**Electron Diffraction and Imaging**
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**Lecture - 15**
**Tutorial - 03**
**Transformation of indices**

Welcome you all to this course an Electron Diffraction and Imaging. In today's class we will talk about what is the need for transformation of indices when we go from one crystal structure to other or what is transformation of indices that spot we will discuss. In the earlier classes you have studied when I crystal structure is there, then we define the crystal with respect to some coordinate system with respect to that coordinate system.

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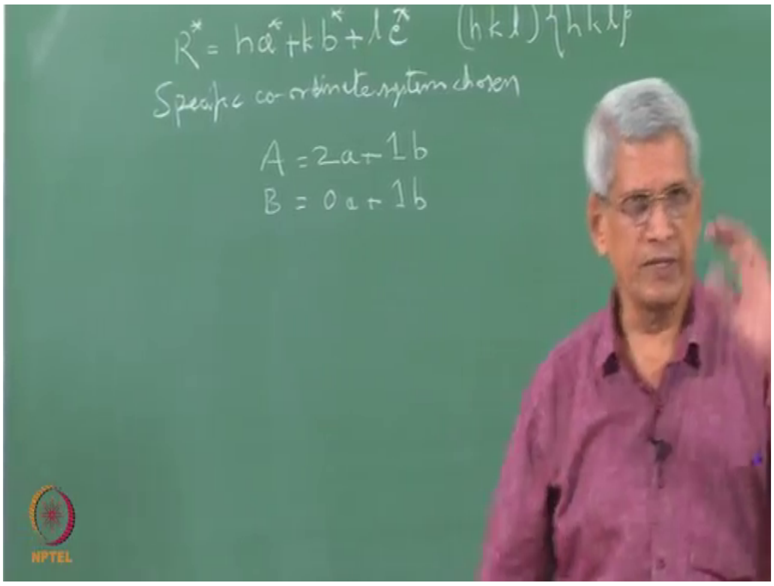


Any direction in the crystal can be a return in terms of R equals u into a plus v into b, plus w into c similarly then the indices of their plane h k l if you wanted to represent, the planes and this is the way vectorially we will represent other ways normally we represent these directions with the coefficients of these vectors this is how it is being done this is for a specific direction if you want to represent it for a family of directions, then this the way we represent you know sorry this will be with respect to correct.

So, if you wanted to represent a plane generally we represent it with respect to h k l this place make plane and family of plane each with respect to h k l, and this h k l are nothing, but if you take a vector R star there is a broken lattice it will be h into a star plus k into b star plus l into c star correct. What can should remember is that all these vectors are written with respect to a specific coordinate system chosen correct; that is how we defining, but we also learnt the crystallography that the unit cell with itself is not unique for any crystal structure that means, that we can choose different type of unit cell, correct.

So, because of the non uniqueness of the unit cell we can have different coordinate system to represent each unit cell, quite often we find that in phase transformations we may have to use different types of unit cell to represent the same crystal structure. So, sometimes it is easy to work with as another type of (Refer Time: 03:10), but normally what happens is that conventionally we use the unit cell which represents the full symmetry that need not be the case always. For example, here this cell 2 dimensional lattice which is shown we have different types of unit cells which we can have.

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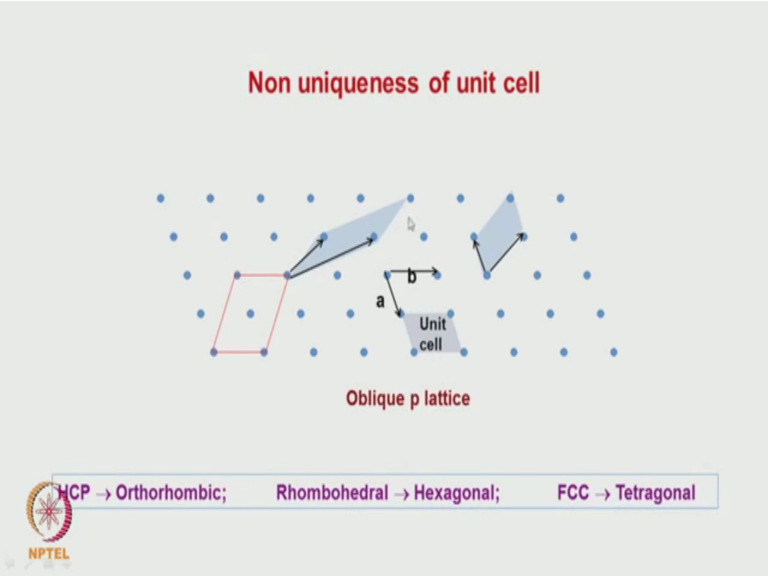


All of them represent the periodicity in the lattice right, we keeping one adjacent to each other we can generate the in this case a 2 dimensional lattice; it could be a primitive unit cell or it could be a non primitive the examples is that we can have an HCP; HCP itself can be represented in terms of orthorhombic, similarly FCC we know that can be considered as a tetragonal unit cell which c by a ratio equals on 1.414.

