An Introduction to Materials: Nature and Properties
(Part 1: Structure of Materials)
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Lecture - 13
Miller Indices Weiss Zone Law

So, this is this is lecture 13 we will continue on hexagonal lattices a little bit followed by Weiss zone law and we would also see some effect of finally, we will see that although in a seemingly cubic lattice the directions may look similar, but symmetry may change that outcome completely. So, with that we will finish the miller indices part.

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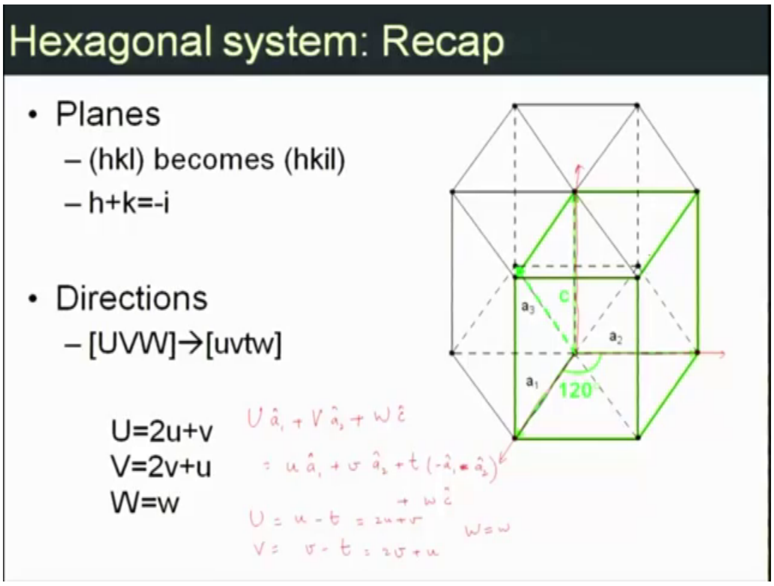

So, if I go to the next slide, so this is the recap of last lecture that we did. So, we have this hexagonal lattice and within this hexagonal lattice you have you have this green colored smaller unit cell which is the primitive unit cell of hexagonal unit cell and then you for the sake of representation you can represent it as a hexagon which consists of 3 of these unit cells.

So, in the normal unit cell you just need 3 axis so, a 1 a 2 and c these are the 3 axis you need this is first axis you choose, this is the second axis you choose and this is the third axis the one which is perpendicular to the basal plane. So, 3 axis system is fine for a smaller unit cell, but when it comes to hexagonal representation you see the problem arises because there are similar planes which are depicted in a different manner if you have if you continue with the 3 axis system.

So, for example, as I showed you last time that and before I go into that let me just tell you that hkl becomes hkil with the condition h plus k is equal to minus i and the direction capital U capital V capital W in 3 axis system becomes uvtw with the condition capital U plus is equal to 2 u plus v, capital V is equal to 2 v plus u and capital W is equal to w.

This is very simple to do you know you can just say capital U x hat plus capital V y hat plus capital W z hat or rather a hat. So, you can say this is a 1 hat a 2 hat and this is c hat, this can be represented as u a 1 hat plus v a 2 hat plus t, now what is t is along a 3 and a 3 is minus of a 1 hat plus sorry minus of a 2 hat plus wc hat.

Student: a 2 a 2 hat.

So, if we now do the matching of variables matching of a b components along a 1 a 2 and c axis. So, what you will get is so, you will get is capital U is equal to so, if you just see this will be capital U will be u and this will be minus of t, capital V will be equal to small v minus t and t is nothing, but minus of u minus of v. So, this will become 2 u plus v and this will become 2 v plus u and w will remain as w. So, this is a very simple equivalence that you can set and determine what is UVW relation.

So, and now what I was coming to is that so, in hexagonal system you have this plane.

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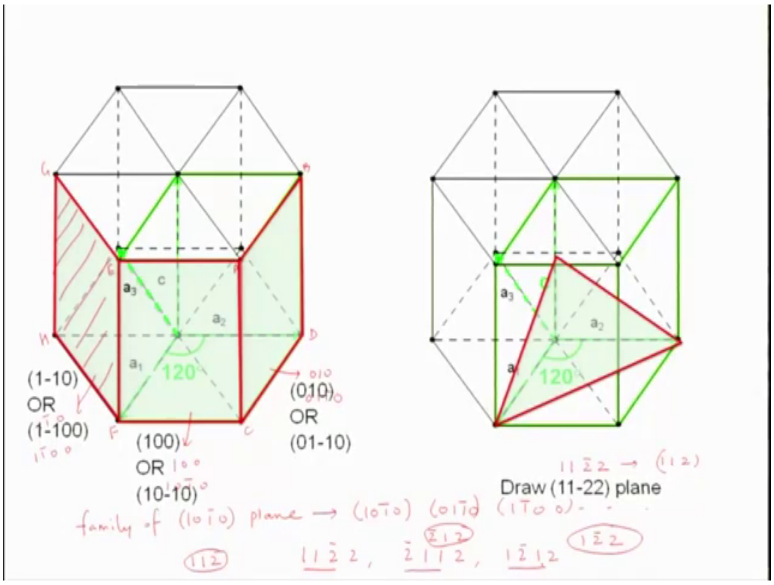

I think it is in the next slide so, you have this plane let us say A B C D and you have this another plane let us say E A C F these 2 are equivalent planes right. So, this plane is you can say it is 1 0 0, this plane is 0 1 0, but if you want to now depict this plane let us say this is G H. So, G E F H this plane if you go conventionally this plane is nothing, but the one which is diagonal and it is smaller unit cell. So, you will say this plane is.

