Crystals, Symmetry and Tensors
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Lecture 5c
Metric Tensor

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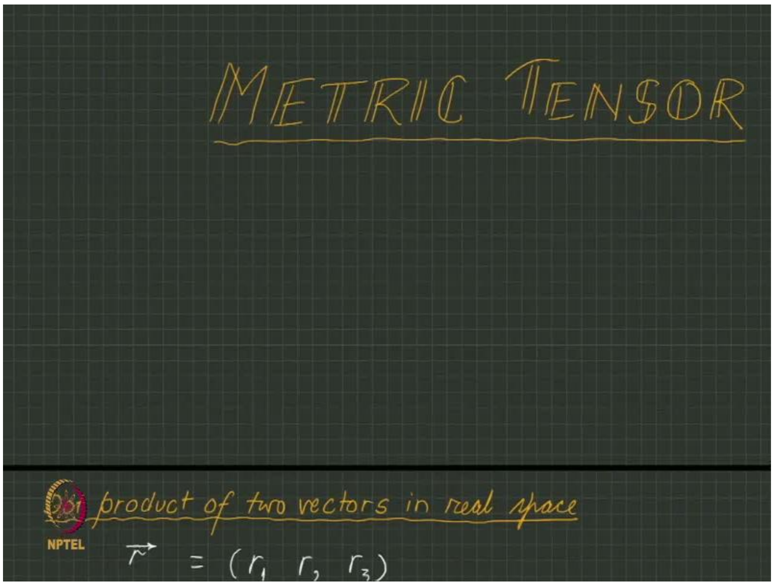

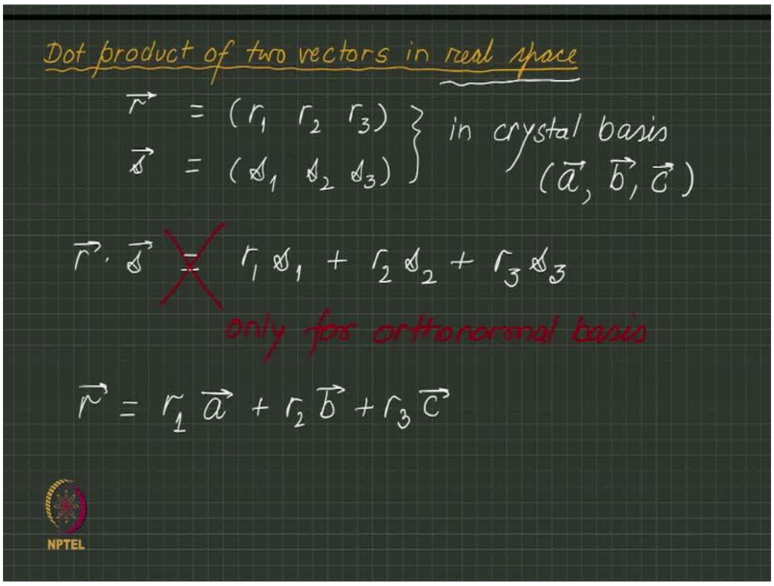

$$\vec{r}\cdot\vec{s} = (r_1\vec{a} + r_2\vec{b} + r_3\vec{c})\cdot(s_1\vec{a} + s_2\vec{b} + s_3\vec{c})$$
$$= r_1 s_1\, \vec{a}\cdot\vec{a} + r_1 s_2\, \vec{a}\cdot\vec{b} + r_1 s_3\, \vec{a}\cdot\vec{c}$$
$$+ r_2 s_1\, \vec{b}\cdot\vec{a} + r_2 s_2\, \vec{b}\cdot\vec{b} + r_3 s_3\, \vec{b}\cdot\vec{c}$$
$$+ r$$

$$\vec{r}\cdot\vec{s} = (r_1\vec{a} + r_2\vec{b} + r_3\vec{c})\cdot(s_1\vec{a} + s_2\vec{b} + s_3\vec{c})$$
$$= r_1 s_1\, \vec{a}\cdot\vec{a} + r_1 s_2\, \vec{a}\cdot\vec{b} + r_1 s_3\, \vec{a}\cdot\vec{c}$$

$$+ r_2 s_1\, \vec{b}\cdot\vec{a} + r_2 s_2\, \vec{b}\cdot\vec{b} + r_2 s_3\, \vec{b}\cdot\vec{c}$$
$$+ r_3 s_1\, \vec{c}\cdot\vec{a} + r_3 s_2\, \vec{c}\cdot\vec{b} + r_3 s_3\, \vec{c}\cdot\vec{c}$$