So, these sort of situations are always there and in many phase transformation also like FCC when a transformation takes place it can go into orthogonal orthorhombic structure, similarly in from FCC to orthorhombic structure transformations can take place FCC to tetragonal rhombohedral to hexagonal, there are various types of especially for rhombohedral to hexagonal what it happens is that it is only a convenience for which sometimes we can represent in rhombohedral coordinate system are in some cases you can represent them in terms of hexagonal coordinate system.

So, today we will talk about if you represent it in one coordinate system or another, how the indices of the planes and directions will change that is very important. Let us take a 2 dimensional that is this is a disordered hexagonal lattice which we are showing.

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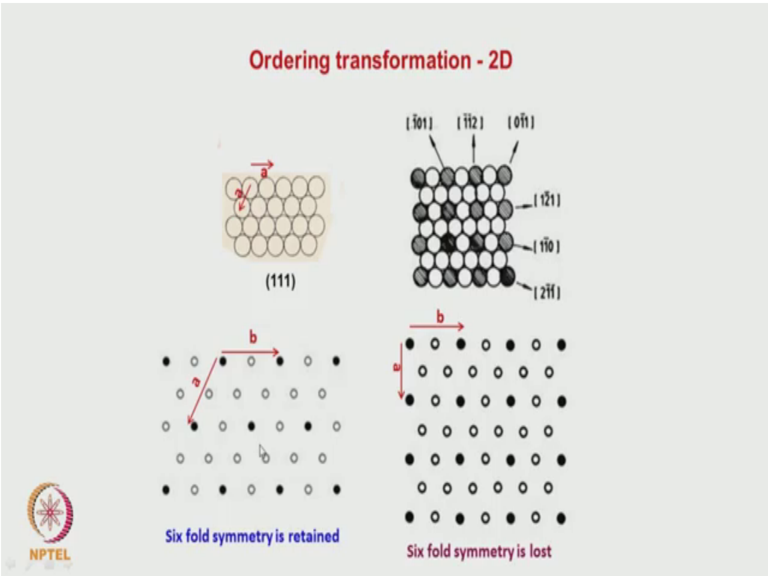


And in this as well as in this if you see it is the lattice translation vectors which is being shown with angle between them 9 120 degree; in this particular case you assume that an ordering is taking place it transforms into an ordered lattice. Now if you look at this ordered lattice, atoms are occupying specific positions if you look at the unit cell this will be the a lattice parameter, this is going to be the b lattice parameter, now what is essentially happening is that the unit cell is essentially in this case has become a rectangle.

So, when we represent the ordered lattice we are going to represent as a rectangular unit cells, when we represent the disordered lattice we are going to represent it as a hexagonal unit cell; and in this lattice suppose you take diffraction pattern where that you have both the structures, now how are you going to index them? Then you should understand what which plane will change into which plane in the ordered lattice, this is what this transformation of indices help us understand. This is an another example where it is on a hexagonal lattice, it is essentially transforming into an another which is an ordered which is hexagonal, but in this specific case which only the lattice parameter s double; that is as far as a 2 dimensional lattice is concerned, we can take the case of a 3 dimensional lattice here I have taken an FCC lattice.

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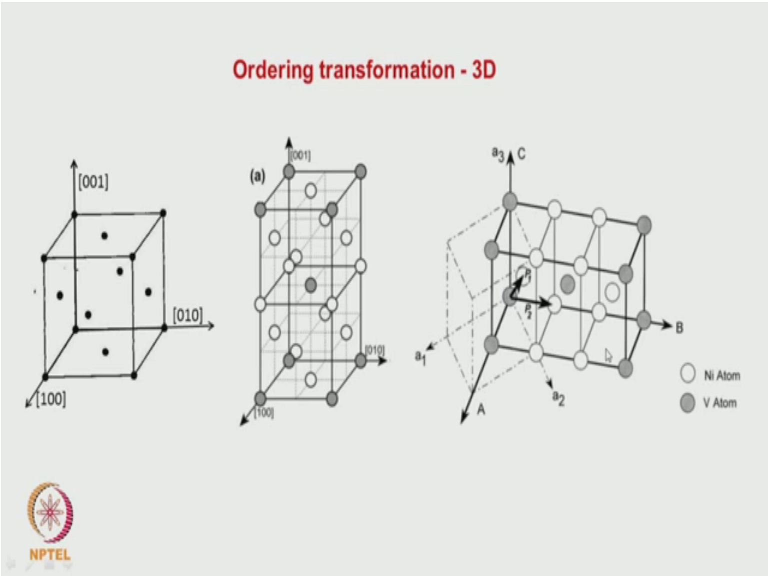


We assume the; this is an FCC lattice ok in this lattice we are showing our unit cells in this specific case, the lattice is essentially infinite. Atoms we assume that it is an alloy which contains 2 types of elements, we cannot distinguish which atom are occupy which position so we call it as disordered one chemically disordered one. Case which I have considered where is an ordering is taking place and the unit cell of the ordered lattice which is being shown here. In this specific case if you look at the unit cell it is as if 2 FCC lattices are kept on top of the other, and then the in this direction as well as in this direction that is a and b the large parameter remains the same, c direction the lattice parameter has doubled because one is kept and some ordering has been introduced at specific position this is essentially a body centered tetragonal structure.