Student: (Refer Time: 04:57).

Some sort of 1 1 0 type plane right because it has a intercept of it is.

Student: It is.

You will you will have to choose a different axis. So, this will be 1 minus 1 0 or minus 1 1 0, but in a 4 axis system. So, in a 3 axis system it will become 1 bar 1 0, but in the 4 axis system this will become 1 0 bar 1 0, this will become 0 1 bar 1 0 and this will become 1 bar 1 0 0.

So, now they look as if they are family of planes there are similar planes and they are. So, you can say that all of these are family of 1 0 bar 1 0 planes so, this will imply 1 0 bar 1 0, 0 1 bar 1 0, 1 bar 1 0 0 and so on and so forth. So, you will have 6 planes, all 6 planes of course, few of them are parallel to each other. So, you will just change that negative signs and so on and so forth. So, these are family of planes that is why this 4 axis representation is better. So, this is what I did show you.

Similarly, as I showed you can draw 1 1 bar 2 2 plane. So, this is 1 bar 1 1 this is nothing, but 1 bar 2 2 plane 1 1 bar 2 2 what is the equivalence basically it is 1 1 2 plane. Now if you draw all such planes let us say if you draw one from here to there, one from there to here they will they may end up with different species. So, if you if you just see 1 1 bar 2 2 this is first, the second 1 will become bar 2 1 1 2 and the third 1 will become 1 bar 2 1 2.

Now, try converting this in 3 axis system this will be 1 1 2, this will be bar 2 1 2 and this will be 1 bar 2 2. So, you can see that this is all right, but these 2 are different. So, it gives you an impression as if they are different planes because that is what we learnt in cubic system or tetragonal system 1 1 2 cubic system 1 1 2 is equivalent to 2 1 2 and, but here we see the planes which are identical in hexagonal system they look differently in 3 coordinate system. So, 1 2 1 bar 2 2, bar 2 1 2 and 1 1 2 they can be represented all by 1 1 bar 2 2, bar 2 1 1 2, 1 bar 2 1 2 and so on and so forth.

So, this is not only true about other this plane, but about that the planes as well I will show you few more examples similarly about the directions.

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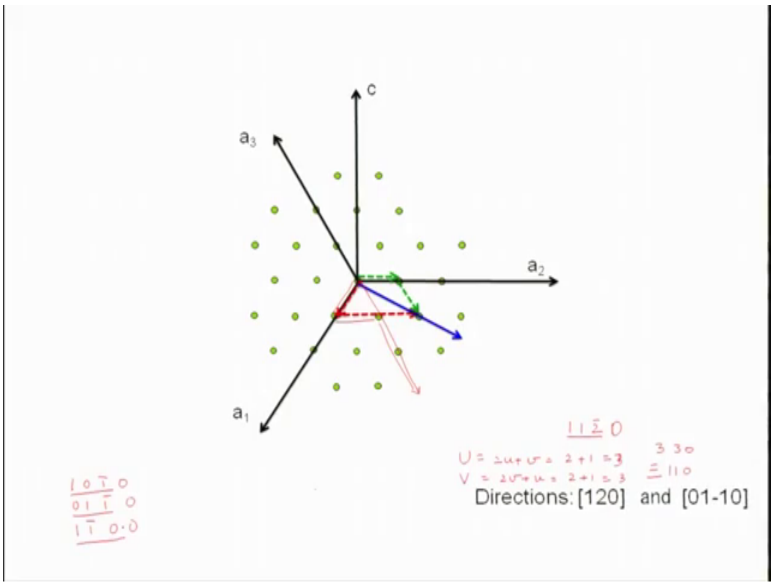

Now, this is a projection of a basal plane of hexagonal system. So, basically we are looking down the c axis and we are looking at a 1 a b plane. So, direction 1 2 0 as we know we can draw 1 2 0 will be 1 2 there is no in c no translation in c. So, this is the direction and the 3 coordinate system this will become 4 coordinate system it will become 0 1 bar 1 0. So, if we draw this now this will be 0 so, 0 there is nothing around a 1, there is 1 along a 2, there is minus 1 along a 3 and if you connect the financial point it is a same direction.

Now, this is again true of the directions so if you so, all the directions of the kind 1 0 bar 1 0, 0 1 bar 1 0, 1 bar 1 0 0 and so on and so forth all the directions will give you can see that what are these directions. So, one is this direction, another one would be that direction. So, if you connect this point if you connect for example, that point so on and so forth, is that clear how to draw the direction in hexagonal 4 axis system? Now let us say if you have I am just thinking of what to give you and you can choose a little difficult example to work on for example, how to draw 1 1 1 1 bar 2 1 direction for example,.