$$\underbrace{+ r_3 s_1\, \vec{c}\cdot\vec{a} + r_3 s_2\, \vec{c}\cdot\vec{b} + r_3 s_3\, \vec{c}\cdot\vec{c}}$$

$$= \underbrace{(r_1 \;\; r_2 \;\; r_3)}\,(G)\begin{pmatrix} s_1 \\ s_2 \\ s_3 \end{pmatrix}\Big\}$$ gives the same nine terms as above

where

$$G = \begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{a}\cdot\vec{b} & \vec{a}\cdot\vec{c} \\ \vec{b}\cdot\vec{a} & \vec{b}\cdot\vec{b} & \vec{b}\cdot\vec{c} \\ \vec{c}\cdot\vec{a} & \vec{c}\cdot\vec{b} & \vec{c}\cdot\vec{c} \end{pmatrix}$$ Metric Tensor

Now, we develop a new concept called metric tensor. So, let us try to take dot product of two vectors r and s, r has components r1, r2, r3 and s has component s1, s2, s3 and we are in real space. So, we are in the crystal basis.

So, what is r dot s the dot product, r dot s in terms of components so, r1 s1 plus r2 s2 plus r3 s3 dot product of two vectors in terms of components this is our familiar dot product this formula at least you should know before the course. No confusion we can proceed only thing is that there is not right this is incorrect that is why I was giving you time because this is only for this is true only for Cartesian system I told you that this is in real space, real space means the crystal space and these are with respect to the crystal bases.

In crystal bases if they are in customer bases, what can you say about r, r now means r1 a crystal basis is abc. So, whenever we say components, components with respect to a given basis so, when the basis is abc the components r1 r2 r3 is with respect to that basis which means the vector is r1 a plus r2 b plus r3 c and similarly, the vector s says s1 a plus s2 b plus s3 c.

Now, if you take the dot product r dot s you can see that you have to take the dot product like this 3 times in each bracket there will be 9 terms 3 into 3 nine terms. So, you will have r1 s1 a dot a r1 s2 a dot b r1 s3 a dot c plus r2 s1 b dot a r2 s2 b dot b r3 s3 b dot c plus sorry r2 s3, r3 s1 r3 s1 c dot a r3 s2 c dot b r3 s3 c dot c.

We are stuck with all these 9 terms. You cannot get away with that. You can see unless and until alpha beta or gamma one of them is 90 degree, none of these dot product is going to vanish. Thanks to Cartesian system, orthogonal system where all three angles are 90 degree. So, all non-similar dot products a dot b a dot c, b dot c all vanish. So, six terms out of these nine terms vanish only the diagonal terms a dot a b dot b and c dot c survived. But that is the property that is the beauty and that is the power and that is the reason why Cartesian system is so much favored.

But in crystallography, once we have decided that our unit cell is abc alpha, beta, gamma, that is the lattice parameter, it may happen that none of these dot products is 0. So, we are left with all these nine terms.

Only way now, to simplify this available to us is to write it in a matrix form like this, we can take the two component vectors r1 r2 r3 one of them as row vector, one of them as column vector, and in between write a matrix G which has this form a dot a b dot b a dot a, a dot b a dot c and so on is a symmetric matrix you can see. And this equality you will have to work out and see if you write this matrix open this out, you will find that you get the same nine terms.

So, the advantage of writing it in matrix form first of all is that it makes it a little compact rather than writing it as nine term some there, you write it in a matrix form like this. The other advantage is that it abstracts out those terms which are depending on the lattice parameter, which is the G the metric tensor and those which are the components of vector which does not depend upon the lattice parameter which can be anything.

So, r1 r2 r3 are component of one vector s1 s2 s3 component of another vector they are variables, but once a particular unit cell is selected in a particular crystal, then there is a dot a a dot b this metric tensor is fixed. So, this is what is known as the metric tensor and gives you is used for calculating dot product in a general non Cartesian coordinate system.

