Defects in Materials
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Lecture – 12
Transformation of Co-ordinates

Welcome you all to this course on Defects in Materials. Today we will be covering transformation of co-ordinates. The first question which arises is why should we study the transformation of co-ordinates, what is the need for that this, is essentially depends upon the type of situation which we are look at that are many situations we have to look at co-ordinate transformation, because there are many situations where we find that we measure. For example, we measure a property in one co-ordinate system, and then we try to interpret it in terms of some other co-ordinate system. The example which if we can take it is the elastic properties of the measure of a single crystal if you wanted to measure.

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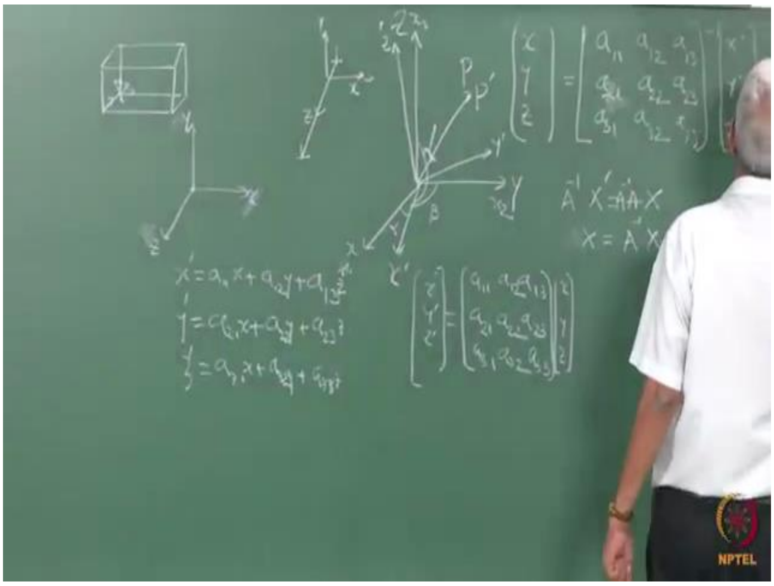

We may be taking a sample with this external shape. So, the co-ordinate system which we will be choosing it is these 3 as their axis.

But in the sample the crystallographic co-ordinate system will be something else, it may be in this particular direction correct; it is a single crystal so; that means, that the property are generally related with respect to the crystallographic co-ordinate system of that samples, but when we do a measurement we do it with respect to an external co-ordinate system right.

Another example is electron backscatter diffraction when we do; there again 1 is the co-ordinate system of the sample with respect to which, but what are we trying to find out the plane normal's for each of the grain, which we are trying to find out with respect to the crystallography co-ordinate system, there also this sort of transformation will be required. The third is stress and strain measurements when we you or the stress and strain field around a dislocation you wanted to find out. We have a crystallography co-ordinate system which is their which we may be you single like Cartesian co-ordinate system y and z, but quite often what or we can choose the system like z x y I am just marking it like this, and when we choose a dislocation the dislocation is not the dislocation lie in if not lying along any of this co-ordinates correct, it is inclined with respect to this.

And stress and strain field around the dislocation is described in terms of a co-ordinate system, where we take this to be z axis that is the slip plane the where the buldge effect is there that is the x axis, and that plane normal as the y axis we choose correct. So, this is another example where we have to go from one co-ordinate to another co-ordinate. In fact, when we consider this location another transformation which is also necessary is that not only Cartesian because of radial symmetry.

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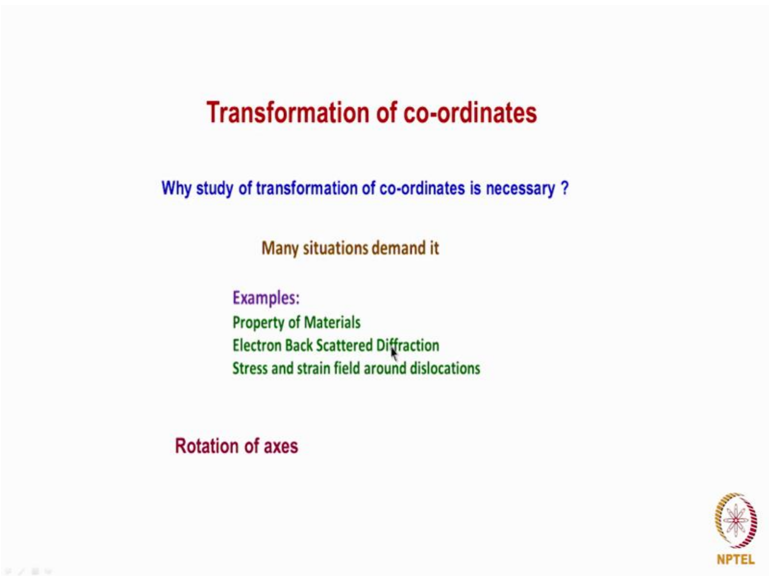

We may have to go from Cartesian to essentially cylindrical co-ordinate system or in there are many cases where will have to go from Cartesian to spherical co-ordinate system, this sort of transformation also will be required. And you may be familiar with this transformation from Cartesian to cylindrical or Cartesian to spherical co-ordinate system.

So, what we will consider in this class is 1 if you look at it like this sort of a 2 Cartesian system which we consider: one is a rotational axis which is necessary to go from 1 to the other correct, then another is that the unit cell dimensions itself might have changed that is an these are all the 2 cases. So, we will consider both the cases 1 is rotation of axis if we do; how that is going to change, how the transformation can be related from one co-ordinate system when we rotate it and come to a new co-ordinate system, how the vectors change this is one aspect which we will consider. The other aspect which we will consider is that in many transformation especially phase transformation takes place, that is certain alloy is in one particular phase and the ordered 1 is in an having an another crystal structure.

But the as far as the atom positions are concerned they remain the same. So, 2 different types of unit cells you have to consider, and as you have as we have studied in crystallography, the unit cell itself is not uniquely different; you can have a square type of a unit cell depending upon the cell or it could be a parallelogram, or it could be a rhombus depending upon the situation the different types of unit types of unit cells which we can choose, then also this sort of trans understanding this sort of transformation is really necessary.