So, this has all the 3 coordinates.

Student: (Refer Time: 10:11) shift.

So, you shift the origin first of all and so, how will you draw that 1 1 bar 2 1. So, you go 1 in.

Student: a 1.

a 1, 1 in.

Student: a 2.

a 2 and then.

Student: Minus 2 in a 3.

Minus 2 in a 3 which means 1 sorry 1 and another 1 you will end up somewhere here and then you need to go 1 up. So, it will be 1 up in the C axis. So, then you connect this point with that point that will take you to.

Student: (Refer Time: 10:51)

Yeah so, as far as plane circuns so, the 4 axis system has more advantage in terms of planes the representation of planes is easier, in case of directions you can live with since direction is just a vector you can draw them with the 3 axis system within the same system, but if you draw a smaller you bigger unit cell hexagonal unit cell then 4 axis system helps.

So, 1 1 bar 2 0 will be you can convert this back to so, this will be basically 1 1 bar 2 0. So, this will be nothing, but if you if you look at the direction 1 1 0 1 1 0 direction is nothing, but 1 1 bar 2 0 direction 1 2 0 is 0 1 bar 1 0. So, you will have to make the conversions for example so you have to use the formulas which I provided you.

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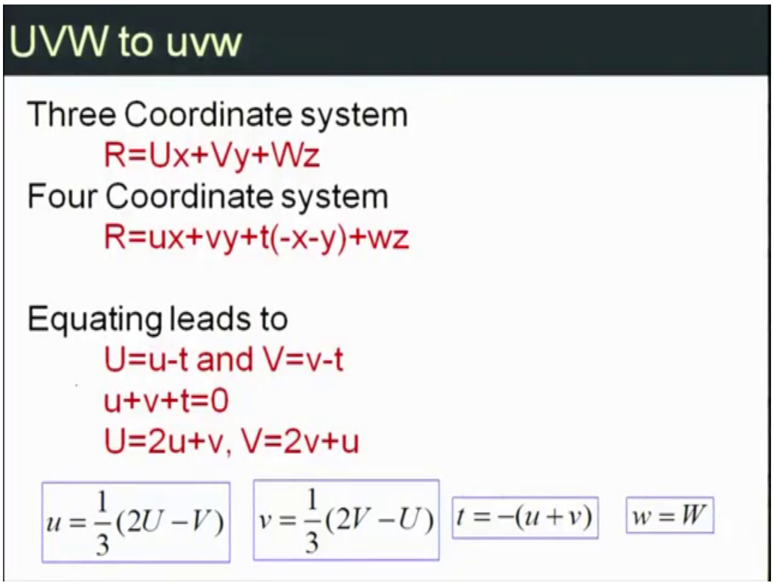

For using small u is basically one - third of 2 U minus V, small v is one - third of 2 V minus U, small t is minus of u plus v. So, you do you will need to these make these conversions. So, if you now convert back so, I said so, this is 1 1 bar 2 let us say 1 1 bar 2 0 what does 1 1 bar 2 0 convert into so, capital U was equal to 2 u minus v.

Student: v.

So, this will become 2 minus 1 1 Sorry 2 u plus v, 2 u plus v I am sorry yeah 2 u plus v. So, this will become 3, V is equal to 2 v plus u this will become again 2 plus 1 this is 3 and w is W. So, this direction will be 3 3 which is nothing, but 1 1 0. So, you could see that you go one step here, one step there, 2 step in this direction which is nothing, but the same vector 1 1 0.

So, this is how you can make the conversion between the directions as well of course, if you draw it along the third axis it will become even complicated, but you can do these exercises at home, is that clear 3 and 4 axis system.

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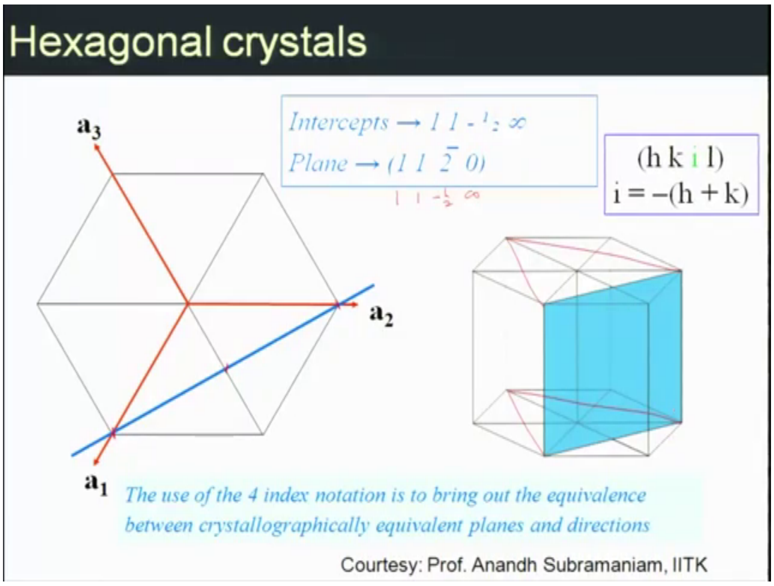

So, now I will give you some more examples of hexagonal crystals you have. So, this is courtesy professor Anandh Subramaniam he has made very nice slides on these crystallography. So, this is about as I said 1 1 bar 2 0 plane. So, 1 1 bar 2 0 plane is nothing, but 1 along x, 1 along a 1, 1 along a 2 and away and by default the third intercept which is minus 2 which is actually half right the intercept will be 1 1 as he has written minus half and infinity all right.