Similarly, we can consider another structure where it is going from FCC to an orthorhombic unit cell. So, these sorts of phase transformations are quite often seen; we will be getting diffraction pattern due to the ordered lattice as well as the disordered lattice. So, there are ways in which and there and these transfer type of transformation when they occur, there is some orientation relationship between the lattices because of that we can index the deflection pattern either in terms of the FCC lattice, are we can index them in terms of the ordered lattice also, but in both the cases the same point we will be representing with 2 types of g vectors, depending upon the whether we have chosen the ordered lattice are the disordered lattice to represent. I have mentioned already that unique cell is not unique here what I have shown it that same the case which I have considered in this specific case is the body centered tetragonal unit cell which I have taken, I had just shown that diffraction pattern corresponding to it.

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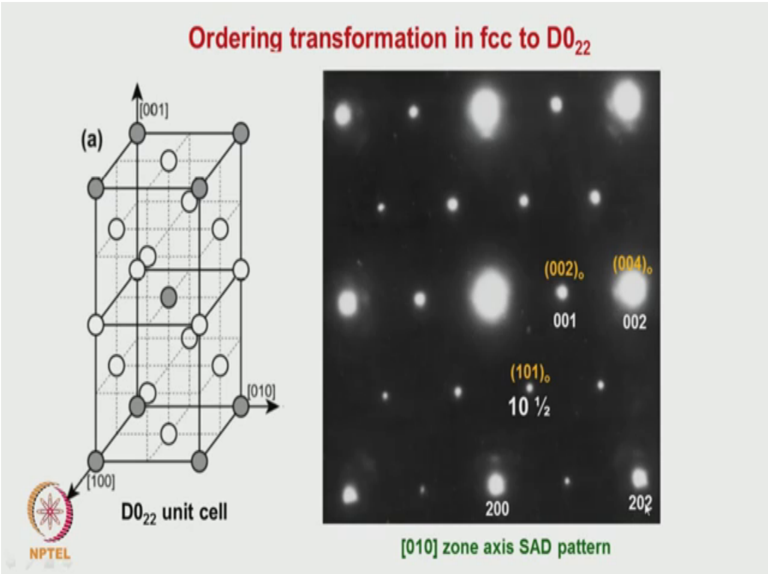


If you see in the literature this diffraction pattern thus parts could be this part could be indexed as 200 this will be indexed at 0 to 0 these are all fundamental reflections, the same fundamental reflection 002 for the body centered tetragonal, the fundamental reflection will be 004, but as far as matrix is concerned FCC we represent it as 002; similarly this 001 is the represent 002 of the ordered lattice, similarly that in terms of matrix are the FCC lattices if we represent, this specific spot we will represent a 1 0 half which in terms of ordered lattice to be represent 0 1 0 1. So, these from looking at this we can make out that some correspondence is there, but is there any procedure by which we can determine this, this is what we are going to discuss in today's class. This is just an example to show; what is the need for it?

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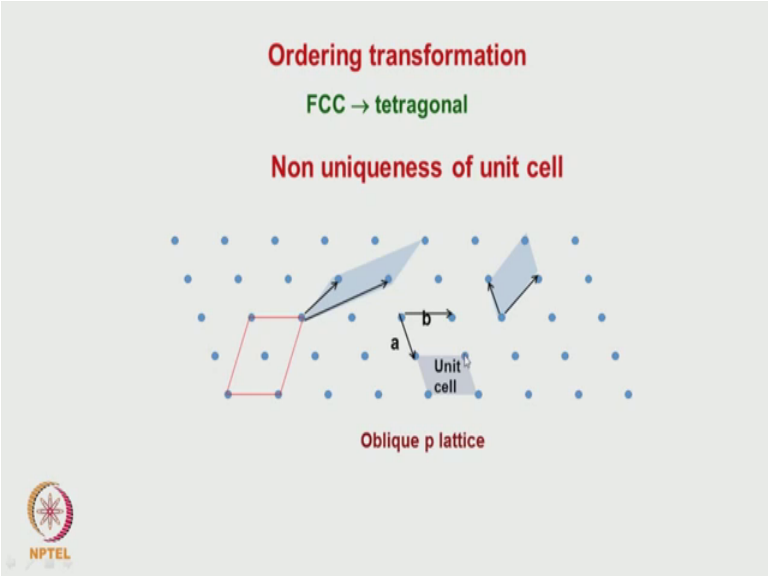


So, FCC to tetragonal is one which transformation which we have considered another I mentioned that this is not the unique one.