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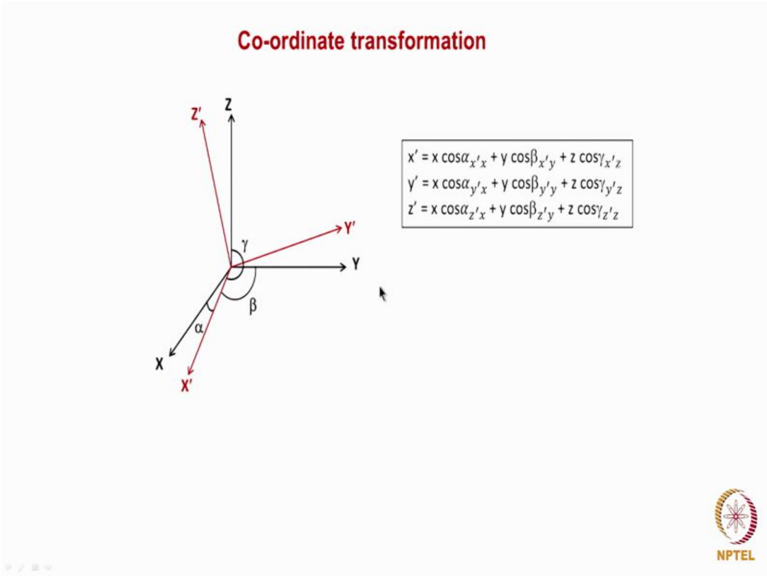

What we will do it is the let us consider the co-ordinate transformation which is essentially rotating from in the Cartesian co-ordinate system. So, here if you try to look at it x y z which is shown in black color, that represents the normal Cartesian co-ordinate system, this co-ordinate system has been rotated to x dash, y dash, z dash. So, when such a rotation has been done we can make out that from the x dash the new co-ordinate which has come, it is rotated with respect to the x co-ordinate by an angle alpha it makes an angle beta with respect to a y co-ordinate of the old system, and a gamma with respect to the z co-ordinate of the old system correct.

So, essentially what we z is z dash, and this is alpha this is beta, and this turns out to be gamma correct. Now what we are trying to do is that what is the component of x in this direction, what is the component of y in this direction, what is the component of z in this direction if all the 3 we take together the same direction if we add it, we get the value corresponding to that x dash, that is what essentially is written in this equation correct. So, this essentially depends upon the angle between the axis, what that x dash makes with respect to x y and z, similarly we can find out the angle which y dash axis makes with respect to x y and z, similarly that z what it makes; this the information which is necessary.

Similar way we can represent the old axis in terms of the new axis also, then what we are looking at it is what is going to be the projection of x dash onto this x, projection of y dash onto x, and projection of z dash onto x, and all we add together we get the value of x y and z that is what we have written here, this is all with respect to the angle between the axis fine.

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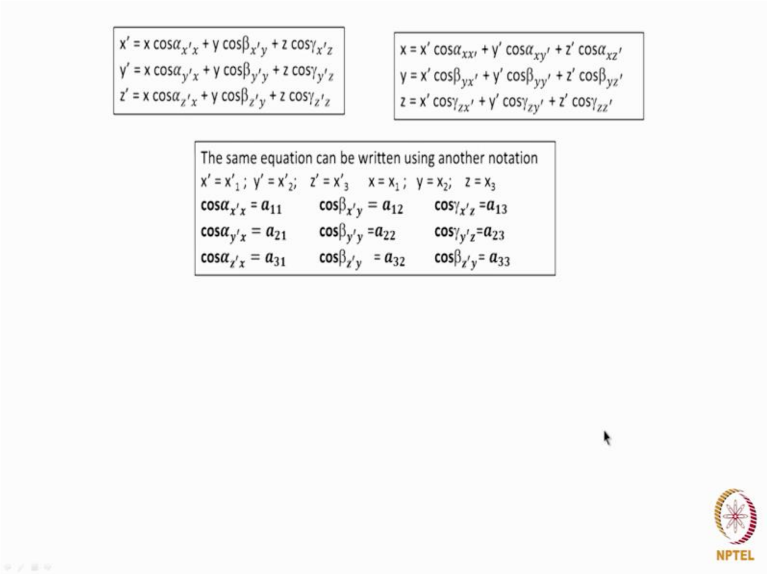

In many books you find that instead of using x y z these may be represented as x 1, x 2, x 3 these sort of symbols are also used that is essentially what I have shown here; and then what I have done it is the this angle I had used suffix that cos alpha x dash x, means that the angle between x dash and x co-ordinate that angle is alpha, that is what we are trying to instead of using these symbols we can just represent them in a nice way in a matrix formation, that is what I had just defined them as a 1 1, a 1 2 like this we can define it ok.

If you try to do this then this equations will turn out to be x dash will be y dash will be equal to k 2 1 into x, a 2 2 into y, a 2 3 into z, z dash will be equal to a, 3 1 into x plus, a 3 2 into y, plus a 3 3 into z correct. This can be written in a matrix form also so as a column vector, we can write x dash y dash z dash this will be equal to a 1 3.

This one also we can write it and this matrix is the transformation matrix to go from one co-ordinate system to the other co-ordinate system. And similarly if you wanted to find out from transform from, in fact then it can be essentially written as a 3 p, the whole inverse x dash y dash z dash is the way also we can write it right. And this inverse of this matrix will turn out to be nothing, but a transverse of that matrix that is what essentially is shown in this transparency; is this clear, because this is here we can write x dash equals A into x correct. So, if you put A inverse multiplied by A inverse on either side, then this will turn out to be x will turn out to be A inverse into x correct, that is what essentially we have done it is a nothing, but a simple matrix algebra; is this clear.

So, using these matrices the transformation matrix, we can go from old co-ordinate system to new co-ordinate system or from a new co-ordinate system to a old co-ordinate system, which is essentially just a rotation of axis.