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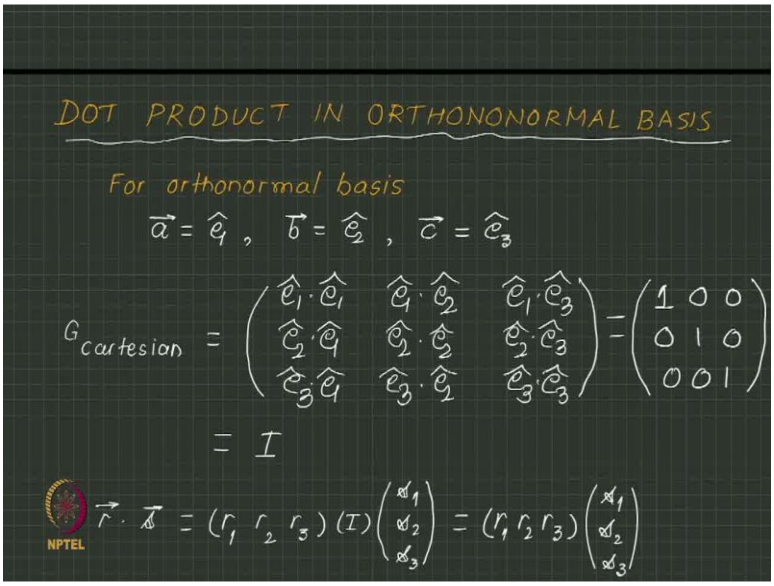


G from lattice parameters

$$g_{11} = \bar{a}\cdot\bar{a} = a^2$$

$$g_{12} = g_{21} = \vec{a}\cdot\vec{b} = ab\cos\gamma$$

$$g_{13} = g_{31} = \vec{a}\cdot\vec{c} = ac\cos\beta$$

$$g_{22} = \vec{b}\cdot\vec{b} = b^2$$

$$g_{23} = g_{32} = \vec{b}\cdot\vec{c} = bc\cos\alpha$$

$$g_{33} = \vec{c}\cdot\vec{c} = c^2$$

NPTEL

$$= \boxed{r_1 s_1 + r_2 s_2 + r_3 s_3}$$

LENGTH OF A VECTOR

$$\vec{r}_{uvw} = u\vec{a} + v\vec{b} + w\vec{c}$$

$$r_{uvw}^2 = \vec{r}_{uvw}\cdot\vec{r}_{uvw} = (u\ v\ w)\,(G)\begin{pmatrix} u \\ v \\ w \end{pmatrix}$$

NPTEL

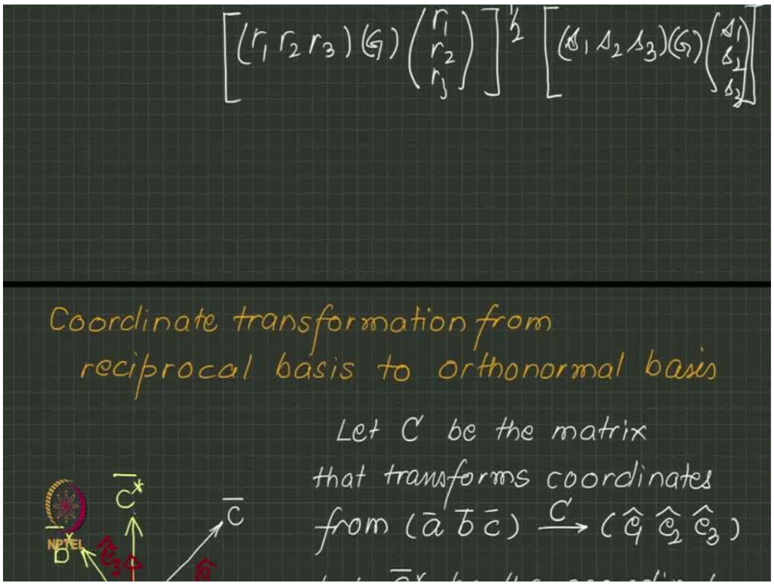
ANGLE BETWEEN TWO VECTORS

$\vec{r}\cdot\vec{s} = rs\cos\theta \leftarrow$ θ angle between r and s

$$\Rightarrow \cos\theta = \frac{\vec{r}\cdot\vec{s}}{rs}$$

$$= \Big[(r_1\ r_2\ r_3)\,(G)\begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix}$$

NPTEL



How do we calculate this G from lattice parameters? It is very simple look at the definition the terms of G are just a dot a a dot b the first term is a dot a. What is a dot a, dot a is a square. So, that is the square of the first lattice parameter g12 which is same as g12 g21 is a dot b. What will be a dot b length of a length of b cos of angle between a and b which we have called gamma.

