Electron Diffraction and Imaging
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Lecture – 23
Tutorial – 05
3-Index to 4-Index System

Welcome you all to this course on electron diffraction and imaging. In today's class, we will talk about how to index planes in a hexagonal system. Two important class most of the structural materials if we look at it either they have cubic crystal structures either BCC or a FCC structures or we have another class which is essentially hexagonal structures especially most of the zirconium based alloys or titanium based alloys. In crystallography when we try to represent the crystals we essentially use 3 index coordinate system.

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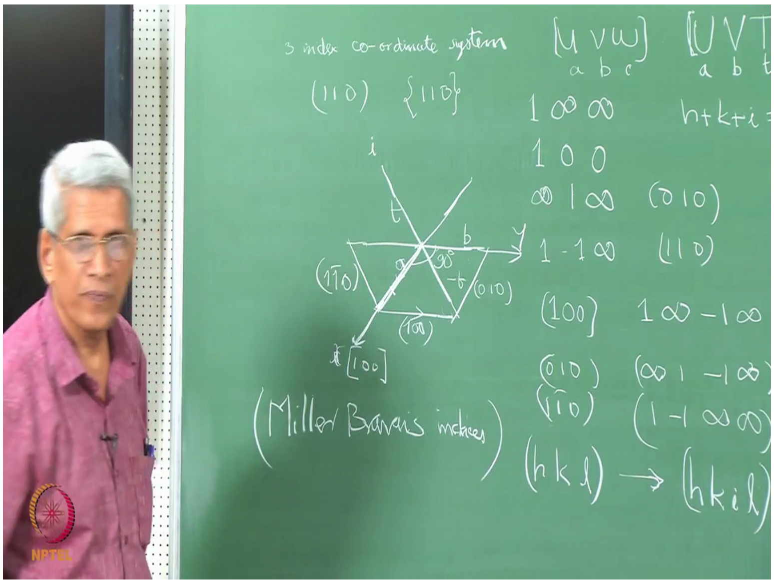

That is how we represent that crystal structure correct including all the 7 classes which are there including hexagonal crystals. Especially if we with respect to a structural materials cubic system or the other one which is zirconium or titanium based alloys or magnesium based there are lots of alloys systems are there which are essentially having a hexagonal crystal structures.

We use a 3 coordinate system to represent the crystal structure and the planes are represented using h k l, we know how to find out the planes, but what happens is that in such a system for cubic crystals when we represent a plane specific one as 1 1 0, if we represent a plane this is specific plane and if we represent the family of planes 1 1 0 with a curly brackets, this means that all the other planes are related by symmetric. But what happens in the case of a hexagonal system is that indices what it represents and the symmetry there is a disconnect this we can look at it if you look at this figure which is shown here.

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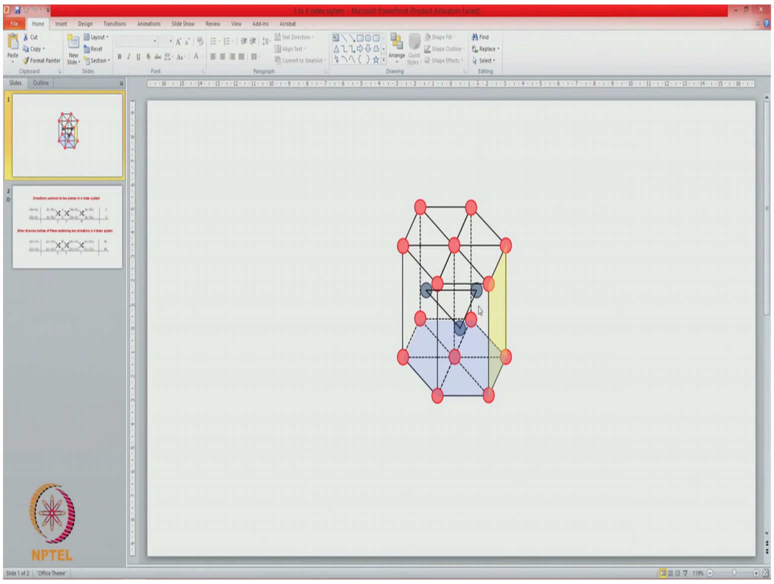

That is in a hexagonal lattice I will just show the base well plane alone, this is the x axis y axis and there is z axis normal to it.