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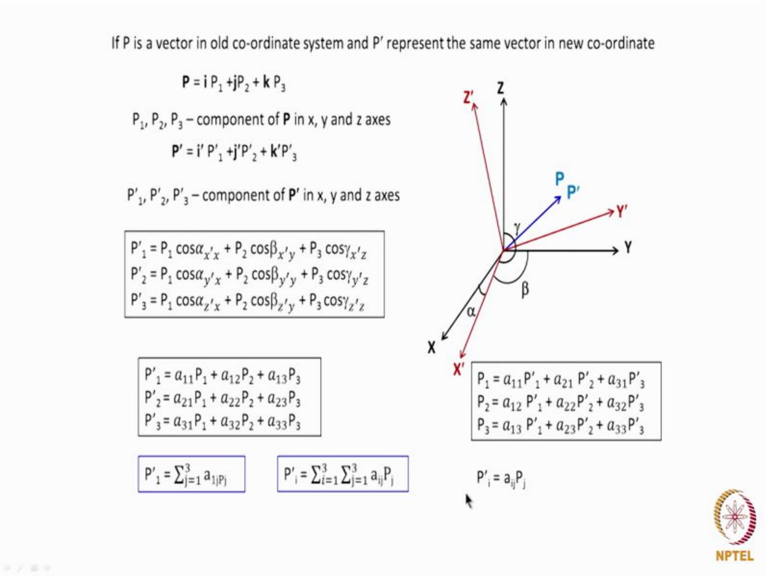

Suppose we have a vector in the old co-ordinate system, which is a just described as the p and the same vector in the new co-ordinate system we are describing it as p dash; like here there is a vector if there p, the old co-ordinate system it is p the new co-ordinate system it is p dash, then we can write this we can have components p 1, p 2, p 3 correct.

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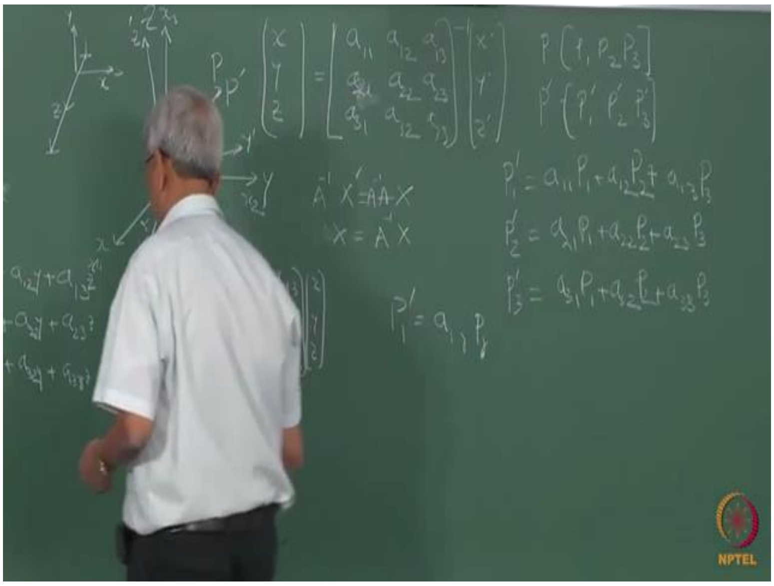

Similarly p dash can have components p 1 dash, p 2 dash, p 3 dash, then these components also exactly similar to the transformation of that from one co-ordinate system to another rotation of co-ordinates which we have considered here the same way we can do it. So, essentially what will happen if that p dash will be equal to p 1, a 1 2 into I am just writing the final result, but you people can work it out.

Similarly from the components of p 1, p 2 in terms of p 1 dash p 2 dash p 3 dash also we can work out on. This generally we use some shortened symbol to represent it, where we write p 1 dash essentially as is shown here in terms of a sigma it is just nothing, but an addition of 3 terms, and as a 1 j, p j that is the way we can represent it and then if it like a p i a set term if we do it, we can you have to take 2 summations will come 1 over j.

Then next over i it will come, this can be represented in a simple form like this p i dash equals a i j p j, and wherever the symbol gets repeated that is at Einstein convention which we if that is the one over which the first the summation will we take, we will take and then the next one will come into the picture.

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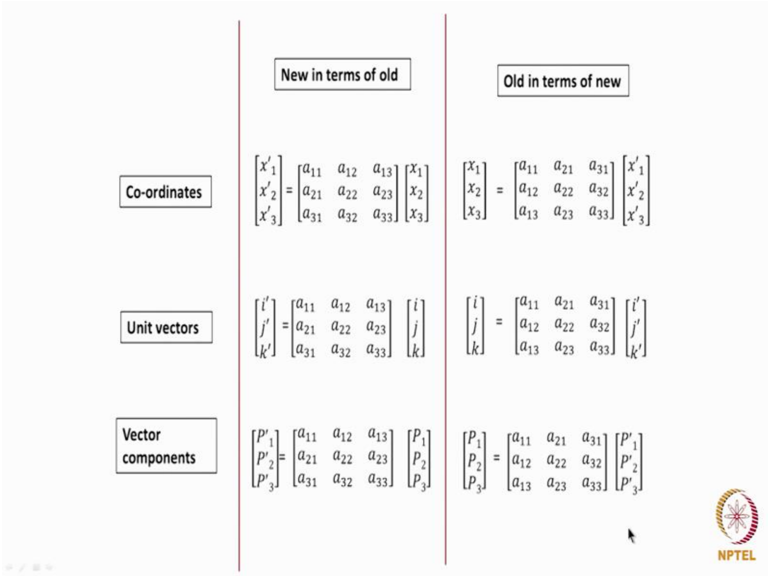

That's it. So, what I have done in this slide is that the transformation matrix from new in terms of old, old in terms of new both for the co-ordinates unit vectors i j k the old co-ordinate system a new co-ordinate system, and the vector components all of them what is the transformation matrix which is to be used is given in this transform transparency.

Now, we will go to change off from rotation of co-ordinates to suppose there is a change in the type of unit cell which we choose, this situation we face quite often in phase transformation. Suppose, from one particular unit cell which we have chosen; we change to another unit cell. The indices of the direction and the indices of the planes will change, what will be the correspondence between them between the old and the new co-ordinate system that is what we will look at.