So, it has a one intercept here, one intercept there, minus half intercept along a 3 and nothing along it is parallel to 3 axis. So, you can see that this is the plane. So, in 3 D the plane will plane is going to look like that. So, all the planes so, this is one kind of plane, this is another kind of plane and you will have which is the other one and the equivalence at the bottom this will be another plane. So, these are all identical plane 1 1 bar 2 0 bar 2 1 1 0 1 bar 2 1 0 and so on and so forth.

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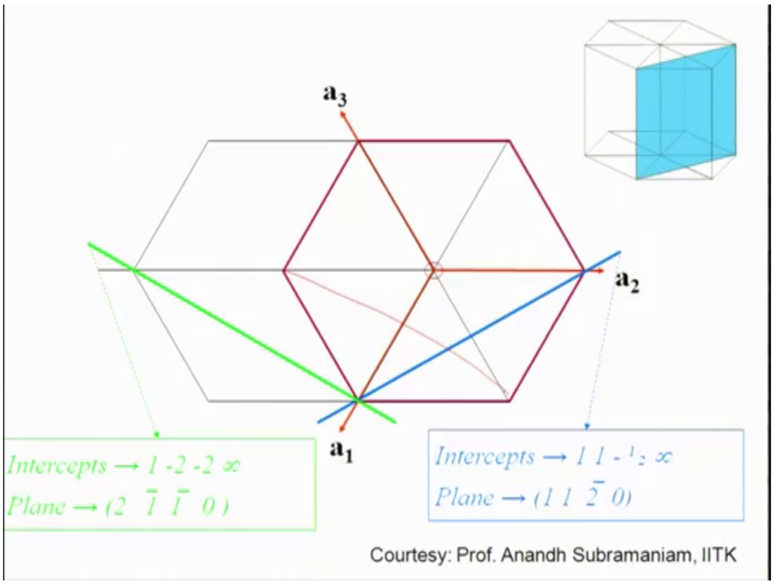

So, now this is the one I showed you 1 0 0 plane example. So, these planes are identical this plane, this plane, that plane, they are identical they look differently in 3 and it is a system, but they look same in 4 indices system this is another example of plane which is 2 bar 1 bar 1 0. So, 2 bar 1 bar 1 0 looks something like remember you should always ensure in all these the sum of the indices is equal to 0.

So, 1 1 bar 2 0 sum of these 3 is 0, sum of these 3 is 0, sum of these 3 is 0, sum of these 3 is 0 that equivalence must be maintained if that equivalence is not maintained that then something is wrong somewhere here also we wrote this equivalence, this equivalence, this sum so, all the sums must be equal to hki and uvt, these sums must be equal to 0.

So, it is obvious, but you might make a mistake so just remember that. So, this is your, this is other plane that you drawn 2 bar 1 bar 1 0 this is 1 1 bar 2 0 you can. So, similar planes you can draw here and this plane is nothing, but parallel to this plane right one which is here.

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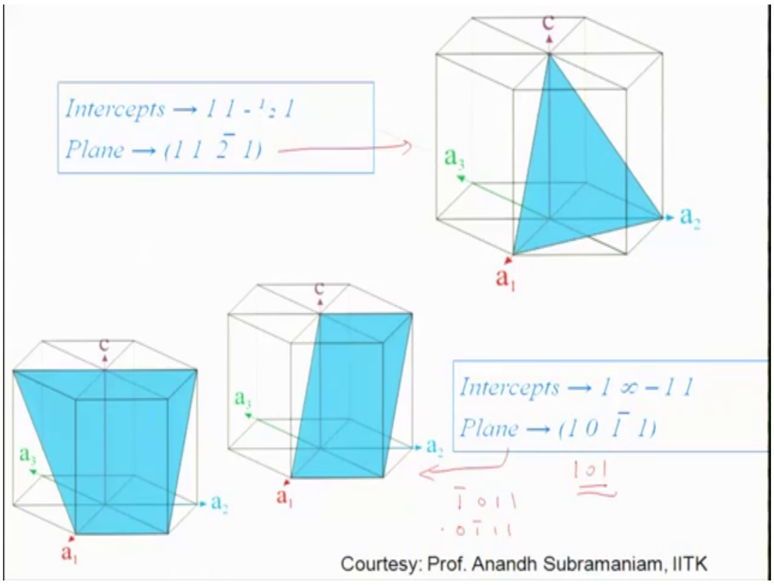

This is 1 1 bar 2 1 it will look like that the 1 on top 1 1 bar 2 1 and the 1 on the bottom is 1 0 bar 1 1 which is parallel to a 2 axis. So, basically this plane is nothing, but 1 0 1 plane, but in 4 d in 4 4 axis system it looks 1 0 bar 1 1. So, 1 0 bar 1 1, bar 1 0 1 1, 0 bar 1 1 1 they are all similar planes.

