# Crystals, Symmetry and Tensors
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## Lecture 4a
## Coordinate Transformation

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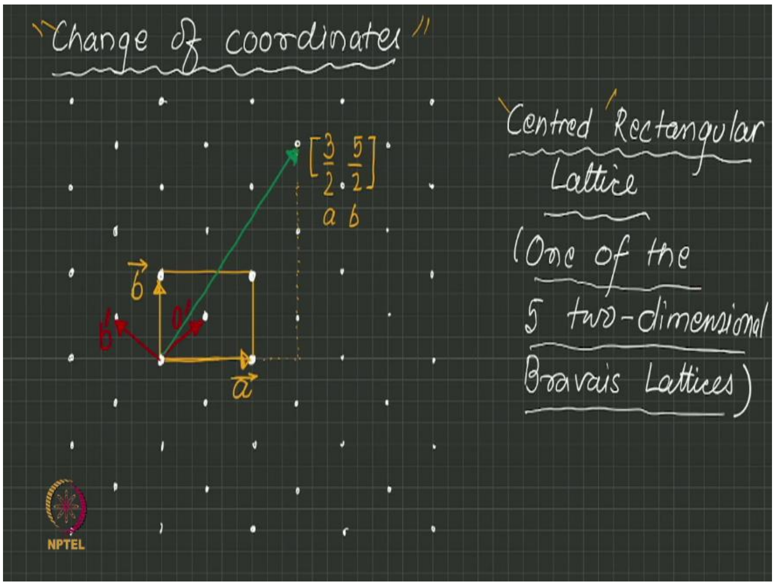


Good afternoon. So, we will discuss now a very important Concept in crystallography and that is change of coordinates. Of course, this is not particularly specific to crystallography as you know, everywhere where you discuss vectors or matrices you need to sometimes use one coordinate system, sometimes other coordinate system, and you need to find out how do they communicate, how you transfer from one coordinate system to another coordinate system.

As an example from crystallography, I am showing you here, what is called a centred rectangular lattice, this is one of the 5, there are 14 Bravais lattices, you must all be knowing in three dimensions, you might not have thought much about two dimensions, but in two dimensions there are 5 Bravais lattices. We will look at them in detail, this is just a preview.

So, here you can see why a centred rectangular lattice, so you can see that the unit cell is a rectangle and the lattice points are not only at the corners but also at the centre, so that is why the name centred rectangular lattice, two-dimensional example of let us say, two-dimensional analogue of face centred cubic lattice.

So, here there is a rectangle and that has a lattice Point not only at corners but also one at its centre. Now, obviously if this is the unit cell, the corresponding crystallographic coordinate system for this will be the edges of the unit cell, and this is the so-called conventional unit cell of this lattice. So, the conventional unit cell is defined by one of the vectors, one of the basis vector along one edge of the rectangle, another basis vector along the other edge of the rectangle. So, a and b are nice crystallographic coordinate system, the conventional crystallography coordinate system of this lattice.

But the cell they generate, as the name itself suggests centred, the cell they generate is centred, so the cell they generate is not primitive, so it is not a primitive unit cell of this lattice, so the correspondingly the basis vectors a and b are not primitive basis vector, but sometimes we do need. So, this is nice because this shows the Symmetry we will see when we discuss the Symmetry that this shows the symmetry of the lattice, that it has a rectangular symmetry, so the two vectors are perpendicular to each other.

But sometimes, we do need primitive unit cell because primitive has its own advantage, that there is only one lattice Point per cell, there is lattice Point only at the corners of the cell and not inside. So, suppose now we select a primitive unit cell for this, so one possibility of selecting primitive unit cell will be to go from the origin to the centre, let us go to the other side also, so call this a prime, and call this b prime.

Now, let us select a vector, a lattice translation vector in this lattice, so let me select arbitrarily, let me select this one, this green vector has my lattice translation vector. So, we see that green vector, what will be its coordinates with respect to a and b, 3 by 2 a, so a we do not write in the coordinate, so 3 by 2 and for b, 1b, 2b and half b, so two and a half, 3 by 2, 5 by 2, that is the difficulty we have to live with if we are using a non-primitive basis vectors.

In non primitive basis vectors, all lattice points will not have integer coordinates, some of them will have integer coordinates, some of them will not have. So, this because the central lattice Point itself is half-half with respect to a and b, the one lattice point within the unit cell is half-half, so it has a fractional coordinate, so this one also turns out to have fractional coordinates.