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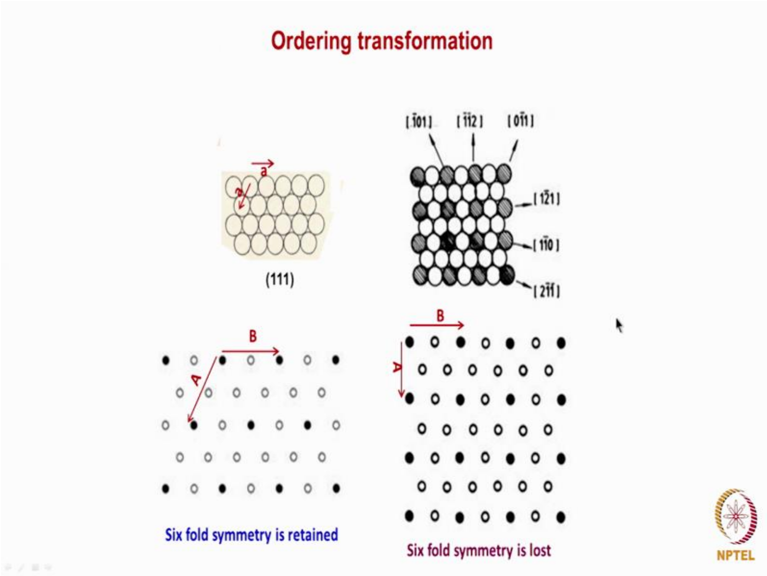

First let us illustrate it with an example; here what I am considering it is essentially a hexagonal lattice. In this lattice this will be the unit cell, and that x and y axis both of them they have to our lab large parameters here angle between them is 120 degree. There are many situations where we can there this could be a situation which can develop, this is just a what we have considered is a only a 2 dimensional lattice which we have considered, if we keep the same lattice one on top of the other, a simple hexagonal lattice will be generated.

There are situations where they undergo a transformation, one such case which you have considered where it undergoes a transformation from hexagonal when ordering takes place, it becomes an orthorhombic structure. Here what happens that you can look at it that every alternate atom now they have become different type of an atom, and the next row nothing has happened the next row again this it gets repeated, the alternate items are a different type of an atom. Now if you look at what is the symmetry which this has, hexagonal lattice has got a 6 fold symmetry that is last.

That is one thing which we can see, another is that the unit cell here now it is going to be this is the type of a unit cell which will be considered for a 2 dimensional lattice right, if this 2 dimensional lattice is kept on top of it, it would be exactly similar to the disordered lattice which you are considered here. So, in such a case the axis the new axis if we can represent it in terms of the old axis, then we can find out information about the planes and directions.

Another thing which happens is that in this specific case which happens in ordered last also, instead of every alternate atom getting alternate atoms are of different types here, it is in this particular direction close packed direction. It can happen in this close packed direction or it can happen in this close packed direction also, so that there are 3 ways in which this tetragonal lattice can orient itself. So because of that to know, what is the relationship between that old and that new co-ordinate system? For each one of them is very much necessary to find out the correspondence between to find overcome between the planes and directions.

Here is these are all the co-ordinates k a n b, there is another type of a transformation which can occur that 6 fold symmetry is within, here if you look at it very alternate atom in a particular row if you consider it, they are of the different they are of different type. Then next row all atoms are of the same type, next row again if you see it is of alternate atoms in the alternate atoms in the particular in this row are of different type, but they are shifted with respect to this one by half the lattice translation vector here. So, this we thinks that this is also an another type of a transformation, and here if you look at it though the directions of that axis remain that same, but the lattice parameter is doubled correct.

So, these are all the different types of situations where we have to get information about a co-ordinate transformation.

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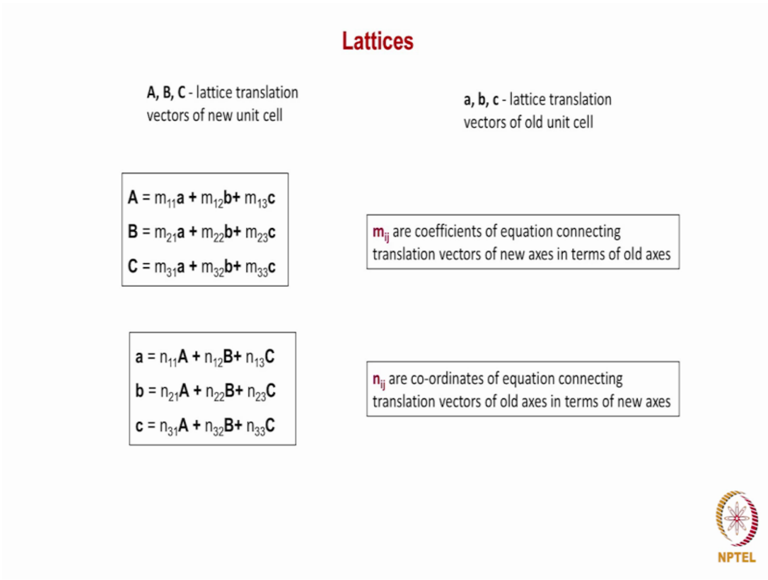

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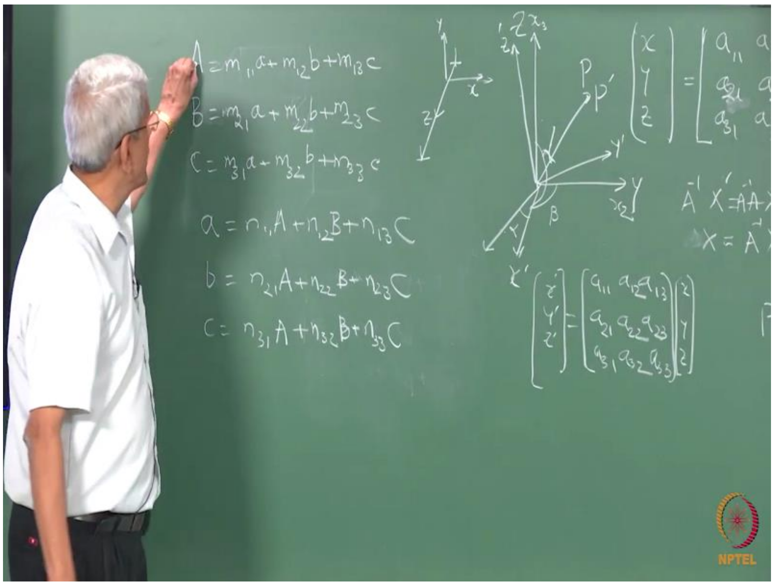

How do we go about it? Suppose A B C are lattice vectors of a unit cell in the new co-ordinate system, that is all capital A B C; and small a b c is the lattice parameters in the old co-ordinate system, and then the relationship between them is essentially will be we are writing it as star ok.

Here m 1, m 2, m 3 these are nothing, but the projection of this vector a in this particular direction right, that is how we are taking it and these values could sometimes or could always be larger than because the case which we have considered rotation of axis, there is a cos theta which we consider it; the value of cos theta can be less than 1, always it is less than 1 by the maximum value should be 1 which it can be having it. Here that is between 0 and 1 equal, here these values could turn out to be higher also. The reason essentially is that if your multiple times cos theta will come if the unit cell dimensions are the well correct, that is the only difference which is going to be there in this particular case.

