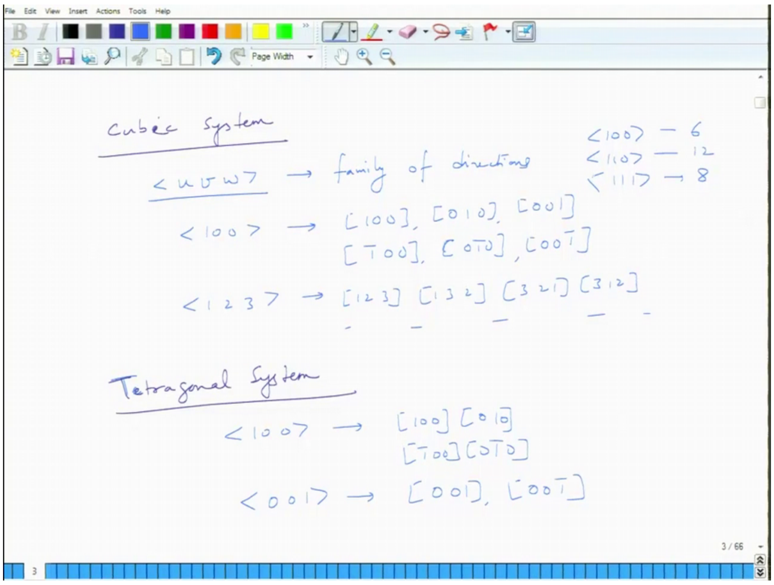

So, again for a cube for cubic system u v w means family of direction right. So, 1 0 0 would mean 1 0 0, 0 1 0.

Student: 0 0.

0 0 1 and bar 1 0 0.

Student: 0 bar.

0 bar 1 0 1 and.

Student: 0 (Refer Time: 00:00).

Taking that negatives into account.

Similarly, for you can say a lot let us say for 1 2 3 direction you can have multiple possibilities for 1 2 3 you can have 1 2 3 you can have 1 3 2, you can have 3 2 1, you can have 3 1 2 and so on and so, forth, you can keep writing the possibilities and you will reach 48 possibilities alright.

So, similarly to and in tetragonal system again; tetragonal again you have. So, 1 0 0 in tetragonal will mean only 1 0 0, 0 1 0, bar 1 0 0 and 0 bar 1 0 and 0 0 1 would mean 0 0 1 and 0 0 bar 1 because these two are because the translation along those two is different right. So, they are two different vectors.

So, this is the difference between tetragonal and orthorhombic. So, again you can work out the multiplicities by yourself. So, for example, for cubic system your 1 0 0 will have a multiplicity of 6, your 1 1 0 will have a multiplicity of 12 your 1 1 1 will have a multiplicity of 8. So, that is how you draw various directions. So, direction is simpler as compared to plane in the sense of understanding it.

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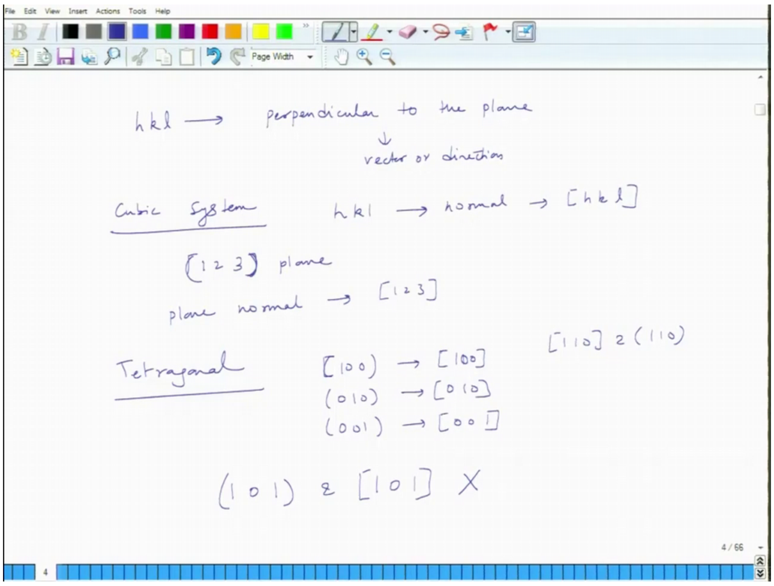

Now, there is a special case which is of well I will before I go to hexagonal system another thing that I want to draw to your attention towards says that in some systems we take. So, when we want to let us say we have a plane h k l the perpendicular to the plane that is a vector right all direction right. So, for cubic system in general h k l plane normal is direction h k l.