So, it is ab cos gamma, g13 a dot c, so ac cos of angle between a and c which is beta, g22 b dot b b square, g32 bc cos alpha, g33 it c square c dot c c square. Maybe here also we can write b dot c and then write bc cos alpha. So, the metric tensor is once we know the lattice parameter metric tensor calculation is not difficult. In terms of lattice parameter, all the nine terms or all the six independent terms of the metric tensor are functions of the lattice parameter. So, given any lattice parameter you can calculate the metric tensor.

Now, how does this reduce to the Orthonormal basis, you can see that for Orthonormal bases a is a b and c are the 3 unit vectors e1 e2 and e3 and they are Orthogonal. So, here you will have e1 dot e1, e1 dot e2, e1 dot e3, e2 dot e1, e2 dot e2, e2 dot e3, e3 dot e1, e3 dot e2, e3 dot e3. But knowing the property of this unit way this vectors you know that this will become 1 0 0, 0 1 0 and 0 0 1. So, that means, the metric tensor for Orthonormal basis is nothing but identity.

So, now, if you use that in the general formula where you had r1 r2 r3 multiplied by the metric tensor multiplied by s1 s2 s3 but the metric tensor now is I and I obviously does nothing it leaves I times s1 s2 s3 s1 s2 s3 so, you get r1 r2 r3 row vector multiplied by s1 s2 s3 column vector which gives you the normal dot product formula with which we had started.

So, you have simply generalized the dot product for a more complicated coordinate system that is all.

Other things just follow. So, if we want to find length of a vector in a crystal coordinate system, so, you have the vector like this the length will again be the dot product of the vector with itself will give you the square of the length only thing now, you have to write the components with G matrix coming in between so, that will become your r square. If you insist on r then, you can take the square root of this quantity. So, the row vector u v w multiplied by the metric tensor sometimes called metric matrix also metric matrix or metrix tensor same thing so that is the length of the vector.

The angle between two vectors again r dot s is rs cos theta where theta is the angle between r and s. So, that becomes this and just using the formula which you had that I have now with r1 r2 r3 into G into r1 r2 r3 sorry these are dot s so, this is r dot s. So, this side will be the s vector s1 s2 s3. So, that is the numerator and the length r will be r1 r2 r3 times G times r1 r2 r3 is square root just like we saw.

So, means writing it by hand is a little messy and complicated what to do you can program it in computer and give any lattice parameter or any components, you can easily find the angle between vectors or length of a vector even though now you are working in a system, which is non Cartesian. So, crystallography just forces you to generalize yourself come out of your comfort zone of Orthonormal Cartesian basis. But it is as you can see that once you have this metric tensor, the discomfort is not so much you can still calculate everything.

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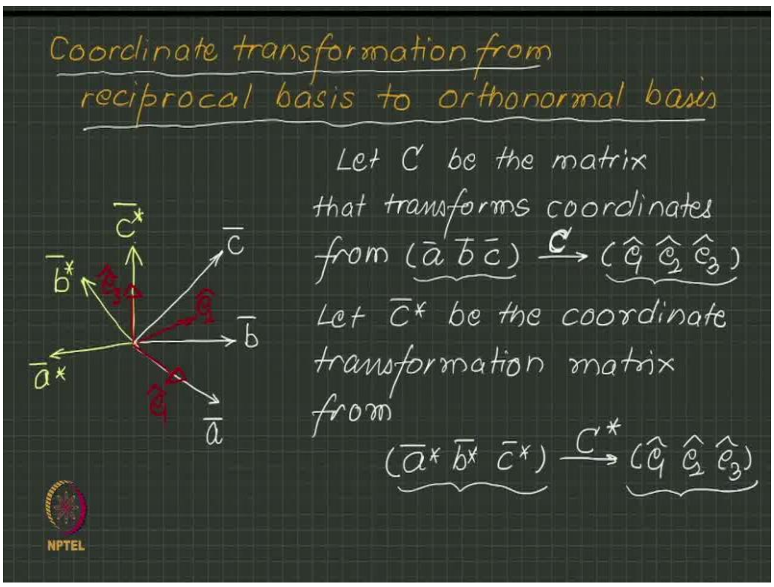