In the primitive lattice vectors, they will always have integer coordinates, so if I transform this into a prime, b prime, so this was with respect to a b, the question is what is the coordinate of the same green vector with respect to the red? So, that exercise is what is involved in change of coordinates. I want to know that I want to represent this green vector, now not in the ab coordinate system but a prime b prime coordinate system, so how do we do that, we will come back to that.

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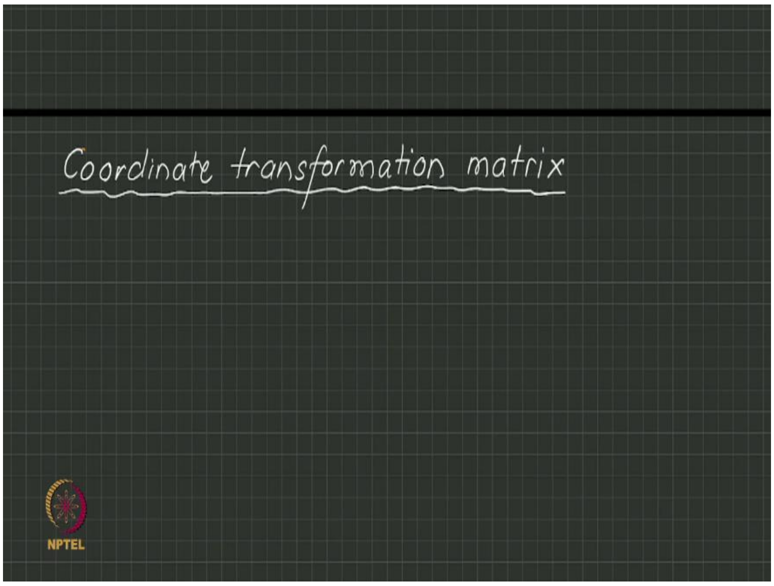


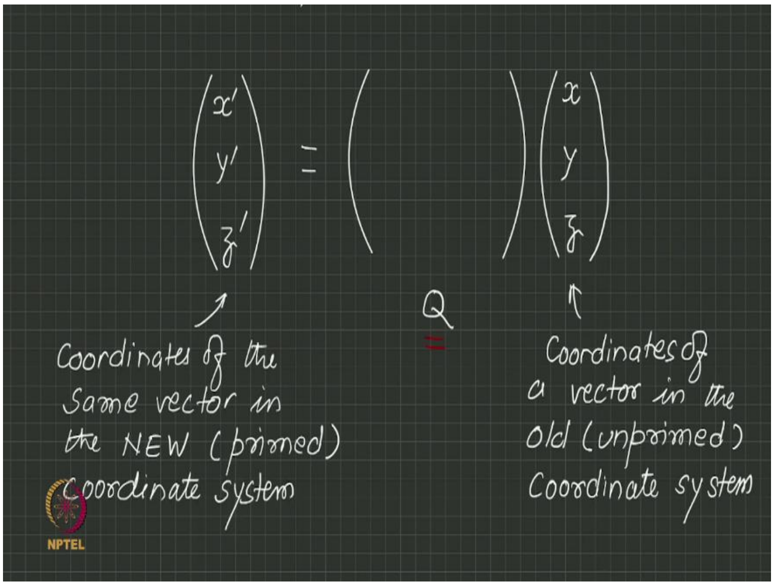


So, the way to do that is to set up a coordinate transformation matrix, that is we want to find out a matrix. Let us say a matrix Q, such that if I give it, if I supply a set of coordinates, I gave you a two-dimensional example, but now I am writing a three-dimensional Matrix, in two Dimension, you will have a 2 by 2, in three dimensions 3 by 3.

So, if I multiply it with coordinates of a vector in a given coordinate system the coordinate transformation matrix, after multiplying it by coordinate transformation matrix the column vector which I should get is x prime y prime z prime, which is the coordinate of the same vector in the new coordinate system.

So, this is of a vector in the old, old or unprimed because in my notation I am using unprime for old, so coordinates of a vector in an old unprimed coordinate system, this is a very simple concept, but I am going slowly and because it is important to grasp this because all those simple leads to often confusion if you are not thinking carefully about it. So, you have to think very, very carefully and that is what I want to do for you.

So, and then this x prime y prime z prime is coordinates of the same vector, there is no change of vector you see. Now, we want to find out the mechanism to transform, the machinery to transform from one coordinate to another coordinate. So, the green vector is existing, but with respect to the yellow axis, the conventional axis, the rectangular axis, its coordinates we have already found is 3 by 2, 5 by 2, what is its coordinate with respect to the red one, you can again separately find it or we can convert this using a matrix which is known as the coordinate transformation matrix, which we are giving the symbol Q.