The angle between this is 90 degree then this plane will be an 1 0 0 plane, correct, this plane is 0 1 0 plane, if we take this plane in this system this is going to be 1 1 bar 0 plane correct. How do you find out this planes? By first finding out take that plane find out what is the intercept which it makes with respect to the axis, take the inverse of it and then try to if it is fraction multiplied by numbers. So, that it is not in fraction and to move the common factor otherwise. So, that it that represents the indices of the plane for example, if we take the 1 0 0 plane, in the case of 3 index system this will turn out to be along the x axis intercept is one on the along the y it is infinity the intercept it makes infinity.

So, this will turn out to be 1 0 0, if we take that inverse of it I am taking it with an example because that is the easiest way to understand and then if it take with respect to 0 1 0 again it will become 0 no infinity then the one infinity for which it will turn out to be 0 1 0, correct. And here it will turn to be 1 minus 1 infinity which will turn out to be 1 1 0 this is the intercept this is what the this is we call it as a miller indices correct, but with respect to a hexagonal system all these planes are similar type of planes correct, but they do not have the same indices or not used to represent when we use 3 index system. So, it becomes quiet confusing how to overcome this that is what essentially it is for which what is done is that since in a hexagonal system there are along the Basel plane there are 3 symmetry axis are there we use with respect to all the 3 axis. So, x y and this we can call it as an I and this axis is going to be the z axis that way we can represent it.

If we represent it that way then now let us look at these planes the same methodology which we adopt in the case of a 3 index system to find out the miller indices.

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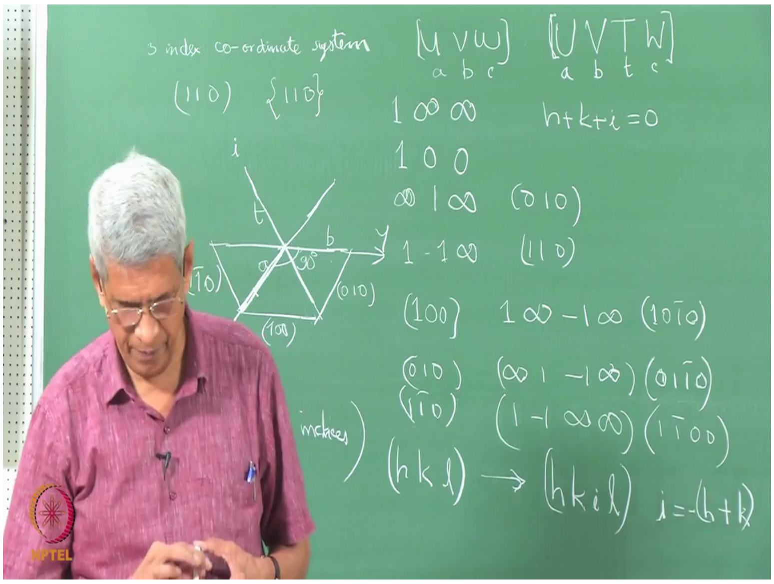

Let us do now what it will happens is that it makes an intercept one here this is for 1 0 0 plane which is in a 3 index system intercept which it makes it is one with respect to the y axis it makes an intercept which is an infinity with respect to the this axis I the intercept which would makes it is again minus 1 with respect to a c it makes infinity. Now if we look at it take the inverse of it this will take turn out to be 1 0 1 bar 0, correct, its straight forward it comes.

Similarly, if we take with respect to 0 1 0 then this will turn out to be in the case of x axis this makes an intercept which is infinity because its parallel to it because of that then with respect to 1 with respect to y z its going to be minus 1 then infinity now if we look this will turn out to be 0 1 1 bar 0 correct if we see with respect to 1 1 bar 0 because in a 3 index system this has the different indices. So, this does not truly represent the symmetry by looking at it we are not able to make out.

Now, if we see it here the indices which may be with respect to x intercept is 1 with respect to y the intercept is minus 1 correct then with respect to this axis this parallel to it. So, infinity the other one with respect to c it is infinity now it turns to be 1 1 bar 0 0 now if we look at these coordinate system in the 4 index coordinate system you can see that its only that indices are positions are changed. So, that symmetry is being revealed with respect to this that is what it happens and another thing which becomes is in a general case if we consider it before we go to general case let us look at what happens this suppose these indices h k with a conventional one suppose we represent this as I then what is going to happen h plus k plus I equals 0 in all these 3 cases correct.