So, this is about the planes and directions in various crystal systems you have seen how we can draw the plane, how we can draw a direction, how we can identify a plane, how we can identify a direction and we have also seen an cubic system that direction lies perpendicular to the plane direction is. So, hkl direction is perpendicular to hkl plane, but that is only true of cubic system in tetragonal orthorhombic it is only true for abc axis or 0 1 0 1 0 0 and 1 1 0 direction in tetragonal it is also true for 1 1 0, but not true for 1 0 1.

So, it is only true for certain directions in these systems depending upon the indices in orthogonal system you still have some cases where perpendicularity is maintained, but in not non orthogonal systems it is not maintained at all. So, in a hexagonal system for example, 0 0 1 direction is parallel is perpendicular to 0 0 1 plane, but that is the only direction which is perpendicular to 0 0 1 plane. So, this relation is true only for cubic system for hexagonal tetragonal and orthorhombic it depends upon which direction in which plane you talking about.

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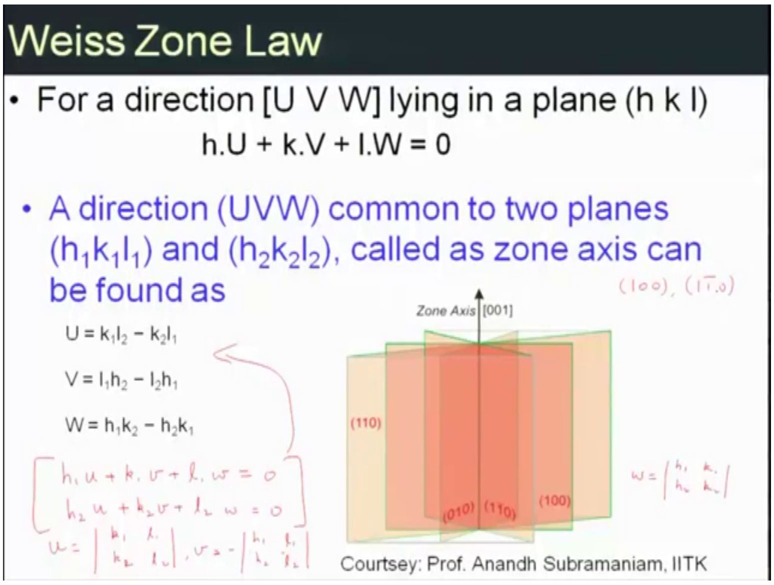

And other crystallographic thing that you need to know is that Weiss zone law, Weiss zone law is basically it is a very useful law especially for plaster deformation any phenomena that happens within the crystallographic planes where you need to know the an isotropy in the phenomena and you need to find out which direction lies common to certain planes.

So, this law says that for a direction U V W lying in a plane h k l the product of that the dot product of the 2 h dot U plus k dot V plus l dot W is equal to 0 so, this is called as Weiss zone law. So, basically what it means is that if you have multiple planes right all these multiple planes they intersect each other and there is a common direction to these planes this common direction is called a zone axis. This is of very much importance especially in transmission electron microscopy when you do that diffraction patterns.

In diffraction patterns what you will do is that when the electron hits the material along a certain axis that may be a certain crystallographic direction. So, all the planes which are containing that direction may be represented on the diffraction pattern. So, sometimes they may be diffraction patterns spots from a few planes and you need to identify, but using the Weiss zone law you can identify which other spots from one particular plane, which other spots from another particular plane because they must have a common zone axis.

So, this is of importance in transmission electron microscopy quite a bit. So, if you have a direction U V W which is common to 2 planes h 1 k 1 l 1 and h 2 k 2 l 2 this is called as a zone axis and it can be found as U is equal to so, basically you write 2 equations h 1 U plus k 1 V plus l 1 W equal to 0 and h 2 U plus k 2 V plus l 2 W because it is a common axis as a result it is common to both the planes.

So, you can write these 2 equations and these 2 equations can be solved in this fashion right. So, U will be equal to basically you can write U to be equal to k 1 k 2 l 1 l 2 and so on and so forth, you can write an expression for V you can write an expression for W in the matrix form and this will give you basically. So, U is equal to this V will be equal to minus of.

Student: h 1 h 2 (Refer Time: 20:42).

h 1 h 2.

Student: l 1 l 1.

l 1 and.

Student: l 2.

l 2 similarly W will be equal to.

Student: h 1 h 2.

H 1 h 2.

Student: k 1 k 2.

k 1 k 2 and you can see that U is equal to k 1 l 2 minus k 2 l 1 V is equal to.

Student: minus (Refer Time: 21:07).