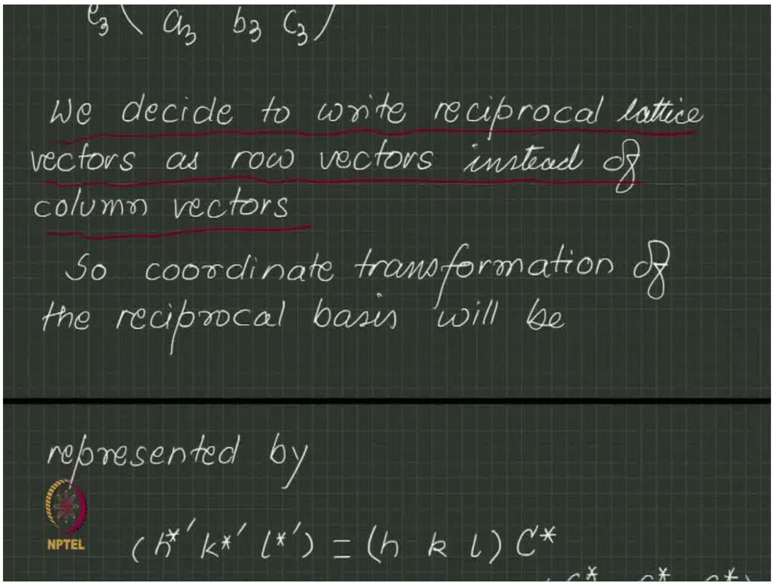

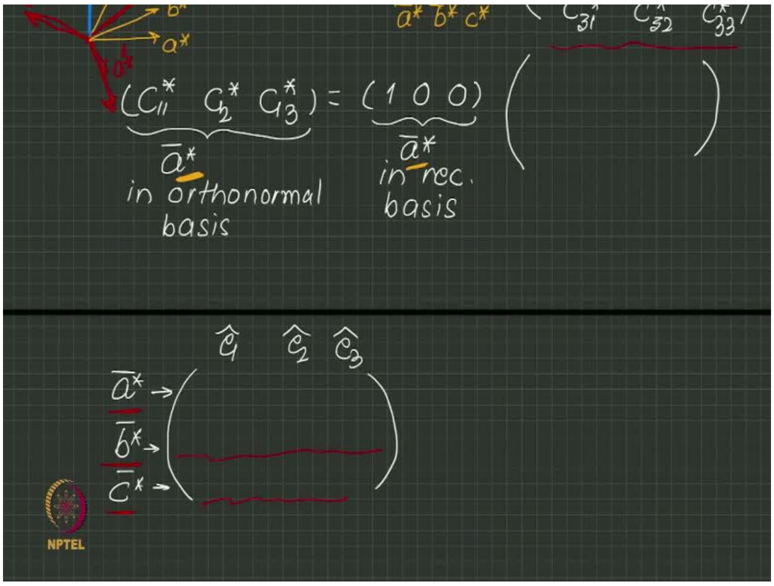

So, coordinate now, we have seen the coordinate transformation in the real basis. Now, can we do that same thing for reciprocal basis. So, let us see this what we want to do we have seen that we have developed this formulation partially and the rest was left as a homework exercise for you the last column that abc if you have abc as your given basis, and you want to go into the Cartesian basis e1 e2 e3 you use the matrix C.

Now, suppose you have the reciprocal basis the corresponding reciprocal basis a star b star c star. How can you go into the corresponding Cartesian basis? So, that will be the matrix c star. Now, how did we write C? We expressed a b and c as column vectors in Cartesian coordinate system. So, a1 a2 a3 are the first column, first column of the transformation matrix C is a1 a2 a3 which is nothing but components of the first basis vector, first crystal basis vector a in terms of e1 e2 e3 so, it is the Cartesian component, Cartesian components of a. The second column is Cartesian components of b third column is Cartesian component of c.

Now, we do means this is not necessary, but this convention is used in international tables. So, we want to follow this that we decide to write reciprocal lattice vectors this is important, this is just a convention you can violate this and decide that I will write the reciprocal lattice vectors also as column vectors like I was doing for the real basis vectors. But, some simplicity comes if you write the reciprocal basis vectors reciprocal vectors as row vectors.

So, coordinate transformation of the reciprocal basis will be represented by now, suppose this was the coordinate transformation matrix. So, you multiply that to the untransformed components, h k l is component of a vector in the reciprocal space h star k star l star is components of the same vector in a new basis. So, now you have two reciprocal bases you have a star b star and c star you also have a star prime b star prime and c star prime.

So, h k l is with respect to this yellow basis, h k l is with respect to a star b star c star h star k star l star is with respect to the new basis a star prime b star prime and c star prime which means the same vector if I draw a vector let us say this vector. So, this vector is being expressed as h k l when I use the yellow coordinate system and is written as h prime k prime l prime. When I am writing they are writing it in terms of the red coordinate system. And how do I go from one to other.