So, here these are all the co-ordinates of the lattice translation vectors of the new axis in terms of the old axis which we have defined the. Similarly we can consider a the old axis in terms of the co-ordinates of the new lattice, and in bet between these 2 are used 2 different types of symbols right correct? Because the axis when we consider what we are trying to find out is, in this case when we look at a what is going to be the co-ordinates of A in terms of the old axis system, what is going to be here the co-ordinates of a in terms of that new system; when we look at these values these coefficients may not be the same there will be different that if why we are representing them with 2 different distinct symbols ok.

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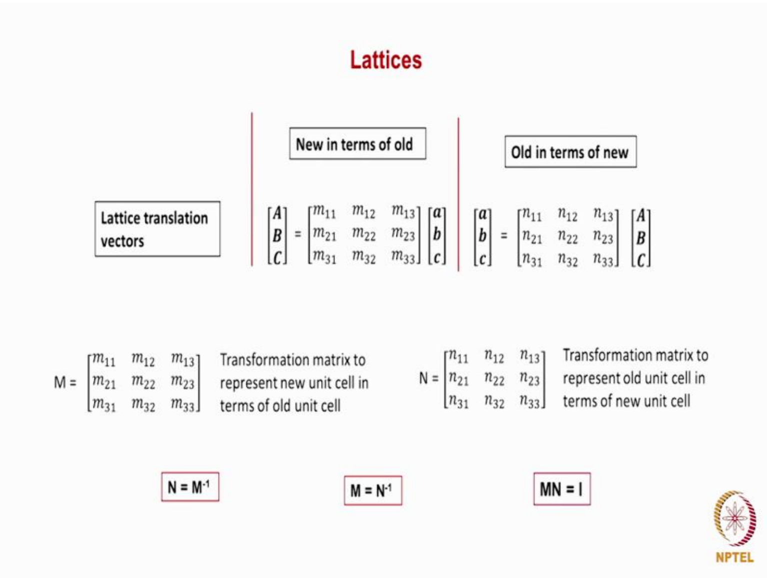

So, this can be represented in a matrix form also that is what is shown here. So, m is the matrix which is use this matrix represents the 1 to transform from old system to the new system, when I use to denote this matrix to transform from new in terms of; the old in terms of the new system. The other one is m is you the matrix which is a transformation matrix is used to denote the transformation matrix from the old to the new system ok. These are all the equation the relationship between n then, m will be 1 will be an inverse of the other the matrix.

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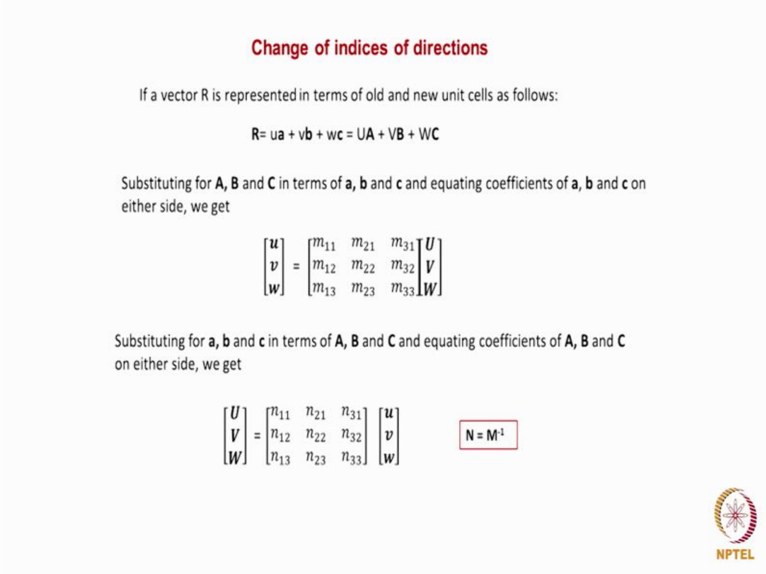

Suppose we have to find out the change of direction like the way we have considered a vector, this vector can have different types of questions because essentially the vector remains that same only the co-ordinates have changed; how do we represent these vectors?

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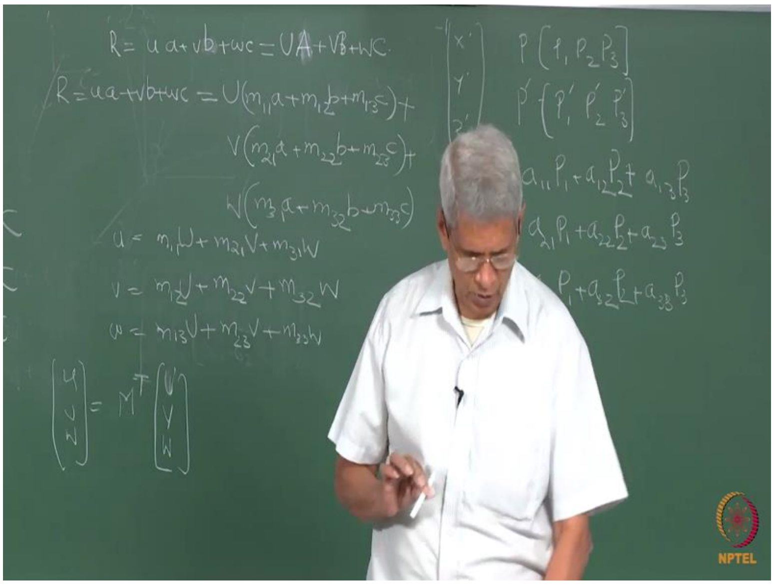

Suppose in the old co-ordinate system we represent that vector R is equal to u into a, plus v into w, v into b, plus w into c. The new co-ordinate system we start capital letters using U into A, plus V into B, plus W into C correct. Now if we substitute for A B C in terms of the old co-ordinate system the values, and then what will happen is that into 2 into b, plus m 2 3 into c, plus m 3 1 into a, plus m p 3 into c. Now if you take the coefficients of a and b on either side and equate it, then this will turn out to be u will be equal to m 1 1 into U, plus m 2 1 into V, plus m 3 1 into W correct. Similarly v will turn out to V, m 1 2 into U, plus m 2 2 into V, m 3 2 into W, W will be equal to m 1 3 into U, m 2 3 into V, plus m 3 3 into W right.