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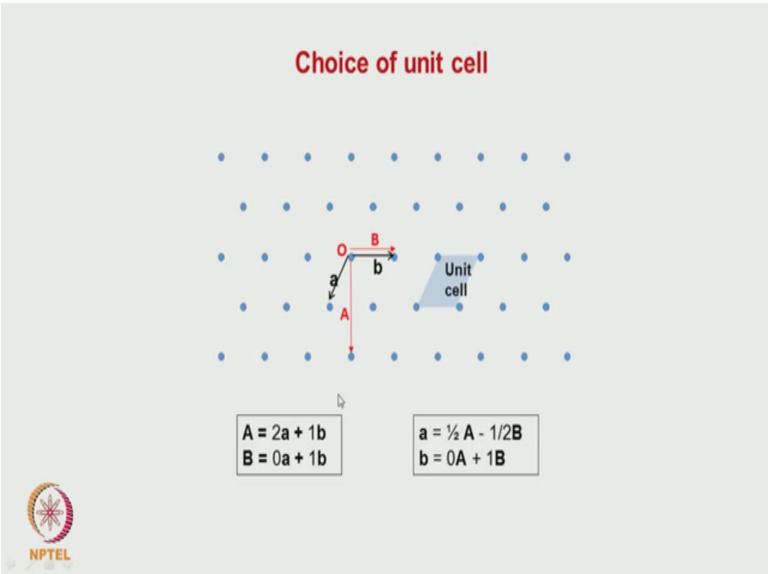


Now before we go into the procedures the general procedure, let us take it with just an example this is again a hexagonal 2 dimensional lattice which I had shown, in this lattice this is the a lattice parameter this is the b lattice parameter which is nothing, but equals to

a. The same as a and b are equal and angle between them is 120 degree, this is how we represent the hexagonal let 2 dimensional lattice. The same lattice can be represented, but this is a primitive one hexagonal lattice and we can represent it as r c centered rectangular lattice. So, in these c centered rectangular lattice if you see the lattice parameter this is A and this is B.

So, in terms of this lattice parameter in terms of the rectangular lattice we wanted to present in terms of the hexagonal lattice, how we will go about? This a will be written as 2 a plus 1 b; b will be represented as 0 a plus 1 b, this is how this is the in that terms of rectangular lattice this is in terms of the hexagonal lattice. In terms of hexagonal lattice we are writing the coordinates ok of the rectangular lattice in terms of the hexagonal lattice. We can do it the other way round also so then what will happen if that, a will be equal to half into A minus half into B, b will be equal to 0 into A plus 1 into B; that means, that when we wanted to represent hexagonal lattice in terms of the rectangular lattice, these 2 cases if you look at the type of equations which you use they are not the same let us take a generalization.

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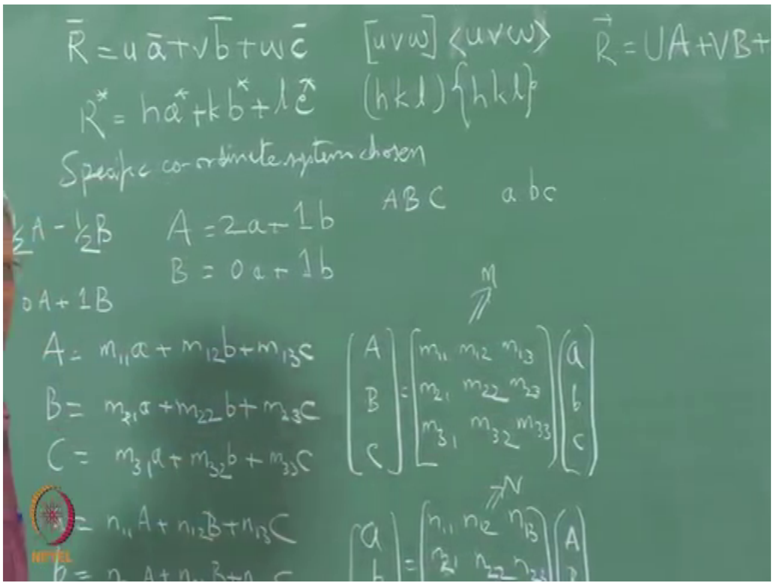


So, essentially what we are trying to do it is that in any lattice if you consider abc are the coordinates which represent the unit cell vectors, then this is for 1 lattice and the original lattice r it is the coordinate of the unit cell of the transformed lattice in terms of the old lattice we wanted to find out; then this can be return us this is I am just writing it in terms of. So, m 1m these are all the coefficient, this I am writing it so that it can be written in a matrix notation that is all. B will be equal to c so that means, that like here what we have written 2 and 1 and 0 and 1 are the coefficients, similarly we are taking some coefficients like this.