So, since I decided to write them as row vectors. So, the row vector multiplies the matrix from front as you know from the left, so, I have written it in terms of the left vector. And if you take the h k l as 1 0 0 you can see this, then what will you get 1 0 0 we will multiply with c1, 1 star c star matrix, we will pick out 1 0 0 , we will pick out the first column, sorry first row, this little pick out the first row.

If you multiply this with 1 0 0, it picks out the first row, which means the first row first row of the transformation matrix is nothing but a star transformed into Orthonormal bases. Because RHS is the vector in Orthonormal bases of a means I was little bit negligent in drawing my prime coordinate system I made it very general.

But if I am writing the C matrix, I am assuming that I am transforming it to an Orthonormal basis. So, you have to allow for a star b star c star you have assume that the star b star c star is Orthonormal and not general. So, the first row is a star expressed in Orthonormal basis and so on. The second row is b star expressed in Orthonormal basis the third row is c star expressed in Orthonormal basis.

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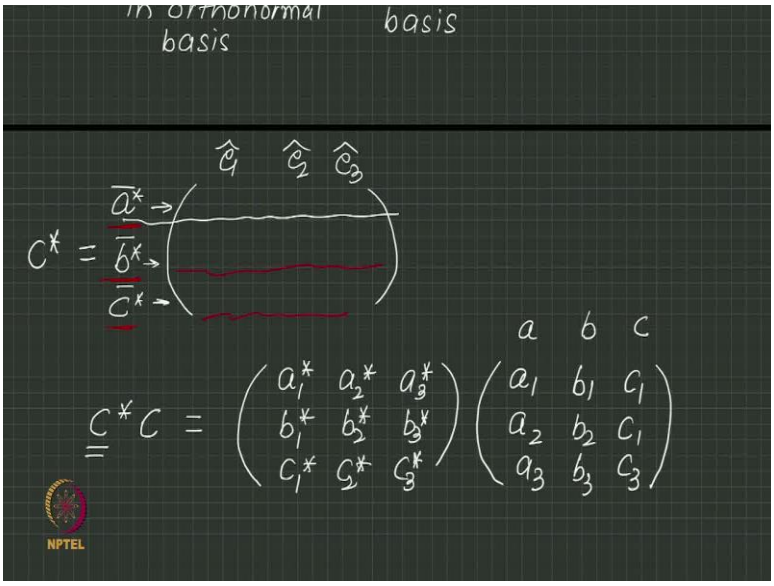

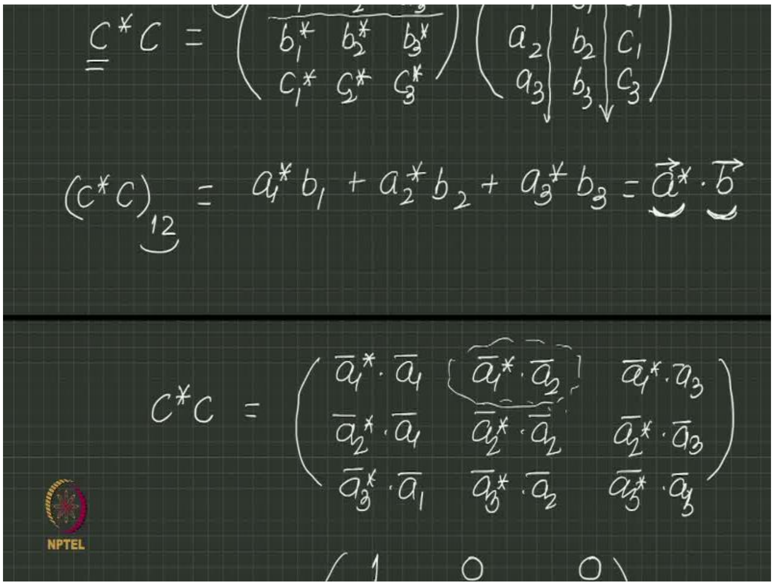

$$\underline{\underline{C}}^* C = \begin{pmatrix} \cdots & \cdots & \cdots \\ b_1^* & b_2^* & b_3^* \\ c_1^* & c_2^* & c_3^* \end{pmatrix} \begin{pmatrix} \cdots & \cdots & \cdots \\ a_2 & b_2 & c_1 \\ a_3 & b_3 & c_3 \end{pmatrix}$$

$$(C^* C)_{\underbrace{12}} = a_1^* b_1 + a_2^* b_2 + a_3^* b_3 = \underbrace{\vec{a}^*} \cdot \underbrace{\vec{b}}$$