So, if you have a plane 1 2 3 sorry. So, 1 2 3 plane normal will be also 1 2 3 ok. So, this is specifically for cubic system it applies to all the h k l planes alright in case of other systems it may apply to certain planes it may not apply to certain planes. For example, in case of tetragonal you can see that 1 0 0 plane and 1 0 0 direction 1 0 0 direction they are perpendicular.

Student: (Refer Time: 11:35).

So they are fine 0 1 0 and.

Student: 0 1 0.

0 1 0 they are fine 0 0 1 and 0 0 1 they are fine alright 1 1 0 and 1 1 0 they are fine, but 1 0 1 and 1 1 0 sorry they are not fine.

Student: Even correction 1 0 1 1.

Even 1 0 1; So, now, so, if you look if you look at 1 sorry that is what I wanted to write actually whatever what did I write. So, 1 0 1 and they are not. So, when you mix h h and l k and l when you mix h k with l, then this normality condition does not hold true which means the plane normal does not have same Miller indices as the plane.

Student: (Refer Time: 12:54).

Plane normal the Miller indices of the plane normal are not same as that of a plane when you go to tetragonal or orthorhombic or other systems especially when you mix up the Miller indices with the Miller indices, corresponding to that dissimilar axis.

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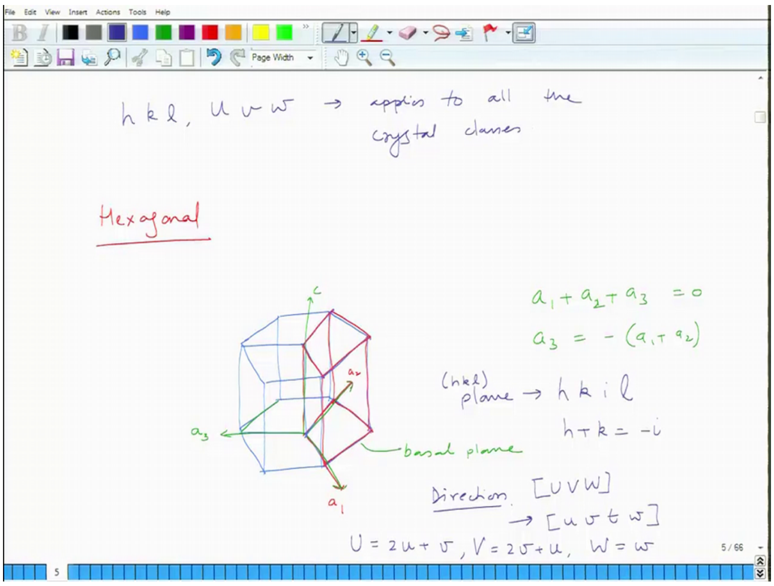

Now, what we will do is that we will move on. So, in case of bar; so, we have taken a three axis system this three h k l u v w sorry u v w system applies to all the crystal systems; applies to this notation applies to all the crystal classes. In case of a hexagonal system we have we can also evolve a new system which in case of hexagonal the hexagonal also follows this system.

But in case of hexagonal because of the because of the geometry of hexagonal system; So, hexagonal system is something like is draw how well I can draw this is my hexagonal system and this is the. So, this is the first one this is the second one, this is the third one oops.

Now, since hexagonal system is not it can be represented not only by this individual unit cell which is here. So, this is the individual unit cell it is not drawn very nicely, but I hope you can see what I am meaning here. So, this is the one third of hexagonal unit cell which is a single unit cell; now this single unit cell can be represented very well by a small unit cell off by 3 axis system by h k l and u v w.

However, what we can do here is the following if I take this as an axis a 1 and this is an axis a 2 then there is a third axis in this direction which is. So, this is a 1 this is a 2 there is this third axis which is called as a 3. So, this can be and of course, the fourth axis remains this one.

So, the h k l plane in this case if I take this four axis systems a 1, a 2, a 3 and c normally in hexagonal system we call this as a axis and c axis because a 1 and a 2 are equal and they are symmetric we call we call both of them as a axis and the perpendicular one is basal perpendicular to the basal plane is called as c axis. So, this plane the base is called as basal plane basal plane.