So, this can be written essentially s into 2 m 23, m 31, m 32 this way we can write this is write. Similarly we can see that when the world coordinates we wanted to represent in terms of the new one then these indices are not the same. So, we can use a different symbol to represent it. So, then it will happen a will be equal to I will write into c n 3 3 into c correct. Here now if we represent a, b, c, this will be in terms of n 11, n 1 2, n 13, n 2 1, n 2 2, n 2 3, n 3 1, n 3 2, n 3 3 you can write it in this form correct. So, these are 2 different matrices.

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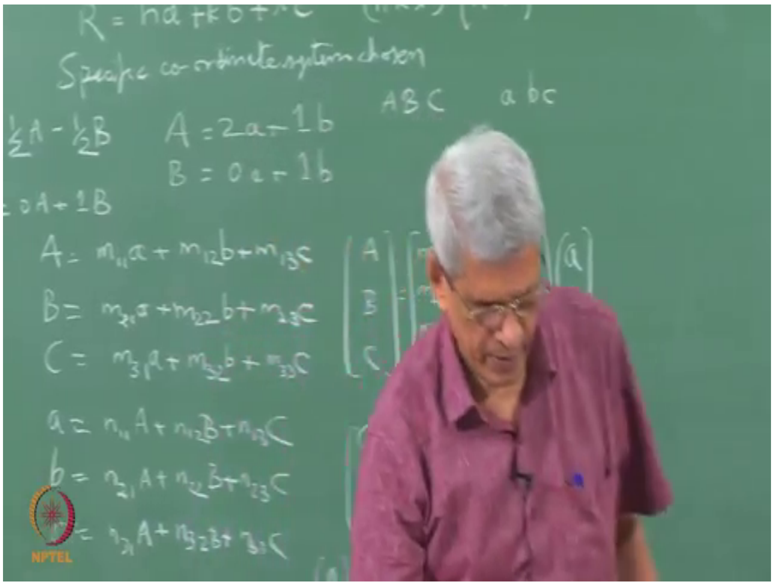


Now, suppose I wanted to represent this in terms of a b c, now this a b c if I substitute this one what it will happen? Suppose this matrix I put it as M and this side I right it has N.

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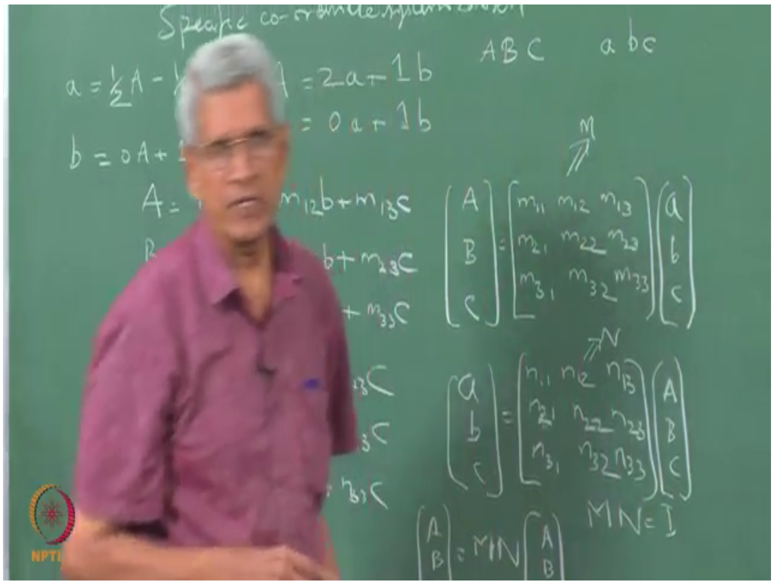


Then what it will happen is that this a, b, c will come in terms of M into N into a b c it will happen correct; that means, are nothing, but M into N equals I and in identity matrix, in which case it can happen if that when they are inverse of each other correct that relationship comes from here. So, this; what we have looked at; it is only the transformation of the coordinates which we have looked at it, how we can go from one coordinate system to the another write it. But what essentially we have to consider is that in this particular case if you take a vector r, the vector r irrespective of whichever the coordinate system which we choose it that remains that same vector it is main tan. So, now, we can represent the same vector as R equals in the world coordinate system, and in the new system suppose we wanted to write this R equal to U into A plus V into B plus W into C we can represent it, correct.