$$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix}$$

$$C^* C = \begin{pmatrix} \bar{a}^* \cdot \bar{a} & \bar{a}^* \cdot \bar{b} & \bar{a}^* \cdot \bar{c} \\ \bar{b}^* \cdot \bar{a} & \bar{b}^* \cdot \bar{b} & \bar{b}^* \cdot \bar{c} \\ \bar{c}^* \cdot \bar{a} & \bar{c}^* \cdot \bar{b} & \bar{c}^* \cdot c \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= I$$

$$C^* C = I \Rightarrow \boxed{C^* = C^{-1}}$$

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Relation between G and C

$$C = \begin{array}{c} \begin{matrix} \vec{a} & \vec{b} & \vec{c} \end{matrix} \\ \begin{pmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{pmatrix} \end{array} \qquad C^T = \begin{pmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{pmatrix}$$

$$(C^T C)_{23} = a_2 a_3 + b_2 b_3 + c_2 c_3 =$$

$$C^* C = I \Rightarrow \boxed{C^* = C^{-1}}$$

Relation between G and C

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3rd col.

2nd row

$$(C^T C)_{23} = b_1 c_1 + b_2 c_2 + b_3 c_3 = \vec{b} \cdot \vec{c}$$

$$C^T C = \begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{a}\cdot\vec{b} & \vec{a}\cdot\vec{c} \\ \vec{b}\cdot\vec{a} & \vec{b}\cdot\vec{b} & \vec{b}\cdot\vec{c} \\ \vec{c}\cdot\vec{a} & \vec{c}\cdot\vec{b} & \vec{c}\cdot\vec{c} \end{pmatrix} = \text{Metric Tensor} = G$$

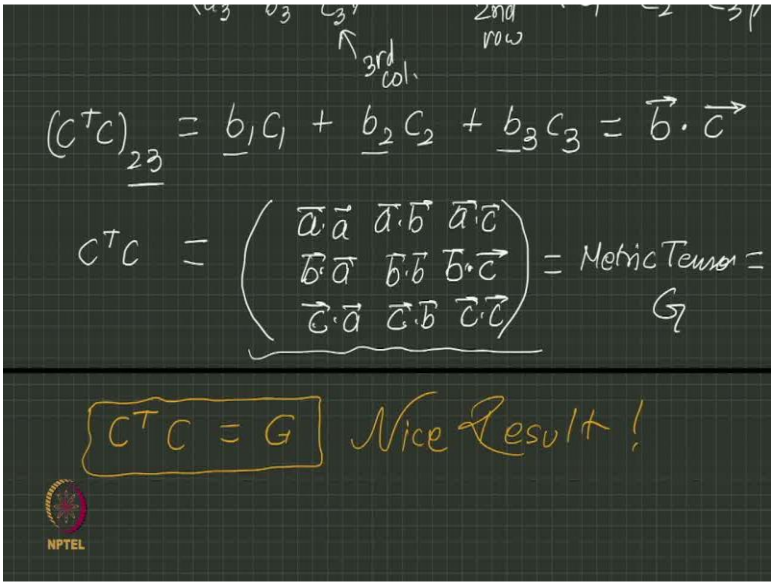
$$\boxed{G = \begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{a}\cdot\vec{b} & \vec{a}\cdot\vec{c} \\ \vec{b}\cdot\vec{a} & \vec{b}\cdot\vec{b} & \vec{b}\cdot\vec{c} \\ \vec{c}\cdot\vec{a} & \vec{c}\cdot\vec{b} & \vec{c}\cdot\vec{c} \end{pmatrix}}$$ Metric Tensor

Symmetric

G from lattice parameters

$$g_{11} = \vec{a}\cdot\vec{a} = a^2$$

$$g_{12} = g_{21} = \vec{a}\cdot\vec{b} = ab\cos\gamma$$



If that is the case, we can derive an important property let us say c star c this product let us take the product of these two matrices c star c. So, c star has a1 star a2 star a3 star this was c star. So, a star expressed in e1 e2 e3 so, I am saying a star has components a1 star a2 star and a3 star, b star has component b1star b2 star and b3 star, c star has components c1 star c2 star c3 star. This is what we get for c star c we have seen that we write as columns of a b and c. So, there is the components of a a1 a2 and a3 these are the three components of b, b1 b2 b3, these are the three components of c c1 c2 c3.

