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Crystals, Symmetry and Tensors
Professor Rajesh Prasad
Department of Materials Science and Engineering
Indian Institute of Technology Delhi
Lecture 6b
Some Properties of Metric Tensor in Real and Reciprocal Space

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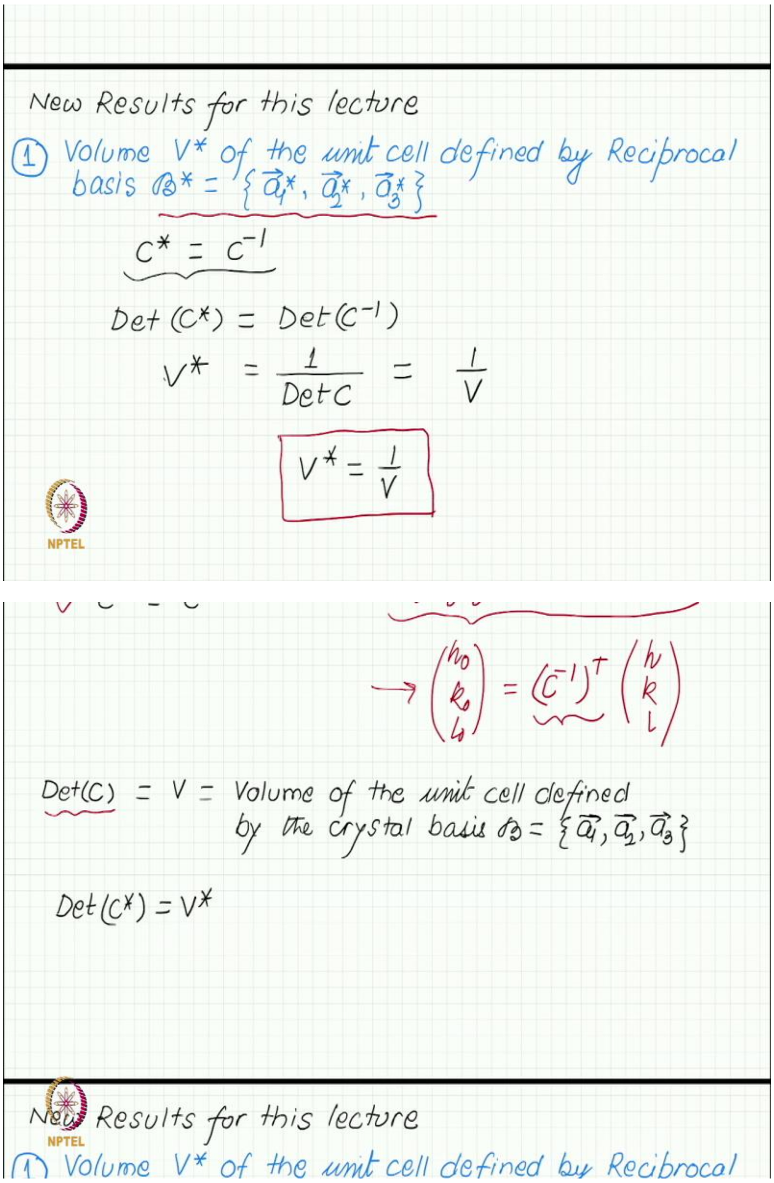

Let us now start establishing some new results based on this, what is the volume of the reciprocal basis V star. So, that is we define a parallel pippin with a1 star, a2 star, and a3 star. a1 star, a2 star, and a3 star are well defined in terms of cross product or dot product whatever definition you like. So, you have found these vectors and then all we have to do is to find the volume of that unit cell.

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We will use this property of the two matrices that C star is nothing but C inverse to find the volume taking the determinant of both sides and you will remember from your maths class that determinant of a inverse of a matrix is just the reciprocal of the determinant and we have already shown that determinant of C is V. So, similarly, this property will be true irrespective of what basis we are using.

So, if we are using the reciprocal basis, so, determinant of C star will become V star. So, LHS becomes V star and RHS becomes 1 by determine and C, but 1 by determinant C nothing but 1 by V, again the reciprocal property comes in very nicely the name is fully justified as you are seeing as more and more property you will explore you will find the reciprocal lattice name is 100 percent justified, we found that C is inverse of C. Now, we are finding V star is inverse of V.

So, this is another important relation. So, if you know the volume of the unit cell of the real lattice you will know the volume of the unit cell of reciprocal lattice just by taking the reciprocal.