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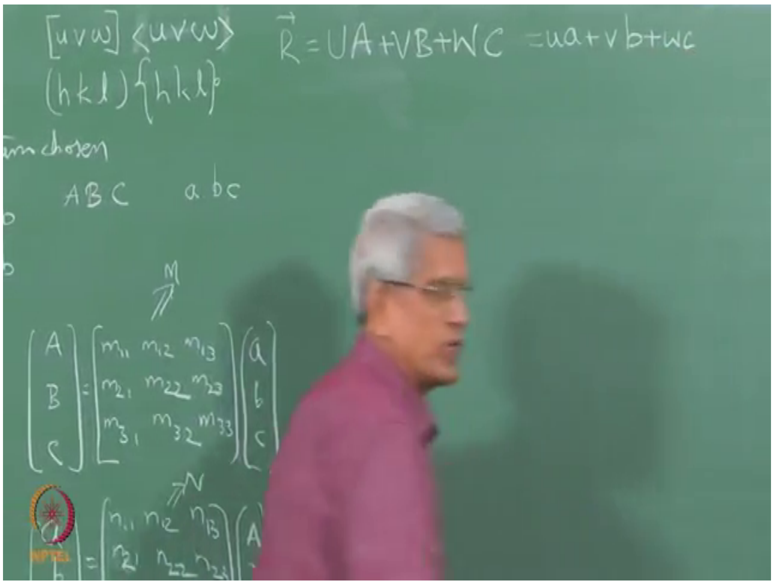


What we can do it is, this essentially means that this equals u into a, v plus w into c correct this what it is value their respective which coordinate system which we chose the vector has to be the same.

Now, we can substitute for a b c in terms of the world coordinate system and e frequent the coefficient of a b and c then we can find out the value of U V and W in terms of this equation we can find out correct? That part of the substitution I am just not doing, but I will give you just what the value is going to turn out to be.

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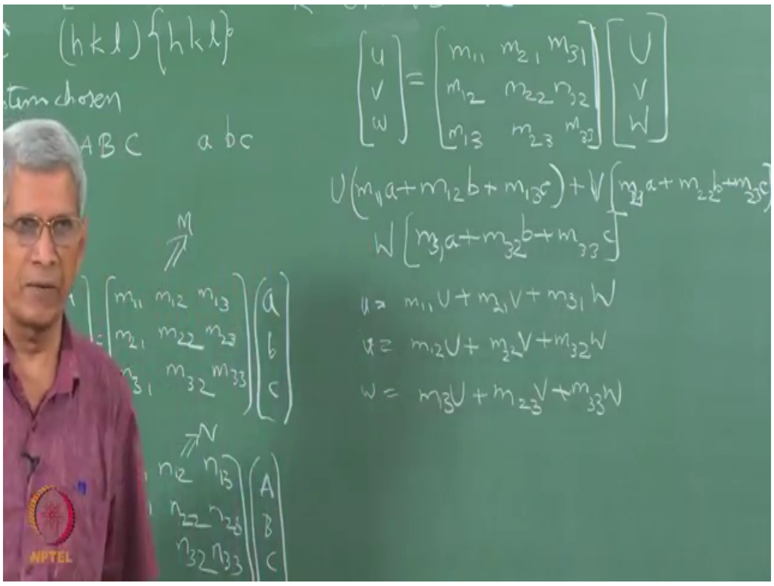

This is what essentially it will turn out to be, what essentially are we can just try to cross check whether it is right or wrong so that we do not make a mistake. I can substitute for here U into a can substitute in terms of m 11 into a, plus m 1 2 into b, plus m 1 3 into c, plus V into e m 2 1 into a, plus m 2 2 into b plus m 2 3 into c plus W into m 3 1 into a, m 3 2 into b, c m 3 3 into c. If we take the coefficients of a alone then what it will happen on that side it is u small u, it equals m 11 into U, plus m 2 1 into V plus m 3 1 into W correct is it right.

So, now similarly we can write it for v which will be m 1 2 into U plus m 2 2 into V plus m 3 2 into W this is V, W equals m 1 3 into u m 2 3 into V plus m 3 3 into W from this we can get this expression this clear.

Similarly, we can get it in terms of the u v and w in terms of small u v w we can find out, but what is essentially is going to happen is that now a b and c we are going to substitute with this equation.

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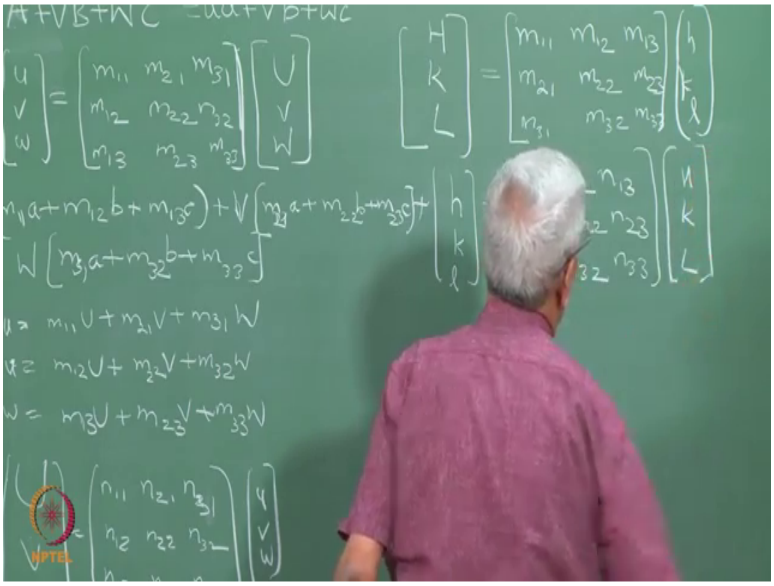