So, now we can see if it instead of taking this small unit cell as the hexagonal unit cell if we take the big unit cell which is the hexagonal cell as the unit cell then we can conveniently choose as four axis system where a 1, a 2, a 3 are three axis within the basal plane and c axis is the axis which is out of the basal plane. And you can see that by symmetry a 1 and a 2, a 3 three are related to each other.

So, you can see that a 3 will be nothing, but by vectors a 1 minus minus a 1 and minus. So, a 3 will be nothing, but you can see that a 1 plus a 2 plus a 3 is equal to 0 right because the they close each other.

So,; so, basically a three in some sense will be minus of a 1 plus a 2. So, we define a new system which is called as. So, instead of three axis h k l system we take h k i l where. So, this is plane where h plus k is equal to minus of i, but the direction if I have three plane system u v w, then that can be written as u v t w where one can prove it vectorially capital U is 2 small u plus small v capital V is 2 small v plus u and capital W is equal to a small w.

So, I am not going to get into derivation of this; this derivation you can find out in many texts its very simple vectorial derivation. So, you can see that u v w. So, the plane h k l can be represented as h k i l. So, plane h k l and three coordinate system can be represented as h k i l in the four coordinate system where h plus k is equal to minus i.

Direction capital U, capital V, capital W can be represented as small u, small v, small t, w where there is a correlation between all the u's and v's alright. So, this is one simple representation of hexagonal system.

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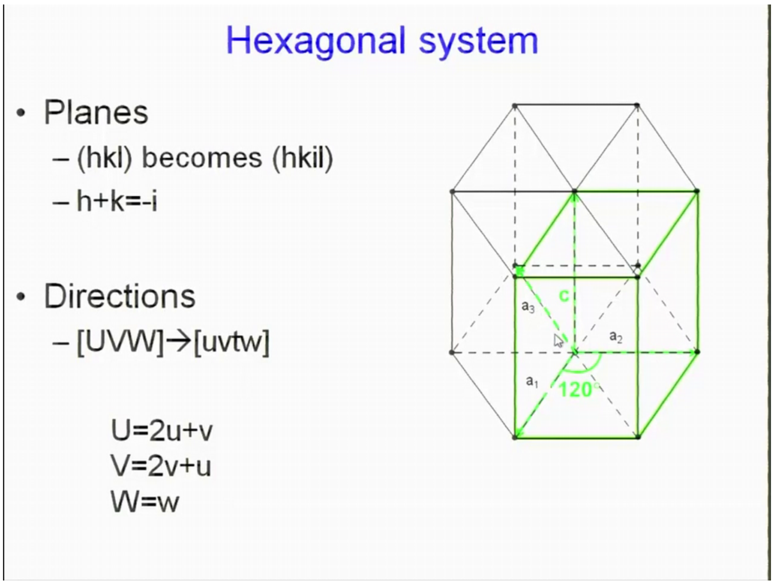

So, what I am going to do now is I am going to give you the knowledge of the system on the basis of some power point it is easier to draw there; l becomes h ki l and h plus k is equal to minus i and direction becomes u v w becomes u v t w these are the relation between small u and capital small u capital U and small v capital V and so, this is the conventional unit cell that we take and the black one the big one is the hexagonal unit cell that you take.

So, this is your axis a 1, this is your axis a 2, this third one is a 3.

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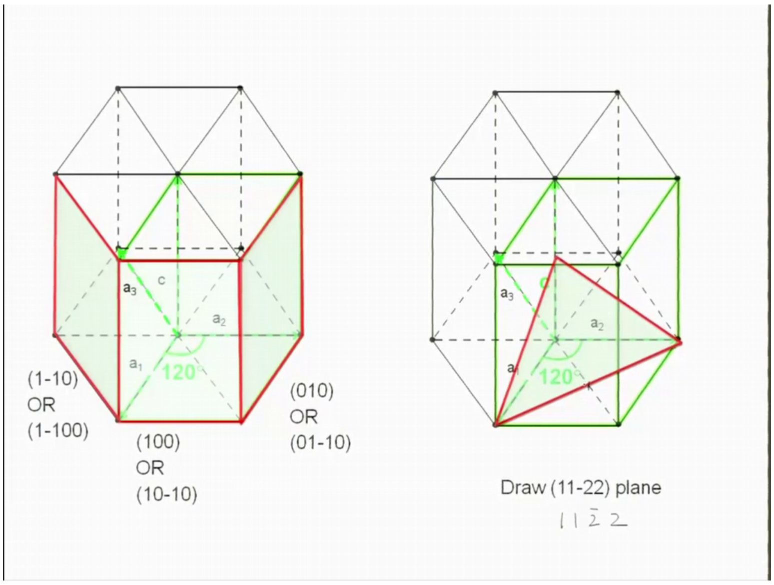