So, what this coordinate transformation matrix should do? The coordinate transformation matrix it is supplied with the old coordinates, the matrix multiplies the old coordinate and gives you the new coordinates. So, the coordinates of the same vector in the new or because of my notation I am calling it prime, prime coordinate system. So, this is the magic which Q should do the matrix should do, but how do I find this magic Matrix?

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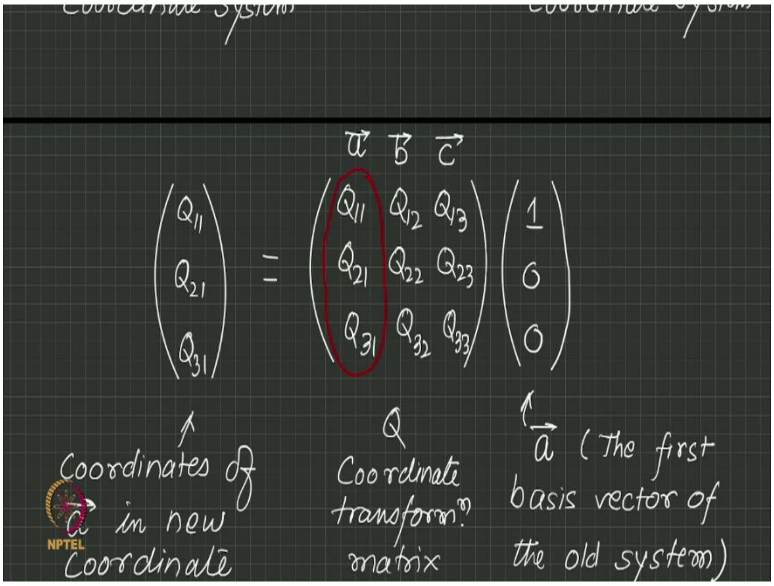


So, let me write the columns of this magic matrix, this is the matrix, now I choose a very special old vector, any old vector will be transformed into a new vector or any old coordinate of a vector will be transformed to the new coordinates of that vector.

So, but since this vector can be anything, I choose it to be a very special one, I choose 1 O O, what does 1 O O represent in terms of my coordinate system, a, so this is nothing but a, because remember this is coordinates of a given vector in old coordinate system, so 1 0 0 in old coordinate system is the first old vector which is a so this represents a that is the first basis vector of the old system.

Now, you all know matrix multiplication, so you can let me know what will be the product column, If I multiply 1 0 0 with this matrix Q 1 1, Q 2 1, Q 3 1. And if you notice, so this is where this will be the coordinates of a in the a prime b prime system or in the new system, coordinates of the first old vector in the new coordinate system.

But notice what you have got, you have got just the first column of this matrix, which means the first column of the coordinate transformation matrix this was your, so this was your coordinate transformation matrix, and the first column of the coordinate transformation matrix is nothing but the transformed first old vector, this is the nothing but the a vector written in the new coordinate system.

A vector written in Old coordinate system is 1 0 0, a vector written in new coordinate system will be Q 1 1, Q 2 1, and Q 3 1. Similarly, if you have understood this, you have understood the coordinate transformation matrix formulation, because the second one, If I multiply by 0 1 0, I get the second column, so second column will represent b, and the third column will represent c.

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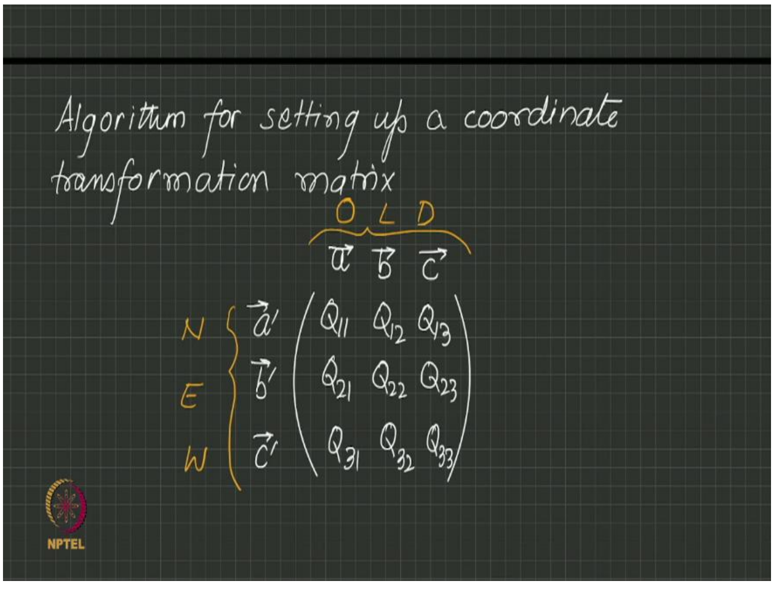

So, this means you have already found the algorithm for setting up your coordinate transformation matrix, it is as simple as that. So, how do you write the coordinate transformation matrix? Write the first column as the coordinates of a in terms of the new basis, and the new basis is a prime b prime and c prime, so you can see that these were the old, in any hierarchy old people are on the top, and the younger people are, younger people are on left, they have leftist leanings, so this is just a mnemonic, I am giving you to keep the row and column in order.