So, this relationship can be used to find out the indices of the directions. Suppose we know the indices of a direction in the new co-ordinate system, then we can find out what will be the indices of the direction the same direction in the old co-ordinates system; which we can write it in this particular form also. So, only what we have to see here what one can make out here is that if it is U V W, this if write it in a matrix form this will be nothing, but m V this matrix is nothing, but the transpose of the matrix which is used to go from you know old co-ordinate system to the new co-ordinate system, that is the only thing which one has to remember.

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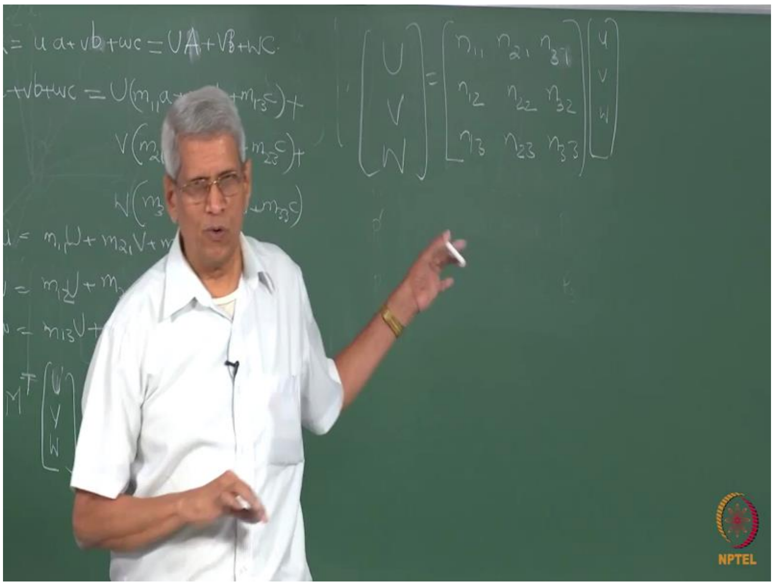

Similar way we can substitute for a b and c in terms of the new co-ordinate system, and then do the same algebra what we will end up with it is that U V W, n 3 1 into u v w this is what essentially it will turn out to be. Here again with respect to a co-ordinate system which we consider or the transformation matrix which is there to go from new to the old co-ordinate system, the matrix for the indices of direction turns out to be essentially a transverse of that matrix.

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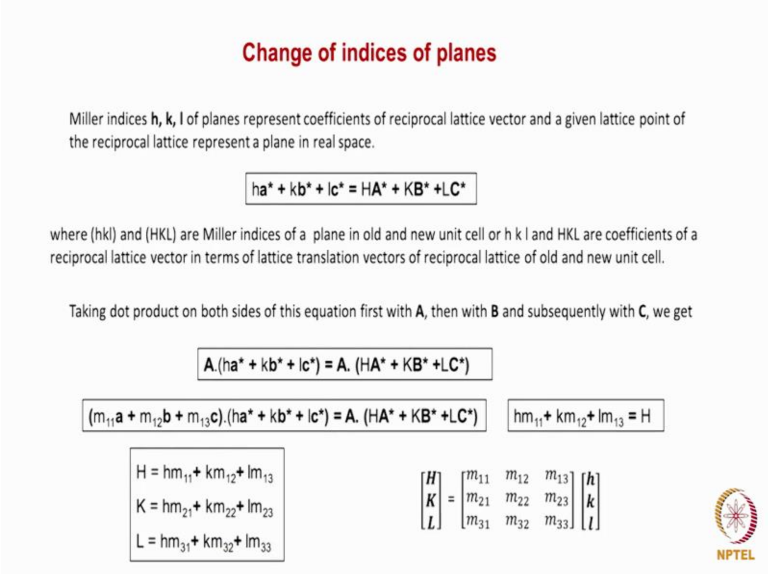

Suppose you wanted to find out that change of indices of planes, but we know that whenever we represent planes, crystal system we use h, k, l miller indices to represent it correct. The way we find out the miller indices is essentially it is a way we take an inverse of the intercept which makes in the real axis; that means, something to do with a reciprocal lattice. Actually miller indices are nothing, but essentially the vector which represents the plane in the reciprocal lattice, it is coefficient that is what essentially miller indices. So, same way we can consider the reciprocal that is how do we represent if a b c is a real lattice, the old co-ordinate system we can have a reciprocal lattice corresponding to that, and it is co-ordinates are a star b star c star we can take it, similarly for the new co-ordinate system which is represented by capital A B and C, we can have a co-ordinate system like this A star B star and C star.

And like in the case of a direct any vector if we take it, and that vector magnitude should remain the same irrespective of which co-ordinate system which we choose it.

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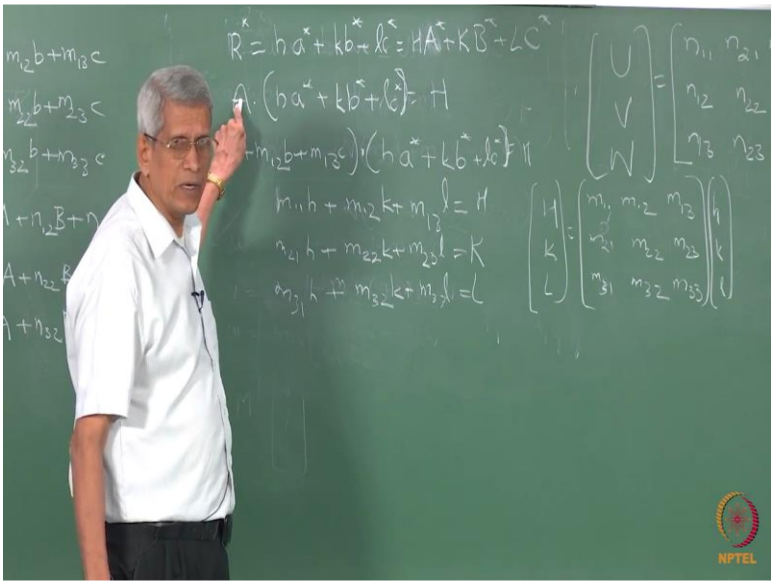

So, in that case R star will turn out to be a star plus l c star equals H into A star plus K into B star plus L into C star correct. What we can do is that it is just an algebra which we are doing it, if on this side of it we take a dot product of this vector with e vector in the vector a in the new co-ordinate system, then this will become a dot h into a star plus k into b star plus l into c star.