Minus of h 1 l 2 minus l 2 h 1 so, it will become l 1 h 2 minus l 2 h 1 and W is equal to h 1 k 2 minus k 2 h 1. So, that is how you can find the common axis between the 2 planes you can see here in this case you have let us say 2 planes 1 plane is 0 1 0 another plane is bar 1 1 bar 1 0.

So, you have a plane 1 0 0 and you have a plane 1 bar 1 0 I will go to the next slide probably that is that will make it little easier.

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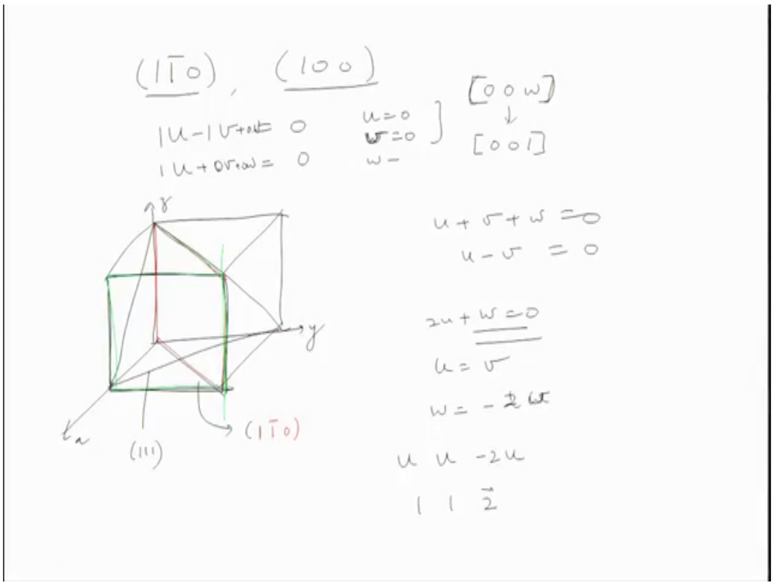

You have a plane 1 bar 1 0 and you have a plane 1 0 0. So, for the first case it will become u minus v is equal to 0, for the second case it will become u is equal to 0. So, what you get here is. So, let me just now draw a cube here I think that is better I think is some mistake there. So, you take this is x y and z let us say you have a plane which is so; obviously, from the examples you can also see what works and what does not work.

So, this plane is 1 1 1 plane right, what is this plane, if I choose this as a origin this is a intercept of 1 along x, intercept of minus 1 along y. So, this becomes 1 1 bar 0. So, now if you have a, you can see that these 2 intersect each other right. So, if they intersect each other in that case in the first one also it is a u minus v plus. So, 1 minus 1 v plus 0 w is equal to 0 and the second one will become 1 u plus 0 v plus 0 w is equal to 0.

So, in this case you can see that your u is equal to 0 and w is equal to 0, which means z u v sorry v is equal to 0 and u is equal to 0 which means your w is undefined you have not defined w over here. So, the direct direction which is parallel to these 2 planes which these 2 plane contain is 0 0 w, 0 0 w direction will mean 0 0 1 direction.

So, both the planes will have 0 0 1 direction common you can see that here, this is 1 0 0 plane, this is 1 0 0 plane the plane which is drawn in red is. So, this is 1 0 0 plane this is

1 bar 1 0 plane the one which is drawn in red you can see this is the common direction this one and this direction is 0 0 1 direction.

But the second case it is one you have 1 1 1 so, u plus v plus w is equal to 0 and the first if this is becomes u minus v is equal to 0 you can see that you are in this case w is equal to 0 sorry 2 u plus 2 u plus w is equal to 0 and u is equal to v. So, you can see that w is equal to minus of 2 u. So, the direction would be u u minus 2 u. So, this is 1 1 bar 2 direction. So, this is how you can find the common directions.

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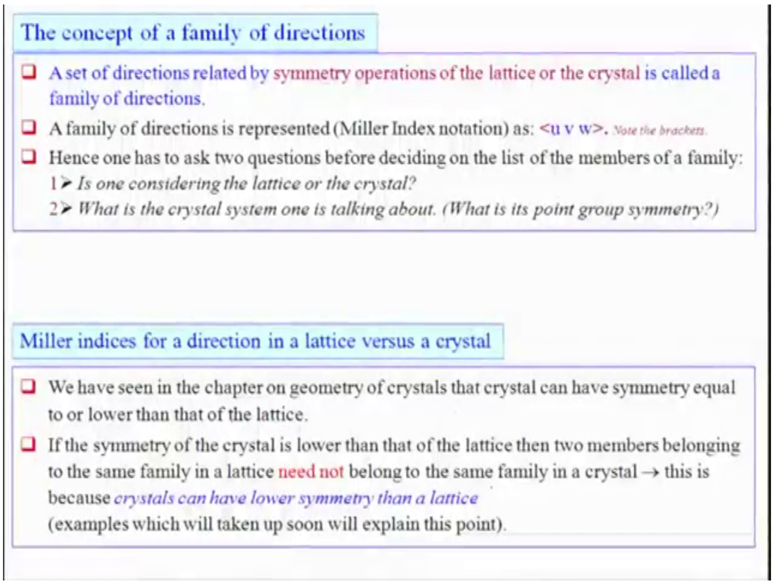

Now, let me finally come to another point which is based on symmetry that the set of direction is always related by symmetry. So, I will skip this slide I will just go to the next slide.