So, each column is an old vector, each row is component corresponding to the new vectors. So, the first row is first component with respect to the new basis, second row is second component with respect to the new basis, first column is the first old vector a second column is the second old vector b. If we have done this, then our job is done and we can now get back to our problem, our example.

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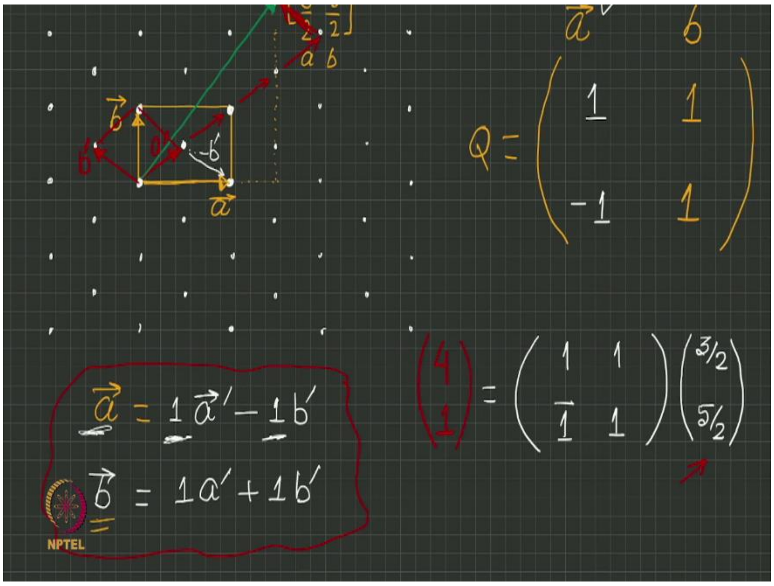


So, let us write down, now our coordinate transformation matrix Q for this problem. So, we have to write a, first column is a, but in terms of a prime and b prime, so what is a in terms of a prime and b prime? a in terms of a prime and b prime, 1a minus, 1a prime minus 1b prime, we are seeing that a prime, and then if you add a minus b to it minus b prime, you will arrive there, so which means this matrix which is now only a two by two matrix has the first Column as 1 minus 1, components of a, components of a in terms of a prime and b prime, 1 and minus 1.

What about b? How do I write b in terms of a prime b prime, 1 prime plus 1, b minus very simple all of you are with me, now I am hearing only one voice, but I hope everybody is with me. If I, if you just add a prime and b prime, you get the vector, b so b is 1 a prime plus 1 b prime, which means by my algorithm the second column of this matrix is the components of b with respect to a prime b prime, so it is simply 1 and 1, so I have set up the Q matrix.

So, now let me do the exercise let us use this Q matrix to calculate the coordinates of green vector in terms of the red vectors. So, 1 1 crystallography as you know we write minus 1 as bar, so we will use that convention, so bar 1 1, my old coordinates the yellow coordinates are 3 by 2, 5 by 2, and this should give me the multiplication if everything works well, multiplication should give me the red coordinates, and what the multiplication is giving 3 by 2 plus 5 by 2, 8 by 2 that is 4 and minus 3 by 2 plus 5 by 2 is 2 by 2 which is 1, 4 1.

So, it is telling you that the same green vector can be expressed as a vector 4 1 in terms of the red coordinates, let us see if that is right. So, we start our journey with a prime 4 a prime, so 1 2 3 and 4, and 1 b prime, so I go in the b direction, 1b prime, sorry for the confusion with the number but I hope you are able to see. So, 4 a prime and 1 b prime, just what the doctor ordered.

The matrix works, so this matrix magically gives me on multiplication with the old vector or the old components of the green vector, yellow components of the green vector, it gives me the new components of the green vector, the red components of the green vector. So, that is all, there is two coordinate transformation matrix, if you keep this in mind that columns are transformed coordinates of the old vector.

So, all you have to do is to take pick up one by one that so you do not have to worry about transformation of all the space or all the vectors in one go, just look at the three old basis vector catch them and one by one express them, this is what we have done here, one by one express them in the new coordinate system force, them to accept new religion.