This if we take it on this side a star into this factor finally, A H A dot A star is going to be equal to 1, others will be 0, this will turn out to b H correct; here we can represent A in terms of the old co-ordinate system a value which we have. So, this will turn out to be m 1 into a, m 1 1into a, 1 3 into c dot v star; and here if you take the dot product what all terms which are going to be there m 1 1 into h, m 1 1 into k, plus m 1 3 into l this equals h correct. Similarly if you take a dot product with b and c also, we will be getting expressions like m 2 1 m into h, 2 2 into k, 2 3 into l equals K, m 3 1 into h, 3 2 into k then 3 3 into l equal to l; from this we can write it that h k l is going to be 2 1, v 1 this will be h k l right.

What one should notice is that here when we go from the miller indices the old system to miller indices of the new system, the same matrix which I had used the transformation matrix to go from old co-ordinate to a new co-ordinate, the same matrix is coming in this transformation also. Whereas, in the case of direction it turns out to be the transpose of this matrix correct is this clear.

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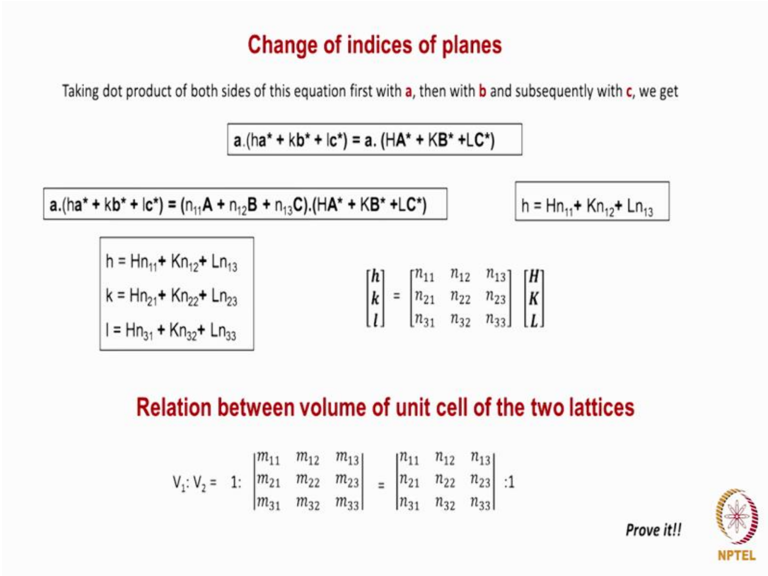

Similarly, we can take instead of taking with the co-ordinate of the dot product with A which is a vector in the new co-ordinate system, we can take with respect to A which is in the old co-ordinate system, then we will be find able to find out relationship between the old co-ordinate system that is the miller indices of the in the old co-ordinate system in respect of the miller indices of the new co-ordinates system right, and that will turn out to be h k l will be correct.

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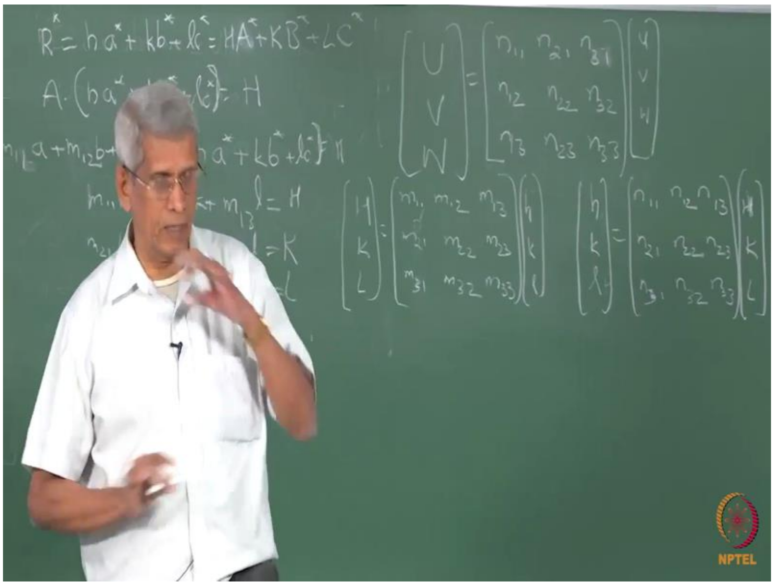

So, these are also only expressions which one has to remember to transform from old co-ordinate system to another co-ordinate system. And when we know between planes and directions also, in fact similar relationship can exist between the volume of the unit cell in the old co-ordinate system and the volume of the unit cell in the new co-ordinate system, the expressions I had given it in the slide, but I would expect you to derive and verify it in ok.

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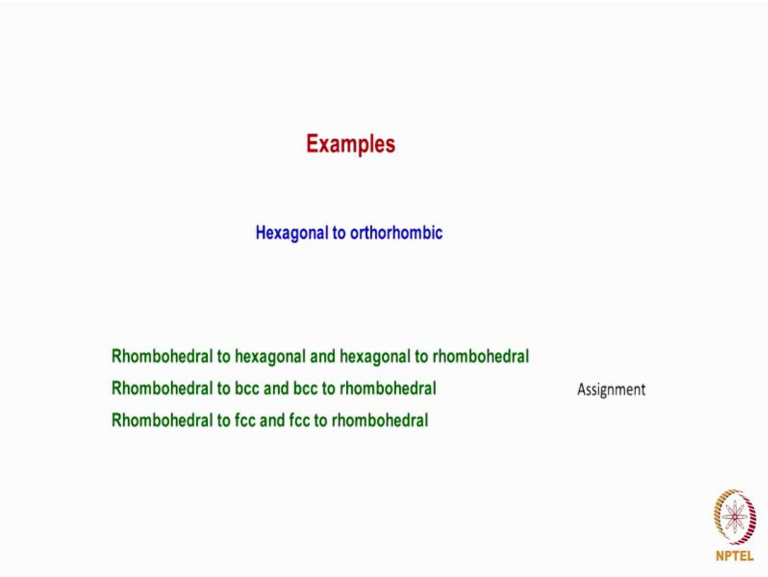

So, in this slide all the expressions which are necessary I had just given in a table form. Let us consider an example to go from one co-ordinate system to an another co-ordinate system, one can take from one transformation from one co-ordinate system to another one can take it that I will give you as an assignment, here what I will consider is to go from hexagonal to an orthorhombic system. Because why we have to do it quite often we find that when we are using an hexagonal system, 3 index system is not convenient we go for a 4 index system, but we are more used to using a 3 index system right.