So, if I take these planes normally these planes normally if you took now remember there are two types of unit cells; one is the smaller set of unit cell one is the bigger unit cell. So, if I look at these unit cell these plane the planes marked in red the first one is 1 0 0 because it is parallel to a 2 axis right. So, it is in the three coordinate if I draw this cell as this will be three coordinate phase on the right will be.

So, this phase on the right will be 0 1 0 system you can see the mouse right. The problem is with this phase how do you phase this phase as this phase is also a phase of another unit cell which is adjacent. So, in some sense this is the phase which is just like 1 0 0 0 1 0 phase, but it can be represent, but basically this phase is parallel to this plane in the middle. And if it is this plane if it is parallel to this plane in the middle, this becomes 1 bar 1 0.

So, there is a discrepancy if you rotate the hexagon this the one on the left this 1 bar 1 0 will become 1 0 0. So, why is it that it is noted differently; it is denoted differently right. So, that is where four axis system helps four axis system will allow us to determine all of these planes in an identical fashion. Because now if I convert this into four axis system, this 1 0 0 will become h k i l. So, h and k will remain same i will become minus of h plus k and l will remain same. So, this will become 1 0 minus 1 or bar 1 0.

Similarly, this will become 0 1 bar 1 0 and if you now look at this what will this become? This will become 1 bar 1 0 0; so, now, they look fairly identical that you just juggle around with that h k i indices and l remains the same. So, basically they are same family of planes it is 1 bar 1 0 0; it is 1 0 bar 1 0, it is 0 1 bar 1 0.

So, they remain same family of planes in four coordinate system and they look like as if they are the same. They are the same family of planes, but in three coordinate system you end up having a indices which is which looks different which feels different in a hexagonal system that is why to make it easier for one to understand the four axis system is invented.

Similarly, now if you draw the for example, if you now want to draw this 1 1 bar 2 2 plane let us say I choose a indices 1 1 bar 2 2 ok. So, this is it is not. So, this is 1 1 bar 2 2 plane. So, how do you draw this plane? This is your 1 1 bar 2 2 plane. So, you have one intercept on a 1 1 intercept on?

Student: a.

1 intercept on?

Student: a 2.

a 2; half intercept on? c the other one is automatic because h plus k is equal to i.

Student: (Refer Time: 23:30).

h plus a is equal minus i. So, that becomes automatic; so, if you look at this it will intercept through half of this length in the opposite direction, this is a three axis and you are intersecting at this point which is half of minus a 3.

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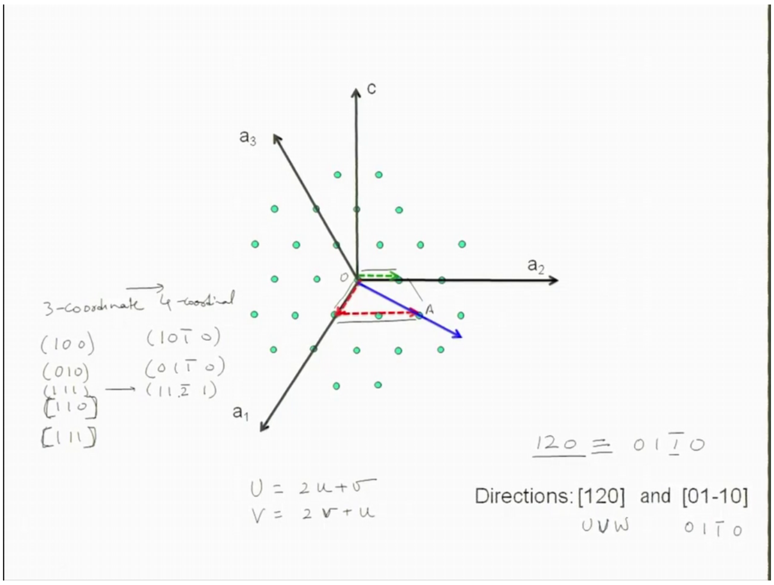