So, when they accept that they change their name so 3 by 2, 5 by 2 becomes 4 1. We are also happy that we were knowing that this a prime b prime, the red ones are actually the primitive, because the unit cell the red unit cell does not have any lattice Point inside, that is a definition of primitive unit cell, and if it is a primitive unit cell we were also knowing that in terms of primitive unit cell all lattice translation should be integer even the fraction one.

So, it was having this fractional roop or fractional Avatar only because it was being represented by a non-primitive basis vector as soon as it realized its primitive origin it became integer coordinates, so that is very nice.

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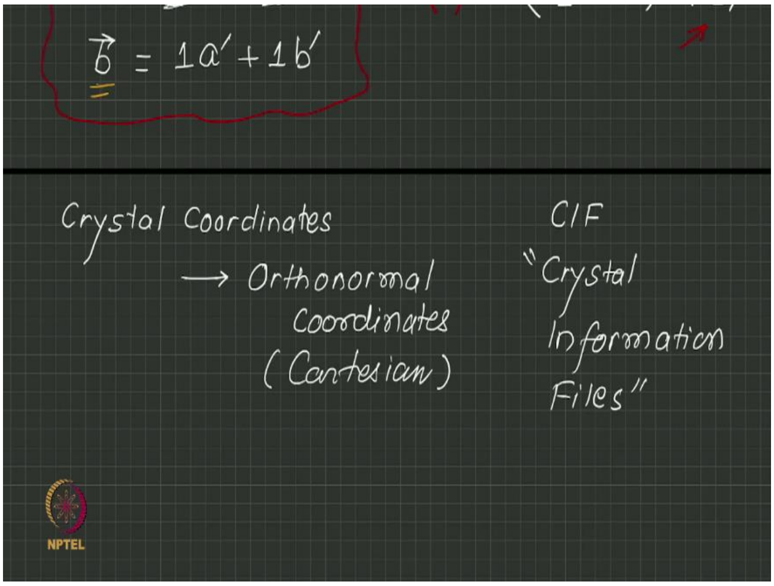


Let us apply this to one special case, which is very common and which is very much required and that is change of from Crystal, now Crystal coordinates system is crazy, a b and c, three different lengths, Alpha Beta gamma three different angles, none of them 90 degree, so it is really crazy, whereas orthonormal system or the Cartesian system with which you are familiar right from your birth that is so simple, all vectors equal, all vectors of unit length and all angles 90 degree, so calculations are quite often simple in your orthonormal system or Cartesian system.

And many of the programs, for example, you want to plot the crystal structure, so you will get the data Crystal structured data from x-ray diffraction or from CIF files, you should look up the CIF files, Crystal information files, so this is how the crystal structure data is recorded and communicated, so there will be always be in the crystal coordinate system, so the coordinates there will be Crystal coordinate system.

Now, you want to plot them and see on your computer how they look like and the plotting routines will always work in the Cartesian coordinate system they do not want to give waiters or recognize directly the crystal coordinate system.

So, if you want to plot your structure you want from Crystal coordinates to Cartesian or orthonormal coordinates, that is the Cartesian. So, out of many possible coordinate transformations which we can do, this one acquires some importance, so let us develop this particular one in detail.

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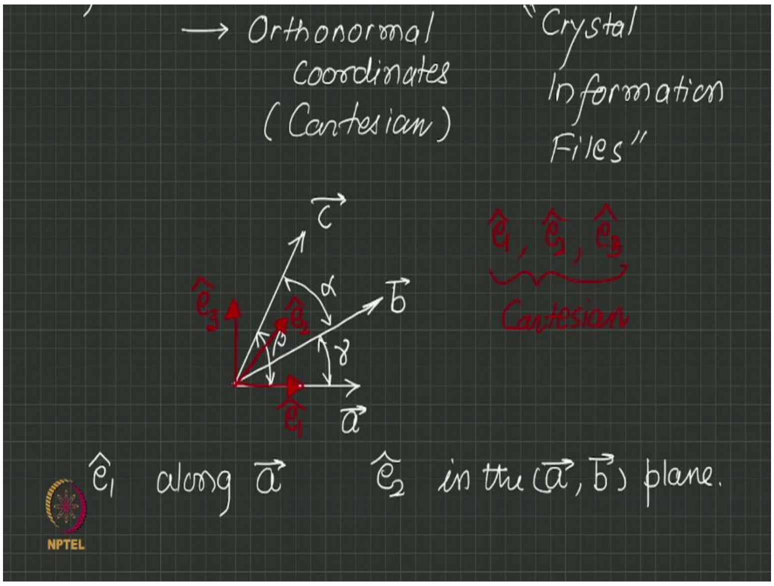


So, how do we do that? of course, the crystal coordinate system as I said, you have a, you have b, and you have c, now if you want to transform it to the Cartesian coordinate system, orthonormal coordinate system, the question is how that orthonormal system, how the i j k or how they e1 e2 e3 is oriented with respect to abc.