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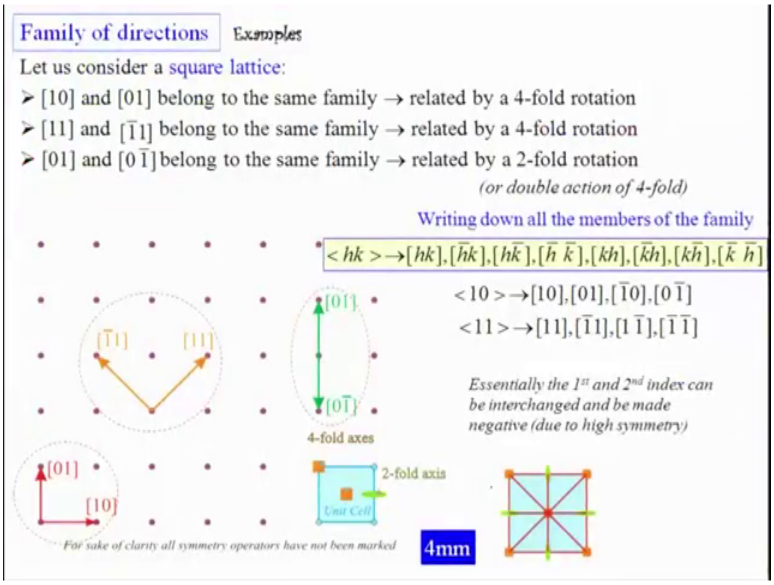

So, this is again courtesy professor Anandh Subramaniam so, here you have a grid of points right you can see that in this case if there is a 4 fold rotation within the plane then 1 0 0 1 direction is equal equivalent 1 1 and bar 1 1 directions are equivalent.

So, you can if you rotate it by fourfold you will get back to same configuration. So, this can be rotated by 90 degree this can be rotated by 90 degree because there is a 4 fold similarly 0 1 is equivalent to 0 bar 1 because there is a twofold axis which is present.

Now, this is about the when the motive is a simple single atom.

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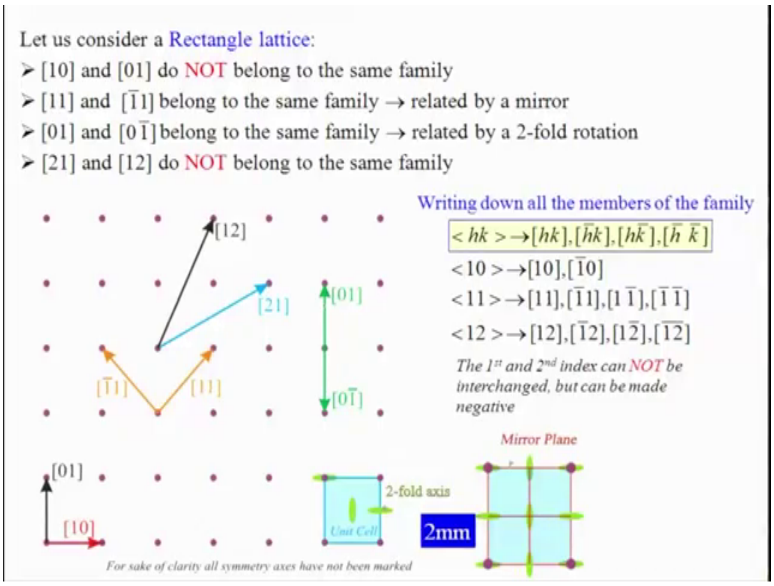

Let us say if the motif becomes slightly different if you do not have let us say in this case this is a rectangular lattice, if it is a rectangular lattice then we do not have a 4 fold there this is what becomes a tetragonal system right in tetragonal system you have only 1 4 fold others are 2 fold.

So, 1 0 0 is equivalent to 0 1 0, but it is not equivalent to 0 0 1. So, this is what is going to happen here in this case 1 0 is not equivalent to 0 1 in the rectangular lattice is that clear and similarly you can see what are the other families of directions.