So, if we represent any crystals hexagonal crystal in a 3 index system h k l is the one which is used to represent the plane then in the 4 index system the same planes are represented h k i l where I turns out to be minus of h plus k this naturally follows then we just chose the axis it is as simple as that generally in the book they will say that this is the way it is written. But it is a natural way in which we are trying to derive that miller indices whatever the method which is being given it is valid for whether it is a 4 index system or a 3 index system from this, this relationship comes this is generally called as the this type of indices are called as Miller Bravais indices .

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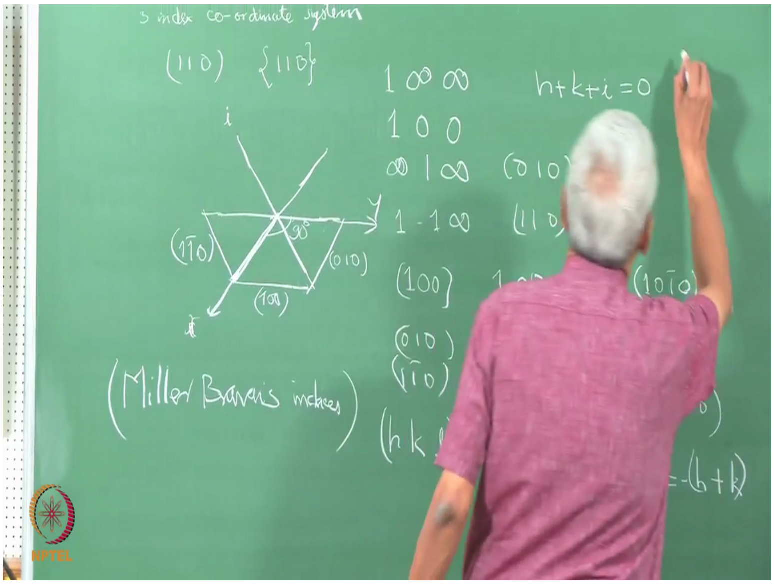

These clear this is as far as the planes are concerned. So, this way we can represent all the planes from 3 index system we are convert to 4 index or from 4 index system we can convert it to 3 index.

Similarly, quiet how we have to represent the directions as well how do we represent that directions generally the indexing which is used is that if u v w are the ones which are used to represent the indices of the directions in a 3 index system in a 4 index system we write it as capital u v t and w this is how this is represented. Now like in these case we have to find out what is the relationship between the coefficients in the 3 index system and so here if the axis the; we represent it as the each unit as into a here if you can represent b and this if you represent it as t and then the other one seems to be c. So, it will be essentially a b c correct here it will be a b t and c this is what it going to be there translation vector in these directions.

But what is essentially important is that now we know that irrespective of the; which coordinate system which we used to represent it the vector has to ru the value has to remain that same. So, we know that r will be equal to.

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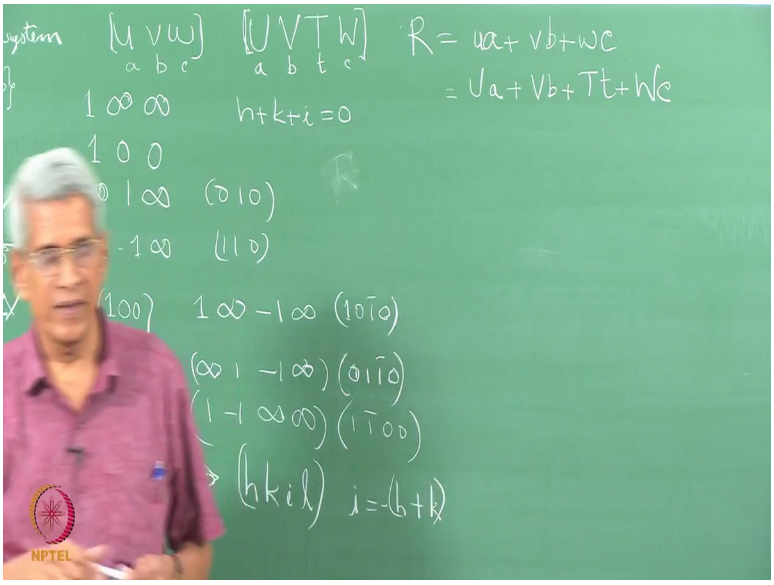

If you try to represent it as R; R will be equal to u into a plus v into b plus w into c correct in the other coordinate system it will be q into a plus v into b plus t into t plus w into c both are equal correct, is what it is if we look at this coordinate system which we have chosen one thing which becomes if this is a and this is b this vector if you see a plus b if we take it this turns out to be minus t right.