One way to do that, if there is no restriction and you are free to choose you want to make it as convenient as possible, and one of the conveniences to choose one of the Cartesian vector along here the first Cartesian vector along your first Crystal vector. So, let us select e1 which is Cartesian basis, so e1 e2 e3 is Cartesian, so we orient e1 along a.

Now, unless and until the angle between a and b is also 90 degree, we will not be able to orient e2 along b, because this angle is some arbitrary angle gamma, this is our convention we have discussed about this, that angle between a and b is known as gamma, angle between b and c will be known as Alpha, and angle between a and c will be known as beta, this is again crystallographic convention.

So, e1, so e2 will not be, so b will not be along e2 or e2 will not be along b. So, e2 will be somewhere but let us now again for simplicity force e2 to lie in the a b plane. So, we had e1 along a, e2 in the a, b plane. So, let us say that is e2 in the a, b plane, then we have no choice left for e3 because that will be defined by the cross product of e1 and e2 and will be mutually orthogonal to both, so e3 will take its own direction.

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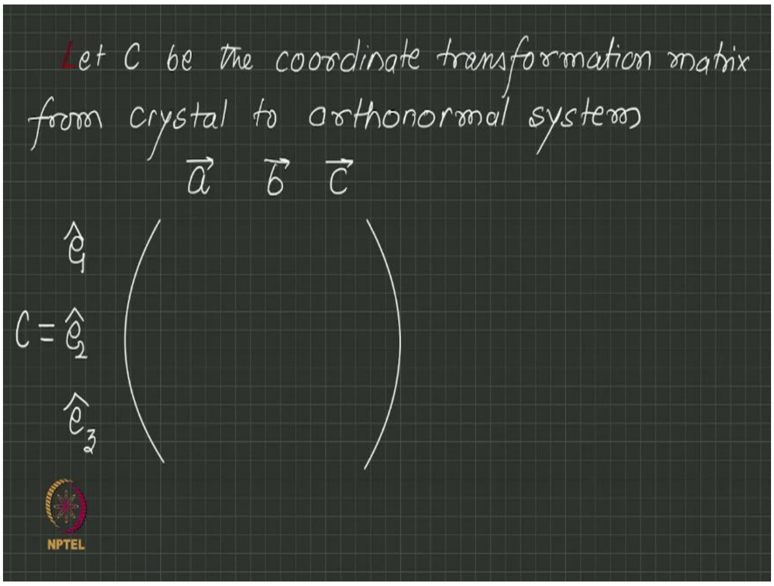


So, now we already know our algorithm for setting, so let c be the coordinate transformation matrix from Crystal to orthonormal system. Now, you can do this exercise easily, because you know your algorithm. Our old vectors are the crystal coordinate vectors, so they are on the top a, b and c, our new vectors are the orthonormal system, so they are on the left, and we just have to write, so we have to write the Cartesian coordinates of a b and c, that is all we have to do to get this matrix c, this is my matrix c.

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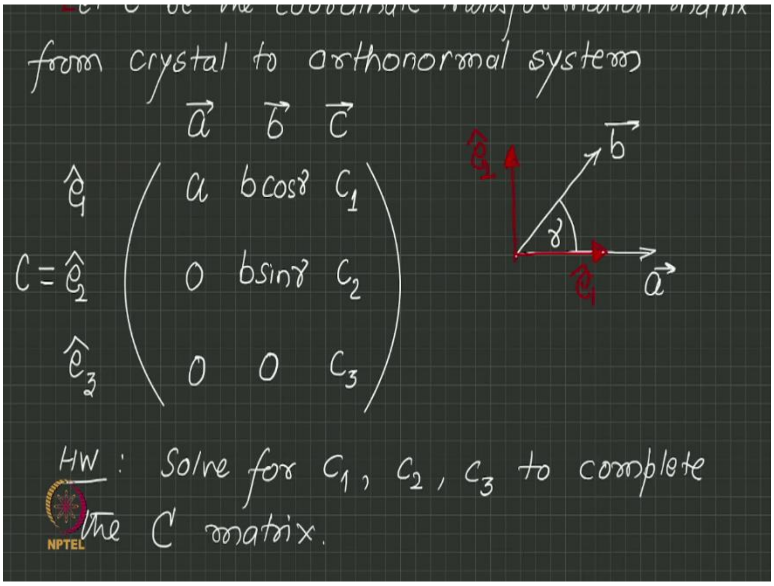


So, what is the Cartesian coordinates of a? a is along e1, so a O, O the first component will be its length Cartesian coordinates of a will be a 0 0, because we have chosen e1 to be along a. What about b? linear combination, yeah.