Now, what will happen is that in that case will be m 11 n 2 1, n 2 3. n m 1 2 n 2 2 now n 3 1 n 3 2 n 1 3 n 2 3, n 3 3 into small u v w this is how it will turn out to be. So, when we have to for a direction if you see with respect to what we have taken for transformation from here to here. So, that is from the old axis to new axis when we come, here for the direction in the new one it is in terms of this u k an understanding it will be essentially nothing, but the transpose of one the other is this clear? Because here what we have done is substituted for a b c in terms of this one now we have found out, what is the relationship this is with respect to similarly we can find out relationship between planes also. In the case of a plane what will happen is I will just write down the if it is in the new coordinate system HKL capital HKL represent the indices of a plane, this will be equal to this is going it will be the same as that for the coordinate system for the plane.

Similarly, for small h k l, this will turn out to be n 2 2, n 2 3 this is how it will turn out to be. Is essentially since for the case of (Refer Time: 26:06) for the going from one lattice to another where we wanted to find out the transformation of indices with respect to a direction k we chose a vector in the space in which the lattice is defined. But h k l is essentially nothing, but coefficients in reciprocal lattice now you take a vector in the reciprocal lattice like the way we have defined it. If we use this vector how exactly it can be done is that? This is in terms of this lattice correct similarly we can define a vector in reciprocal space also, if we choose that for both the lattices which over be the indices which we have used both we will have 2 types of lattices which will be there, then essentially what will happen is that. Suppose we take h into A star plus star plus l into C star this is all in capital which we have taken.

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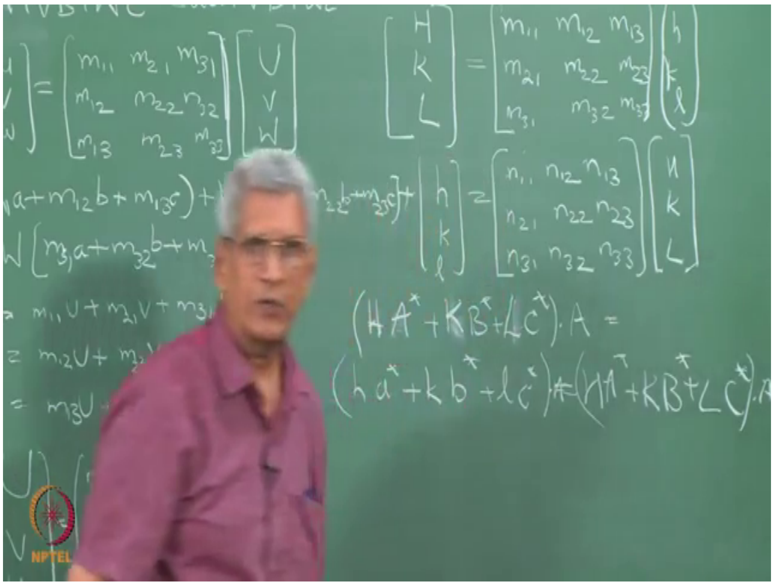

With respective which if we take a dot product with respect to a then what will happen? See this will be getting some value correct, but similarly in reciprocal lattice also no sorry this is H this is K the coefficients have to be L correct and with respect to the old lattice the reciprocal lattice vectors will be h into a star, plus k into b star, plus l into c star correct. So, these 2 vectors this has to be the same in the reciprocal lattice also because the way we have transformed from in real lattice from one unit cell to another, similar way in the reciprocal lattice also we will have corresponding to old lattice one unit cell of reciprocal lattice and for the transformed lattice also they will be an another reciprocal lattice a vector has to have the same magnitude that does not change right. So, we can write an expression like this and if we take a dot product of these with respective a, and we take a dot product here also on this side also we have to put to a to take a dot product.

Now, if you substitute what is essentially is going to happen is that this a can be written in terms of the world coordinate system then we will be finding that value. Here what it will happen A; A star this will turn out to be only h the rest of the terms will not be there. So, from this expression we will be able to derive this. This part of the derivation I am not going into the detail this you can do it this is how the final formula comes. So, now, essentially you have got transformation matrices for going from one unit cell to another for direction as well as in as well as for planes, is it clear? This can be used to go from one lattice to the another we can find out the transformation of indices. Let us just take one example that is what we will do it is yeah from a simple hexagon it transforms to an orthorhombic unit cells.

So, if we come back to this lattice which is shown in this slide this is essentially a hexagonal lattice, a b we have defined it and if we assume that next layer is kept on top of it at a distance c then it forms a simple hexagonal lattice and here this is a and b lattice there for a rectangular lattice, and the c direction remains the same then it becomes a orthogonal not orthogonal orthorhombic this becomes an orthorhombic lattice. So, it is an hexagonal to orthorhombic lattice which is going. If you look at the expression for a b and c what it will turn out to be ok.