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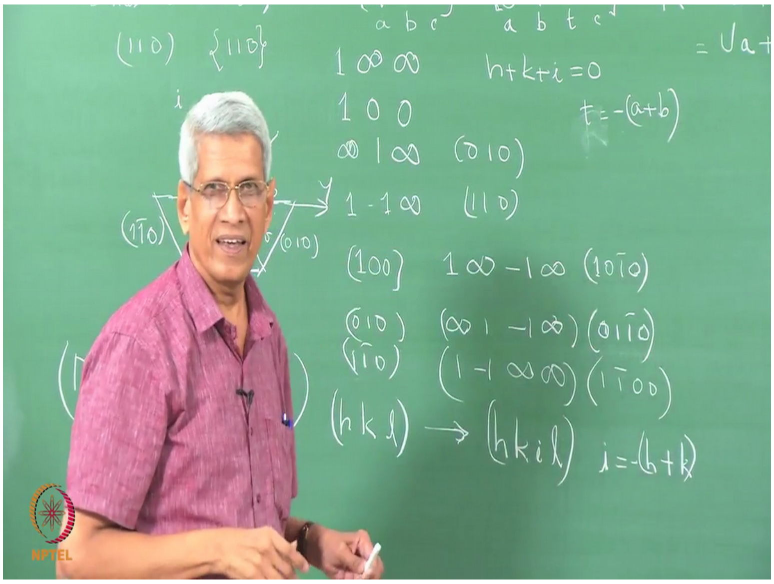

So, now we have that other relationship is that t equals minus of a plus b correct we substitute this onto this equation then u into a plus v into b minus of a plus b into t plus w into c it will come.

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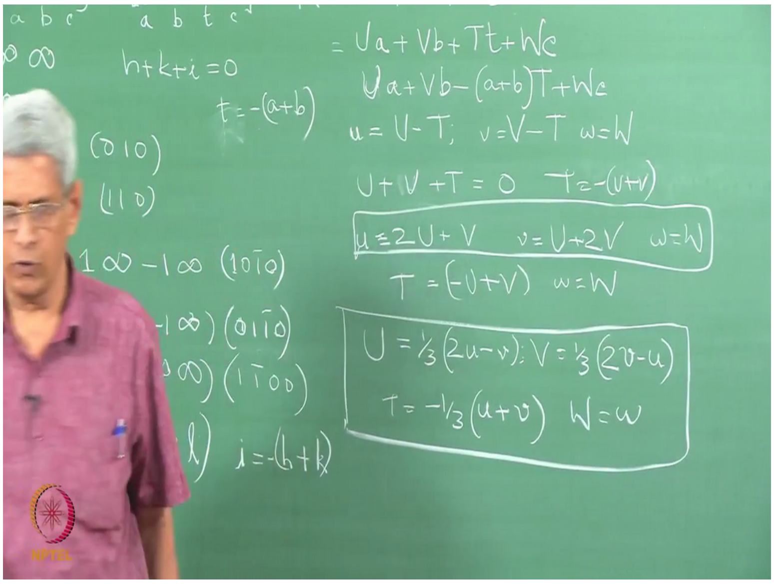

Now, we have a b c are there, we can find out the coefficients a b c and that will give raise to what is going to be that expression these expression will turn out to be u equals u minus t v equals v minus t w equals w this is how it will turn out to be. Now what is important is this fine we should know what is t what the relation to which it is related this is something I think in mathematics its quiet often than when we do not another unknown is one of the simplest thing which we can take it is these coefficients which are there u plus v plus t this can be taken to be equal to 0, this is 1 of the things which it is an assumption there are many ways in which can be done.

Let us not bother about all these things the simplest case we take it if we make this assumption then t will turn out to be minus of u plus v correct this is the only place we have mathematics otherwise all of them are coming out as a natural consequence of the crystal structure itself correct you are not done anything. Now if we substitute t with respect to this and now I try to find out what it will turn out to be u will turn out to be 2 u plus v small v turn out to be u plus 2 v t equals minus of u plus v or w equals w. This is what the expression which will turn out to be this is now we have represented or we can write w equals w; that means that we have represented the 3 index system coordinates of the direction with respect to 4 index coordinate system you have represented.