So, let us look at this plane, this was a, and this was b, and the angle was gamma, and we also chose our e1 along a, and we chose e2 in the plane of a and b, so it is very clear that, what is the components of br, in the e1 e2 e3 system, the x component or the e1 component is b cos gamma, the y component is b sin gamma, and the z component, z is perpendicular to this plane, so b will not have any component, because b is lying in the e1 e2 plane, so its z component is 0.

Similarly, you can solve for, I have done the easy part I am leaving the, little bit, is not really all that difficult but little bit more algebra is required. I want to do here in the class, so similarly you can solve for c1 c2 c3. Once you have this matrix, you essentially, if once you have set this matrix and you really hate Crystal coordinate system, hopefully not crystallography, you can always transform everything to Cartesian using multiplying by the c, and happily do your calculations.

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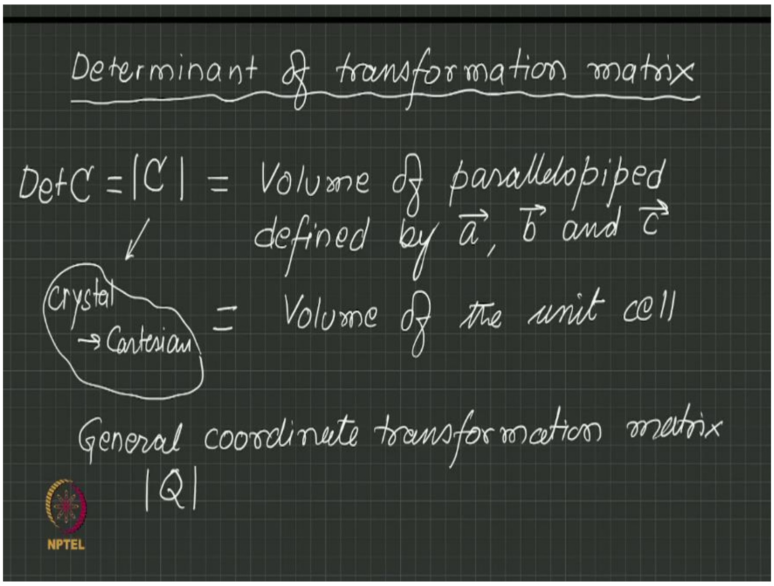


This matrix gives us also a very important interesting property of the determinant of the transformation matrix. What is the determinant of c matrix? So, what does that represent? If you have three vectors, I have three vectors a b c, and I have written their Cartesian components in the matrix form as columns and I am finding the determinant, what is the determinant represent from vector algebra? Volume of the parallel pipette, volume of the parallel pipette defined by a b and c, but abc was defining what in terms of our crystal structure it was defining the unit cell.

So, the determinant of c is nothing but volume of the unit cell. And therefore, it is volume of the unit cell, so if you expand this you will get the formula for, if you solve for c 1, c 2, c 3 and expand it you will get the complicated formula for volume of a triclinic unit cell.

Now, what about a general, so determinant of transformation matrix, so c was a special transformation matrix from Crystal to this was from Crystal to Cartesian the determinant of that is volume of the unit cell, what will happen to the determinant of a general that matrix Q from one Crystal coordinate system to another Crystal coordinate system?

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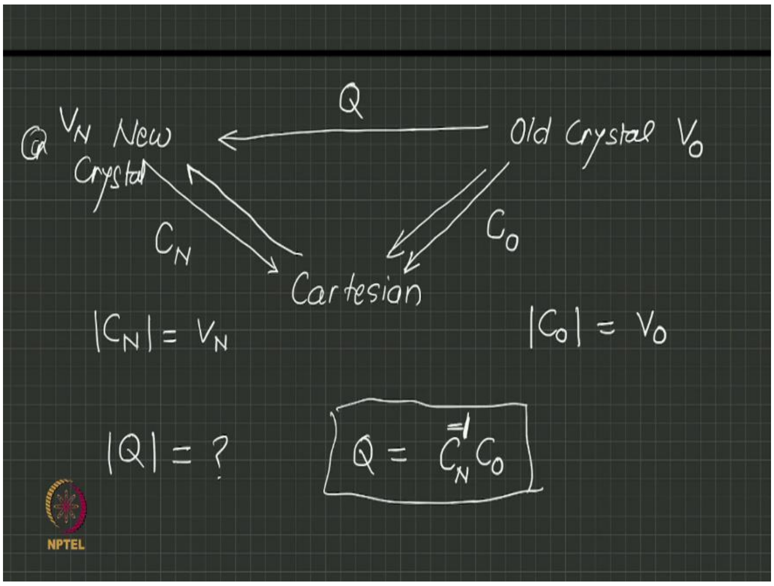