Now, you can use this property of the first row, first row is a star expressed in Cartesian coordinate system. First column is a express in Cartesian coordinate system. So, when you multiply c star c and let us say let us take a particular component let us take 12 component. Let us first row multiplied by a second column let us say. So, that will be a1 star b1 plus a2 star b2 plus a3 star b3.

In Cartesian component term by term dot product and sum is what, is just the dot product of a star and b there is a dot product of a star b. So, the 12 term is just the dot product of first vector a star and second vector b. So, similarly, you can write the entire matrix c star c the 12 term we just worked out currently 12 term as a star I am using a little bit of confusing terminology here so, let me write it out completely.

So, c star dot c these nine terms the 12 terms we worked out as a star b. The 13 term if you work out it will come out to be a star a star dot b a star dot c. Similarly, this is a star dot a. Then you will have b star dot a b star dot b b star dot c c star dot a c star dot b c star dot c.

But then by definition of the dot products of real and reciprocal vectors only a dot a star dot a the diagonal terms will be 1. The off diagonal terms will be 0 which means c star c is identity that simplifies our life a lot that we do not have to calculate c star separately. If we have calculated c the transformation matrix for their direct basis to a Cartesian basis c was transformation matrix for direct basis to Cartesian basis. Then, the transformation matrix for the corresponding reciprocal basis to the same Cartesian basis is nothing but the reciprocal of the direct transformation matrix.

This relation will be important in establishing some other relations. So, let us look at that let us find out what is C Transpose C. So, C we just saw that c has columns of a b and c expressed in Cartesian coordinate system. So, C transpose will have rows of rows expressed as just the transpose of the previous matrix. So, now the basis vectors are written as rows. And if I multiply again so, let us say let us again calculate 12 term.

Now, let us try to do some other term 23 term. So, we take the second row and multiply it with the third column. So, what do you get a2 a3 b2 b3 c2 c3 but this is a2 b2 and c2 sorry I multiplied it wrongly. So, let us get rid of this because transpose comes first so, I should take this matrix first, so, I this is c c transport.

So, let us do that again c transpose c 23 so, I take the second row here and multiplied by third column from this matrix so, b1 c1 b2 c2 plus b3 c3 second row from here multiplied by the third column here. This is b1 b2 b3 are components of the b vector and c1 c2 c3 are components of the c vector so, this is nothing but b dot c.

So, similarly, you can see that CTC matrix we just calculated the 23 terms. So, second row third column this was be dot c by same analysis you can keep working out you will find that this is a dot b for a dot a a dot b a dot c b dot a b dot b c dot c c dot a c dot b and c dot c.

Some algebra is there and some thinking is required. So, you have to you have to do that on paper yourself also because I can see that in lecture it is not a very easy way to communicate, but all I can do is to work it out with you. So, you get this matrix but what is this matrix? They should now be familiar to you. We but we defined it as some matrix just in this lecture. The G matrix, the metric tensor this is the metric tensor which we called G.

S, it is an interesting way of getting this one 23 terms. In the transpose matrix, the second row is b1 b2 b3 that is the components of the basis vector b in Cartesian coordinate system, because C is transforming the basis vectors to Cartesian system. So, b1 b2 b3 are components of b, c1 c2 c3 are components of c in Cartesian coordinate system, where the dot product has this simple form b1 c1 plus b2 c2 plus b3 c3 despite all our problems with metric tensor in Cartesian the metric tensor is identity.

So, that is not appearing here. So, this simply becomes b dot c so, just like now, I am taking a jump of faith that just like 23 became b dot c 11 will become a dot a, but you can check that and it is not that difficult and 12 will become a dot b so, that the whole matrix CT dot c the product matrix becomes the metric tensor. So, this is an interesting relation we stop here the time is up.

So, this is an interesting relation that if you have the transfer we wrote let us c we wrote very different things. So, in a sense the relationship is interesting and I will say to some extent surprising also, because our metric tensor was a tensor define in terms of the basis vectors it has nothing to do with Cartesian coordinate system. It was not asking for any Cartesian coordinate system a b and c were three vectors totally non Cartesian totally non equal angles not equal.

So, the set of dot products was the metric tensor, the set of dot products written in terms of this matrix is the dot product, c had to do something with the Cartesian coordinate system c was taking a b and c to Cartesian coordinate system.

But then now, we find that if we have that transformation matrix, if we have the transformation matrix then the transpose of the transformation matrix multiplied by the matrix itself is nothing but the metric tensor. So, this is a great result I will say nicely despite appearing to be quite boring during the lecture rather than nicer establishing the relationship between the two matrix, so, thank you very much.