Suppose we wanted to do the other way round 4 index system if we have to do it, it is just solving this equation which are there all these 4 equations if we do that I will just write the final expression what it turns out to be this one can work out oneself and try to find out v equals 1 by 3 t equals w. This is what essentially these expression will turn out to be this one can just since these equations are there we can just substitute it and solve it its very simple using this expression we can find out; that means, that this equations can be used to find out in the 4 index system any direction which being given by u v w what will be the coefficients of u v t w in terms of 3 index system we can find out.

Let us take a simple example suppose in these this direction if we see it, it is 1 0 0 correct for this direction suppose we wanted to calculate let us substitute this u is v and w are 0.

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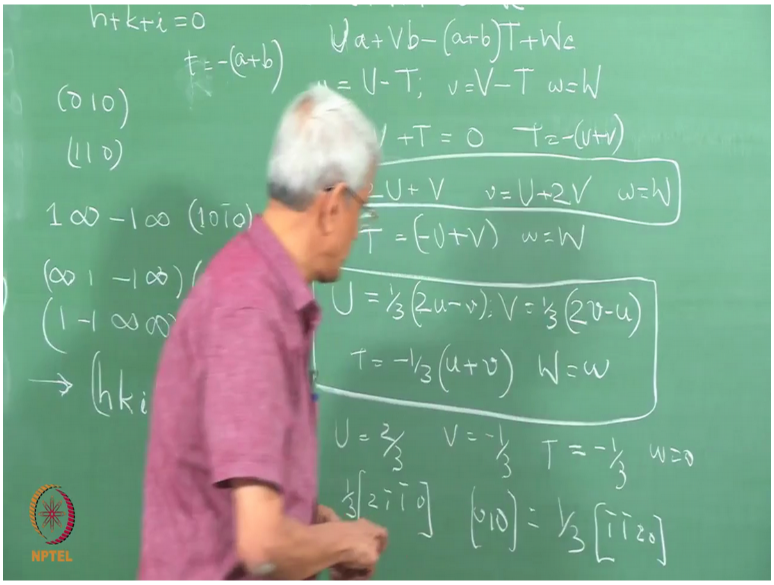

So, what if it u are turn out to be u will turn out to be 2 by 3 in this case correct v will turn out to be minus 1 by 3 t will turn out to be minus 1 by 3 w will turn out to be 0. Now if we write this; this will turn out to be this vector if you write 1 by 3 into 2 minus 1 minus 1 0 that is 1 0 0 direction the magnitude this turns out to be this vector or 1 0 0 is nothing, but 2 1 bar 1 bar 0 direction.

So, compared to planes if you look at it indices change a lot using method we can find out indices of directions in 4 index system when we know indices in 3 index system is it clear. Now generally when we use another one is formula which we use is the sound law the sound law.

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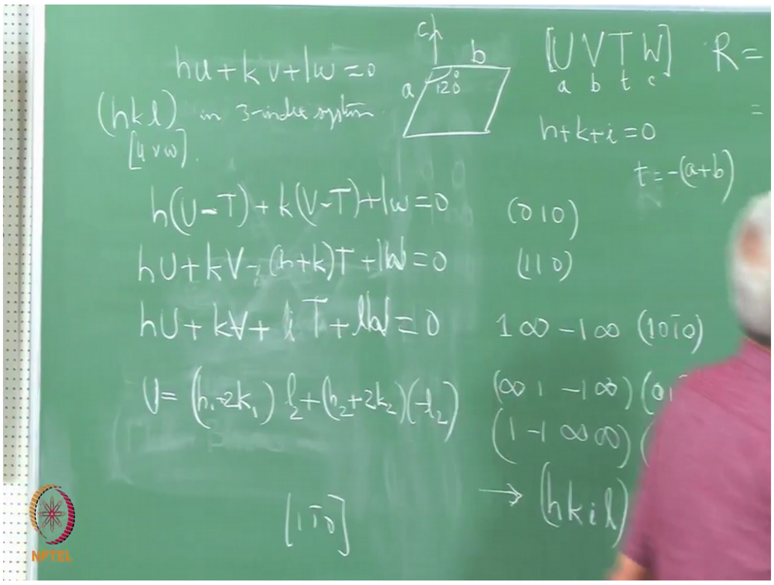

Essentially what we write sound law is nothing, but h u plus k v plus l w equals 0 this is the 0th order sound law which we consider it. So, where h k l are indices of planes in 3 index system right and u v w are the corresponding direction correct. So, essentially what it means is that h k l represents the indices of the planes.