So, if are the if you make a unit cell which is essentially because as we have discussed earlier unit cell is not unique, even for a hexagonal lattice we can make a unit cell which is essentially yet orthorhombic type or a rectangular type of a unit cell.

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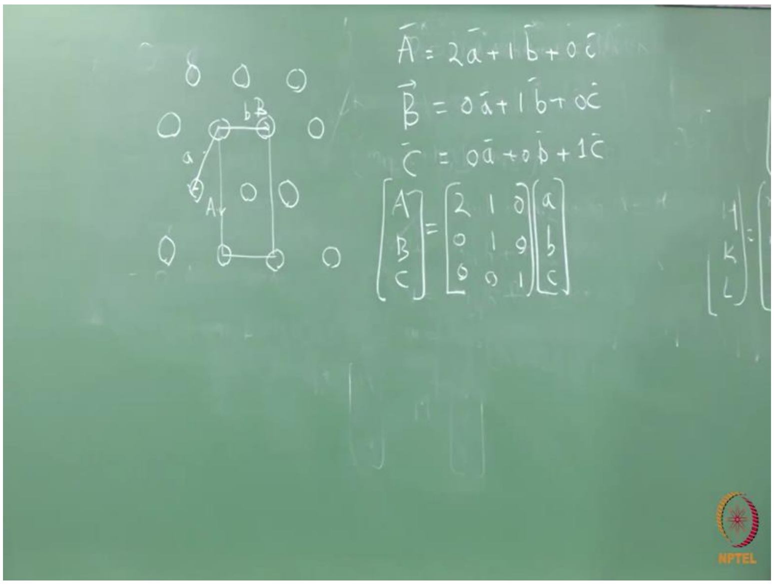

Let us consider such a case; in this particular case if you consider this will be the a with respect to a hexagonal lattice, this is the b co-ordinate, and assume that the next layer is just sitting on top of it, it generates a impel hexagonal unit cell, and this can be considered in this particular way also a unit cell, it has entered 1 item at the center and A becomes the lattice parameter for this, and B is the lattice parameter for in this particular case.

Now, what will happen in this case? If you try to represent a in terms of the old system A will be equal to 2 times A correct plus B correct. So, this will be 2 a plus 1 b plus in this plus 0 into c correct, what will be B? 0 into a, plus 1 into b, plus 0 into c correct; what is C going to be 0 into a, plus 0 into b, plus 1 into c correct. So, now, you if write it in a matrix form this A B C will turn out to be 1 0 this is right. So, this is the from old co-ordinate system this one to the new co-ordinate system we can get that information.

Similarly, when we wanted to represent A in terms of the new co-ordinate system how we will represent.

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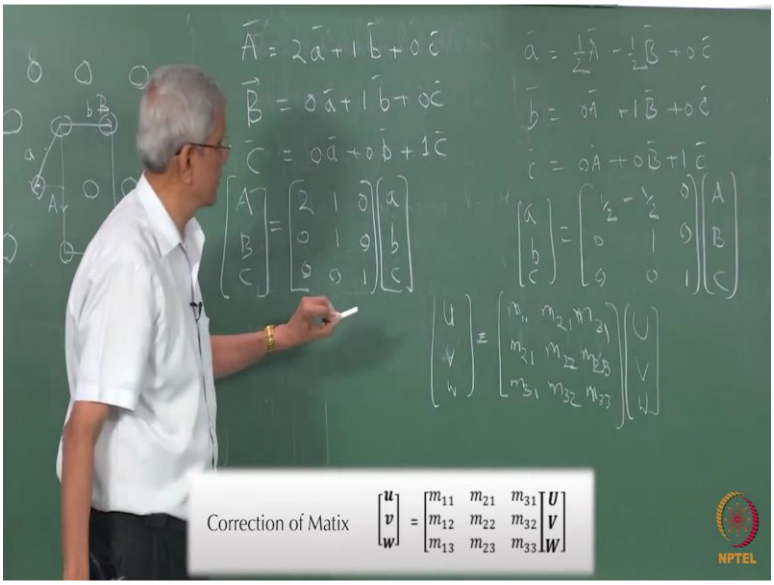

A will be half into A correct half into right minus half into B, plus 0 into C. B will be 0 into A plus 1 into B correct plus 0 into C correct and C will be 0 into A plus 0 into B plus 1 into C. So, this A B C will turn out to be of minus of 0 1 this is right. So, these are all the relationship to go from one co-ordinate system to another. Once this relationship is there using the formula which we have written to go from directions as well as in their planes we can immediately find out what is going to be there correspondence which is will be there if it is take a vector in the old co-ordinate system, what will be the direction in the new co-ordinate system; that we can get suppose it is the U V W for vector is there in the old co-ordinate system in terms of the new co-ordinate system m 3 2, m 3 3 , to U V W this matrix is nothing, but this one correct.

So, we can use this to find out if you know the vector what is going to be; similarly if you wanted to find out a vector the old co-ordinate, new co-ordinate system in terms of the old co-ordinate system, then we have use the transpose of the matrix other not put the inverse of that matrix and then we can find out, this you can take some directions take an example and work out for yourself.

So, essentially in this lecture what I have tried to do is to derive expressions to go from one co-ordinate system to another co-ordinate system. If that co-ordinate system involves only just a rotation of axis, and another if the co-ordinate system is essentially changing from one lattice to an another lattice where it is not only just a rotation, even the dimensions of the lattice parameters change that is the volume of the cells also change; both the cases which we have considered. In this particular case I had given or I had the just mentioned about it that one can go from rhombohedral to hexagonal, similarly the primitive lattice for f f c c is rhombohedral.

Similarly, primitive lattice for b c c is rhombohedral. So, one can transform from one to the other and vice versa also how to go from that; this one can work out as an assignment when you do that then this concepts will become much clear and similarly as a winter class talk about how the stress field and strain field around dislocations are calculated; in that case also you will understand what is the need for going from one that cryptography co-ordinate system is essentially a Cartesian co-ordinate to an another Cartesian co-ordinate rhombohedral system, which is nothing but rotation of the axis.

I will stop here now.