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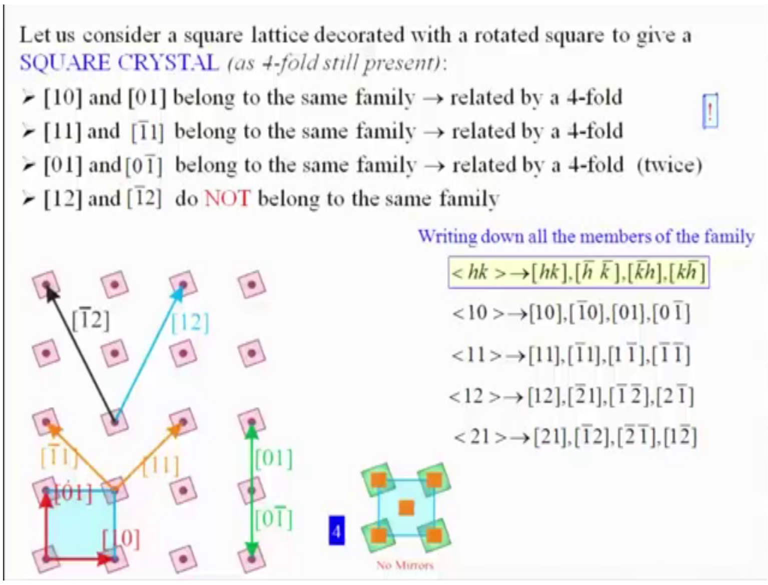

If we change the motif you have a 4 fold, but again there are no mirrors, if there are no mirrors then the two directions which could be equivalent because of a mirror they will not be same.

So, for example, 1 2 and bar 1 2 do not belong to the same family 1 2 and bar 1 2 do not belong to the same family because there is no mirror. The symmetry changes the classification of direction quite dramatically.

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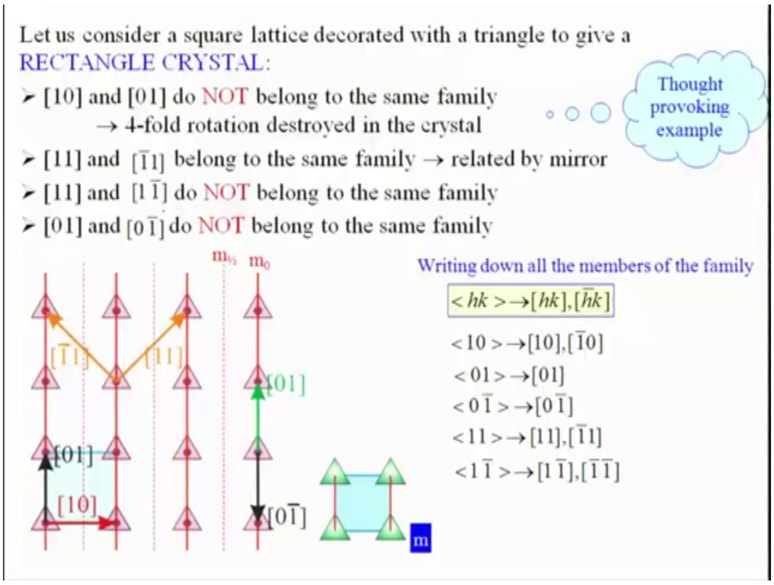

So, this is again an example where which directions are equivalent and which directions are not equivalent it depends upon the type of motif. So, in a square motif if you have a different motif then also it changes, but in an non square lattice non square lattice with a simple motif again things change.

So, it depends upon the symmetry whether you have 4 fold present whether you have twofold present whether you have mirror present and not there is no mirror present. So, direction equivalence the family of direction the concept changes from system to system which is determined by symmetry.

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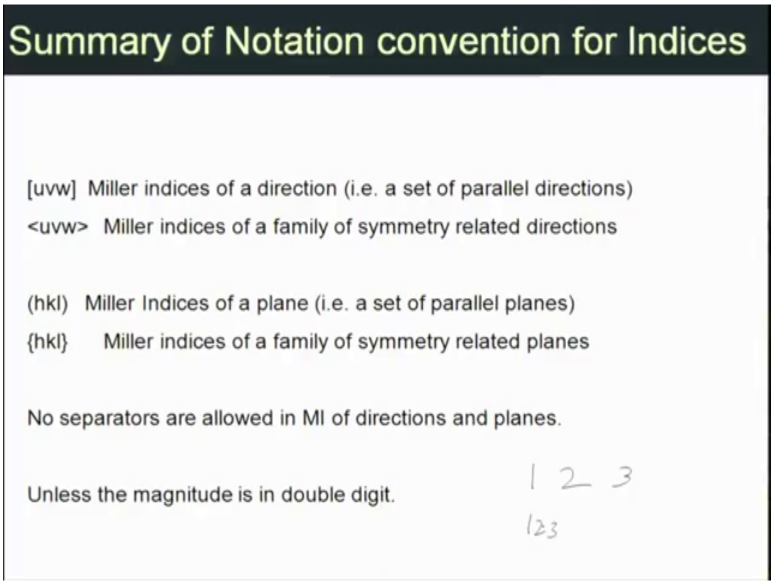

So, to summarize you we have learnt about the direction UVW which are Miller indices of a direction which is nothing, but a vector and UVW in a triangular bracket is Miller indices of a family of symmetry related directions. So, since cubic is the most symmetric system all of them happens to be of same type, but in tetragonal system they become different.

Similarly in hkl plane is a single plane, curl bracket hkl planes are family of symmetry related planes and we do not typically allow separators in the miller indices of directions and planes they are written together. So, you do not write them as 1 space 2 space 3 you write them 1 2 3 and unless of course, the magnitude is in double digit.

So, that is where we will finish this particular part, we now go to the next part which is structure of metals.