So; that means, the direction which is perpendicular to that plane this is normal t this is normal to it that is what the physical meaning of this. So, if we want to substitute for u v w what will happen in the 4 index system? Now what we can do it is that this is the expression for u v and w if we substitute this what it will happen into u minus t plus k into v minus t plus l into w this is turn out to be 0 correct. This will be nothing, but h u plus k into v plus minus of minus of h plus k into t plus l w equals to 0 correct what is minus of h plus k it is equals I right that is I into t plus l into w will 0. So, exactly the similar expression you get it in sound law is identical whether it is a 3 index system or a 4 index system the same it will turn out to be.

Then the other one which we will require is that when we wonder to index diffraction pattern there are so, many directions. So, many reciprocal lattice vector which we see the indices of the reciprocal lattice vector how index is nothing, but they are indices of the planes if we wonder to find out the direction perpendicular to it or we can consider it an another way that is we have 2 planes are there these 2 planes will have a common direction in which they will be meeting if they meet how will we find out the indices of this direction. Suppose the planes are given in a 3 4 index system we wondered to find out the direction in 4 index system common direction the way in which we can go about is convert this each of this planes into 2 index system, and then try to find out using the sound law what is going to be the directions corresponding to that and then when you know direction using this formula we can convert it back into a 4 index system the same thing is done in is given in this slide also here.

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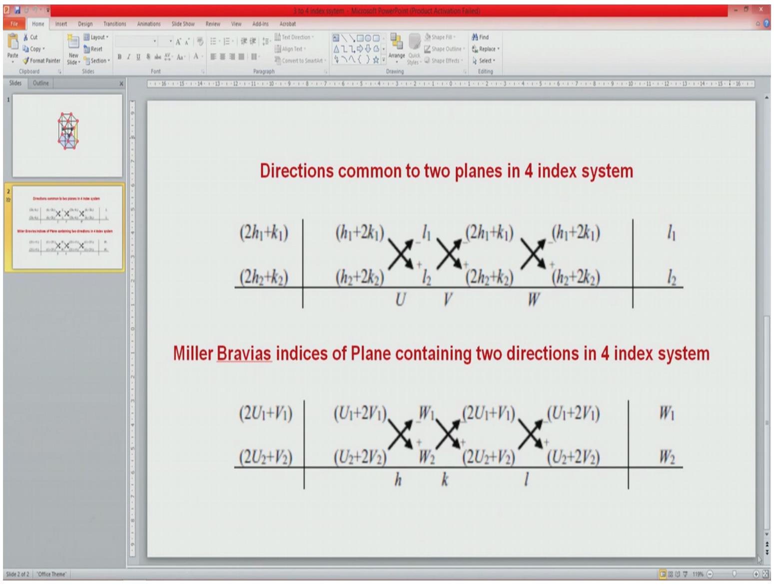

What has been done is that the planes are given it is given in some formula which one can directly use it there is h k and del this is for one plane. So, what all the what it means is that h 1 plus 2 k 1 and this and this here U and V W are mentioned directly. So, to find out u you take a product of this and take a product of this, this will turn out to be this one what it will turn out in that case is that you will turn out to be h 1 plus 2 k 1 into l 2 h 2 plus 2 k 2 minus l 2.

So, similarly we can write expression and we can get it that is what essentially this sort of table which represents similarly suppose you are given 2 directions in a 4 index system you wandered to find out the planes which contains that direction we can use these expression which is given here this table its exactly the same way h will be equal to you multiply this by this one this term by this one add them together you will be getting the value of h h k and l if you know h plus k equals i. So, we have that 4 index plane system is the way it can the other way as I mentioned earlier we can do it convert this directions into a 3 index system that is exactly what it is its only the final expression which is given in a form mammogram which one can just remember and use it this is the way in which we can convert from 3 index system to a 4 index system.

From these example you can make that this is 1 0 0, similarly 0 1 0 also we can find out and similarly this will turn out to be this you have just verify it may be one bar one bar 2 0 I am not sure, but you can do it. Similarly the direction 1 1 bar 0 it will also be turning out to be in terms of this because this is the 3 coordinate z y and I which you are chosen they are symmetry of the related. So, they will have the same type of an indices which will happen this one can work out as an exercise and verify it t.