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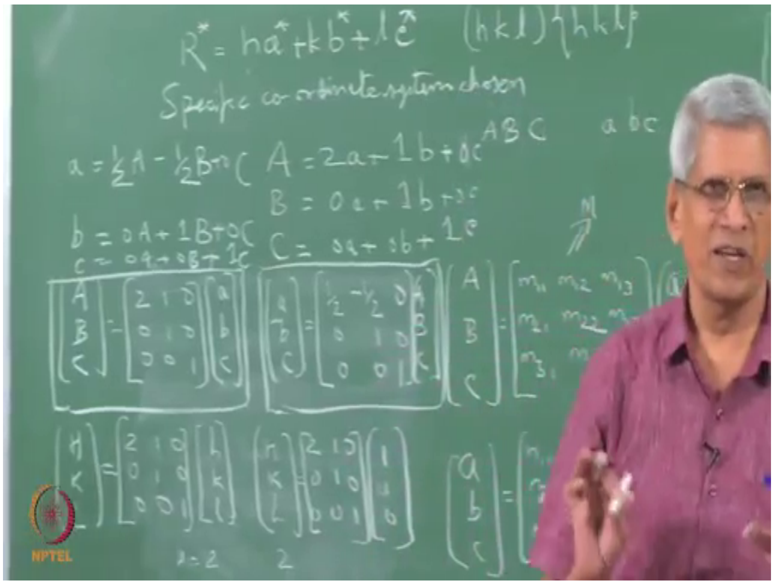


We have written this expression here it will become 1 into c correct for this lattice; here also what it will become b is no a will be this is 0 into c, because the 0 direction there is a vector a when we represent it there is there is no projection correct no component of a in the because it is in the basal plane correct. Here it will become 0 into c and what will happen to c 0 into a, plus 0 into b, plus 1into c correct. So, now, this matrix if we look at it ABC, this will turn out to be 2 1 0, 01 0, 001 into a, b, c, correct.

Similarly, we can do a substitution here as far as a is concerned there is no component in. So, this will become 0 into C, this will become 0 into C and the small c will be 0 into A plus 0 into B plus 1 into C. So, this if we look at it a b and c will turn out to be half, minus half, 0,01 0, 001 into this is how it will turn out be these 2 equations; this is one this is the equations for going from one coordinate system to the other; hexagonal to rectangular the orthorhombic are from orthorhombic to hexagonal. No planes we know that how it has to be indexed, if we know suppose we wanted to find out h k l; HKL also is the same matrix which works will be equal to correct suppose we wanted to find out 1 0 0 plane in this lattice hexagonal lattice, then what it will happen for then h k l will turn out to be 2 1 0,01 0, 001 correct what will HKL will turn out to be 2 0 0 correct. That is h k l this will turn out to be 2 correct yeah r h will turn out to be here 2, k will turn out to be 0 correct l will turn out to be 0.

We can take an another one that is suppose you wanted to take 1 1 0 now what it will happen? H will turn out to be 2, k will turn out to be 1, l will turn out to be 0. So, 1 1 0 in hexagonal lattice will be represented as 2 1 0 plane in the orthorhombic lattice. So, this is how we can found out correspondence between planes similarly we can find out correspondence between directions also. So, that I want to be able to work it out as an exercise; this you can think of various planes one can choose and try to find out how correspondence. In fact, for any crystal structure similar type of correspondence we can find out this is we have initially took for a 2 dimensional case, now we extended to a 3 dimension similarly for all the lattices when you know the unit cell in one and how it is oriented with respect to that when it transforms into the other lattice, we will be able to find out directions. And this method is what is used here to represent these planes in the ordered and the disordered lattice is it clear.

Similarly, I mentioned about that another case like from that is from Rhombohedral to hexagonal; because sometimes in some cases the Rhombohedral has to be expressed in terms of hexagonal lattice, that also you know what the coordinates of Rhombohedral are if you use a hexagonal lattice what will be the coordinates, one can write the transformation matrix to go from one coordinate system to the other, then using these formulas which are returned for directions as well as for that planes, one can immediately find out the correspondence between the planes and directions between the 2 lattices. In fact, the same this formalism could be used to find out direction between planes in one coordinate system to an another coordinate system in any type of transformation.

Most of the time will see that in ordering transformation is essentially where the atoms are replaced had some positions in the disordered lattice and then an order lattice forms; when that ordered lattice forms it could have a symmetry which is lower than that of the disordered lattice, not only that it can have the lattice parameter which could be either the same as that of the order lattice or that of the disordered lattice or the lattice parameter could be more this sort of far transformation could occur. So, in all such cases using this formalism one can easily find out the correspondence between planes and directions, and this is very much necessary when we wanted to index diffraction patterns in terms of either in the matrix in terms of the disordered lattice are in terms of the ordered lattice we will stop here now.