Scaling Factor, so which way we should do the scaling? Volume fraction ratio? You are right, just be a little bit more precise, let us do it this way from old to new we went by a matrix Q, from old to Cartesian we went by a matrix c, we can also go from new to Cartesian there will be another matrix c, so we distinguish, let us call this c old and let us call this c new.

So, we have now three bases, old crystal bases, new crystal bases and in between we have a Cartesian basis, C naught transform from old Crystal to Cartesian, CN transforms from new to Cartesian and Q transforms from old to Cartesian.

We have already established some property of, so let us call the volume of the old Crystal, Vo not the volume of the crystal, volume of the unit cell, volume of the unit cell of the old Crystal volume of the unit cell of the new Crystal even old Crystal new crystal is also a wrong phrasing I think crystal is the same old basis or old unit cell.

So, volume of the old unit cell, volume of the new unit cell and is V naught and VN, we have determined that the determinant of C naught is V naught, we have determined determinant of

CN is VN, just our current argument here, that C naught and CN are column vectors of a b c, so the determinant is volume.

What we want to find out is what is the determinant Q? Whatever is being achieved by Q will also be achieved by the product, suppose we first transform to C naught, and then we transform to the new, so from old we come to we first take the root, we are now going by the circuitous route. So, whatever Q is achieving CN inverse CN inverse C naught will also achieve the same, because if you give it a coordinates, old coordinates and you multiply by C naught, what you will get the Cartesian coordinates.

Now, instead of CN, I am multiplying by CN inverse because I am going in the opposite direction, so I want to transform from Cartesian to Crystal. So, if CN was bringing me from Crystal to Cartesian, C N inverse will take me from Cartesian to the crystal. So, CN, so if you are convinced with this that Q should be CN inverse minus C naught.

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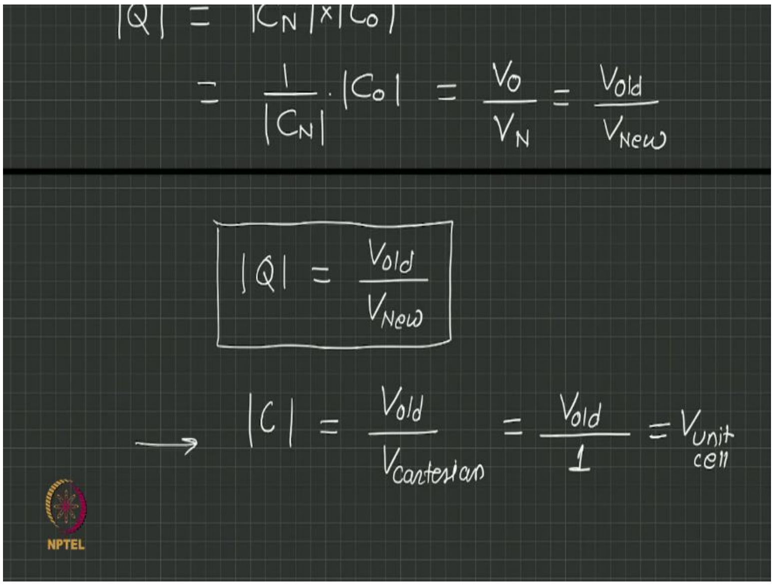


And that you know the property of determinant, the determinant of product is product of determinants, so you just multiply these two determinants. And you also know the determinant of an inverse matrix is 1 by the determinant of the matrix, but you have seen that C naught is V naught, determinant of C naught is V naught, and CN is VN. So, determinant of any coordinate transformation matrix, determinant of any coordinate transformation matrix is just the ratio of two volumes, the old volume divided by the new volume, so this is a interesting result which we will find some use later also.

So, the Cartesian was a special case, because you are going from Crystal to Cartesian, what is, so the new is Cartesian. If old is Crystal and new is Cartesian, what is the volume of Cartesian unit cell is unity, because it is a unit cube, so that is why there you got volume of the unit cell of the original, which we first saw.