Now, let us let us look at this problem in a slightly different manner. So, you know how to draw the plane now for drawing the planes it is easier to follow the same convention; it is just that the third will be drawn automatically. If you wanted to draw for example, 1 bar 1 0 0; so, you wanted to draw 1 0 bar 1 0, you have one intercept along this direction, one intercept along minus this direction and the other ones are parallel. So, this is parallel to a 2 axis and c 2 axis c axis. So, this is 1 0 bar 1; it only has intercept along a 1 and minus a 3 axis nothing else.

So, now let us try to draw the direction. So, in this case let us say I want to draw a direction 120 this is a hexagonal basal plane and I am drawing 1 2 0; 120 is simple I go one along a 1 axis and two along a 2 axis and then join with the origin. So, that is what I will do 1 1 sorry 2; this will be 120 vector.

Now, what will I do if I want to draw in four coordinate system; in four coordinate. Now if I want to draw one bar 1 1 0 plane this is 1 0 1 bar 1 0 plane one along a 2. So, if this is a direction 0 1 bar 1 0 direction. So, this direction will be; so, 120 can be converted into.

Student: 0 1.

0 1 bar 1 0 because you know that capital U is equal to.

Student: 2 u.

2 u plus v capital V is equal to.

Student: 2 v (Refer Time: 25:37).

2; 2 v plus.

Student: u.

u; so, since So, these are capital U, capital V and capital W you can determine small u, small v, small w which will come out to be 0 1 bar 1 0. So, to draw this direction you can see you are at this origin; you go one along a 2 minus 1 along a 3 and you will end up at the same point right.

So, whether you follow a two axis system, whether you follow a three axis system you end up with the same direction if you end up with a different direction; that means, something is wrong is that clear to you?

Student: Sir if you not (Refer Time: 26:19) a 1 (Refer Time: 26:20).

I have converted it. So, 1 to 0 is equivalent to 0 1 bar 1 0. So, in the first case this is 120; 1 along a 1 2 along a 2. So, I move from o to a in the second case I convert this into four axis system. So, now, this becomes 120 becomes 0 1 bar 1 0.

So, I do not have to go along a 1 now; I have to go 1 along a 2. So, I go 1 along a 2 I go 1 minus 1 along a 3. So, minus 1 is this is a 3; so, this is opposite direction. So, this is minus 1 along a 3 I end up at the same point I should end up at the same point, if I do not at that end up at the same point which means there is some problem the conversion alright.

So, this is how you draw the direction in four coordinate system in hexagonal ok; So, in the previous case I showed you how you draw the plane the four coordinate four following the four coordinate plane and in the three and in the in this slide I showed you how to draw the direction in three coordinate and four coordinate system ok.

So, this is a distinction between you can do the exercise. So, the home exercise would be for you which you can for which you can do for example, you can try drawing 1 0 0 plane 0 1 0 plane; this is in three coordinate system 1 1 0 direction. Let us say 1 1 one direction sorry directions 1 1 1 directions; this is three coordinate system.

And in four coordinate system, then you convert these into four coordinate convert these into four coordinate system. So, this 1 0 will become 1 0 bar 1 0 this will become 0 1 bar 1 0 you can choose another plane let us say I take a plane 1 1 1; 1 1 1 will become 1 1 bar 2 1 plane.

So, try doing these conversions and drawing these directions and planes in three and four coordinate system at home this will make it clear. Follow the same routine which I have told you in this lecture alright. So, we finish it here.

So, we can we have seen that you know you can you can describe the unit cells with the use of Miller indices and planes and directions are nothing, but vectors and which can be drawn very easily and determined very easily in hexagonal system because of the symmetry of the unit cell.

If you want to represent the unit cell in hexagonal form, you can conveniently choose a system which is you can choose conveniently choose a notation system which is easier to comprehend for a hexagonal system than for a normal unit cell.

So, I can take up little bit more some more problems in the next class on hexagonal system to make it little bit more clear.

Thank you.