His is the way in which most of the crystallography work or when we wandered to index diffraction pattern you can do it this when you work out a lot of examples one will become quite familiar with it because in the text book as well as in many of the research papers when you go through them you will always see that they use a 3 index system very frequently. This, only through experience one can understand quickly how that system is being used another one which is being done is that quiet often this is to how to represent in a 3 index system to 4 index system, how hexagonal crystal system is to be represented another way in which hexagonal system can be represented is in a another way of 3 index system. Because in this case what we considered as the unit cell if we consider it this is a this is b and the c will be turn out to be in this direction the angle between them is one twenty degree correct there is an another way in which it can be represented is that in any hexagonal system if this is the v a and b.

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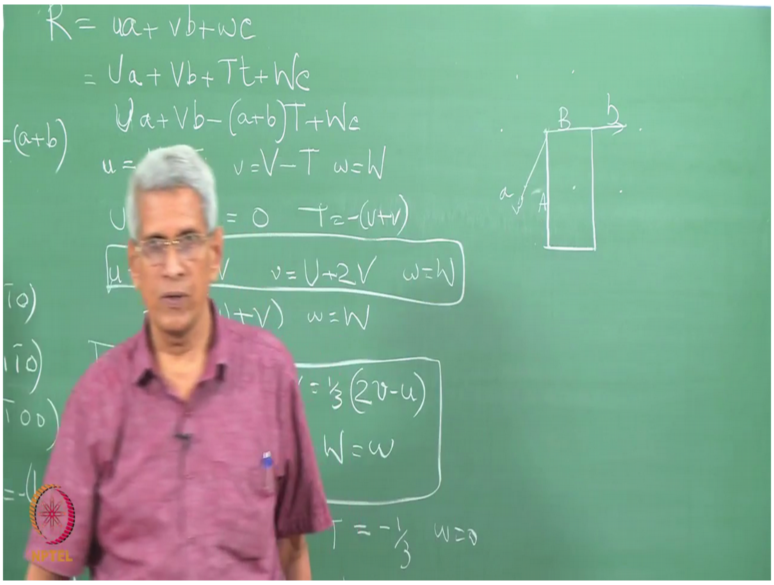

Another way in which we can represent it is this can be represented in this particular way this can be a this can be b this can be the c axis an as an orthorhombic unit cell also because we know that unique cell is not unique. Generally we use a unit cell which represents the full symmetry of the lattice the best example which we can take it is if we take a cubic system the primitive unique cell of the cubic system is triagonal that does not represent the full symmetry that is why we choose either a simple cubic or body centered or phase centered the unit cell which we used to represent them.

Here are here we can use a crystal which is for convenience if we consider it this is an orthogonal 3 index system with which one can work where it becomes very important is suppose on a hexagonal lattice an ordering has taken place and because of that ordering the atom positions have shifted slightly then it is no more hexagon it can be a orthorhombic structure. So, in such cases we can use the orthogonal unit cell to represent it even for a hexagon this can be represented because and un-similar lines here essentially from one 3 index system to an another 3 index system this aspect of it I will take it up in the next class similarly an another one which will happen is that trigonal. If we take it trigonal system also it is essentially an a stacking of hexagonal layers one on top of the other there is gen as a general sons if we look at it all the cubic system trigonal hexagonal they are all arrangement of hexagonal 2 dimensional lattice one on top of the other keeping some distances in some symmetric positions that is how this lattice.

So, all of them can be represented in terms of hexagonal unit cell especially in trigonal it can be represented on a trigonal coordinate system or it can be represented on a hexagonal system also because in material science when people work on many of this compounds one will find that many of them are either in rhombohedra's structure. Those structures when we have to represent them what is the type of a indices which we have to use to represent them that is where sometimes we will use trigonal itself in some cases it can be indices in terms of hexagonal lattices these are all the possible way which it can be done.

So, essentially in the today's class what I had just shown is how to go from one crystal structure from one indexing system to an another indexing system which is the cubic in the that is the 3 index system which is normally used to represent all the crystals. But generally when we use this sort of indexing system it if the indexing system also is also is chosen such a way that it represents the symmetry which is associated with the crystal then just looking at the indexing the planes we can tell that this belongs to a per this sort of planes correct. That is the advantage; it is there that is the primary reason which motivated to go from 3 index system to 4 index system for hexagonal crystals.

I will stop here now.