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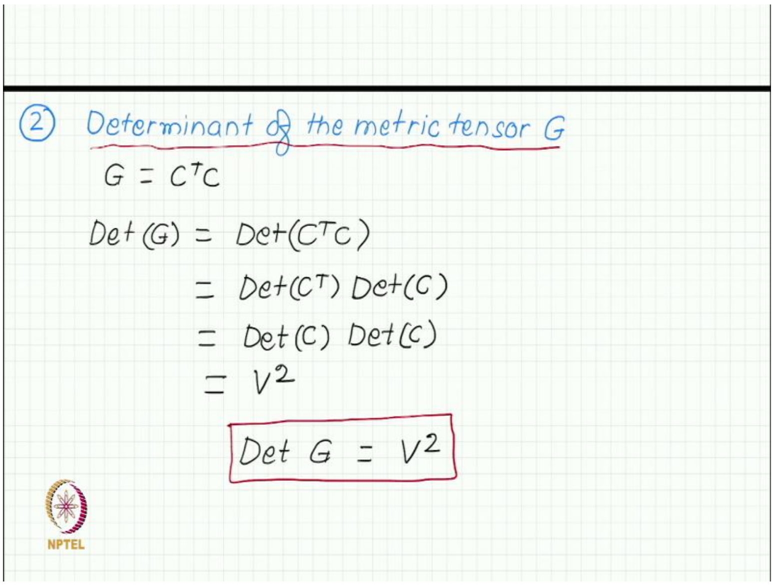

Now, what is the value of determinant of metric tensor? This this is another interesting thing. So, let us explore this the equation here must be suggesting you that what you will get? What should we do? We want to find what is determinant of G. So, we take the determinant. So, this becomes the determinant of C transpose C, again from the properties of determinant, determinant of product of two matrices is product of their determinants. So, we can write this

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as determinant CT times the determine C, but then determinant of a transpose of a matrix it is same as determinant of the matrix transposition does not change the determinant.

So, you get determinant C times determinant C but both are the volumes of the unit cell we have just shown. So, this quantity becomes V square. So, another interesting result that determinant of the metric tensor is nothing but a square of the volume of the unit cell.

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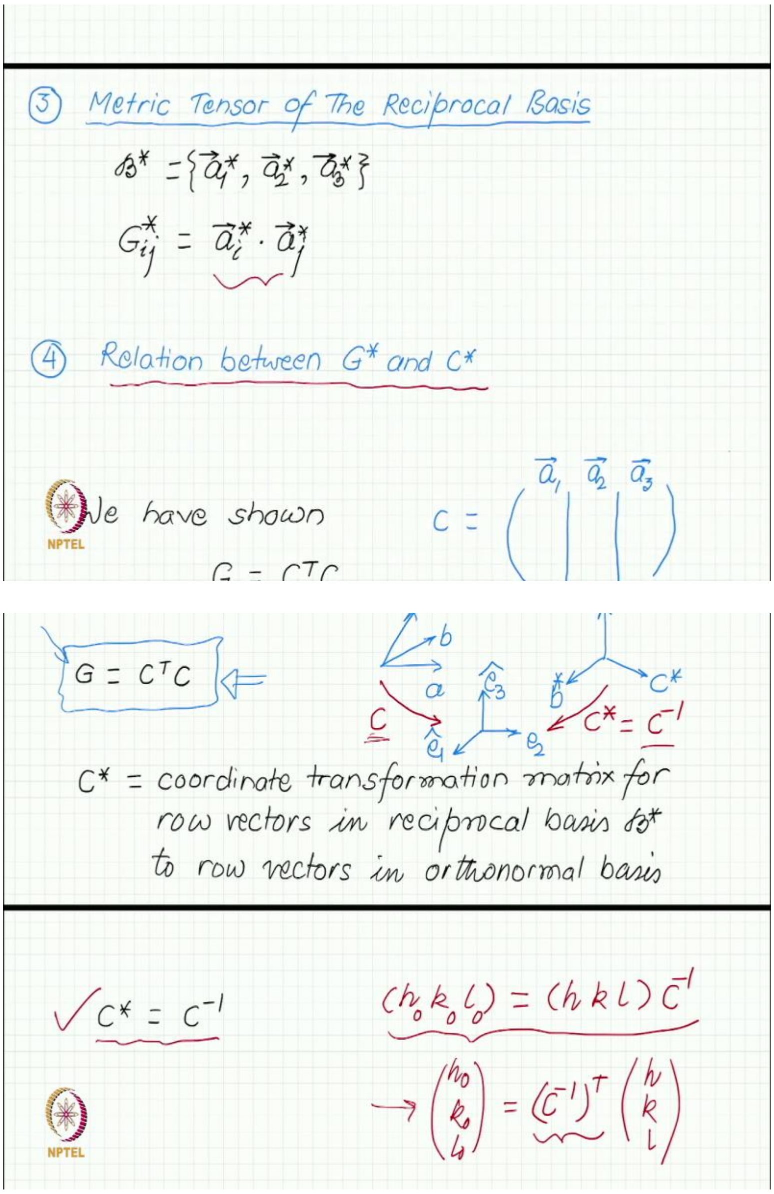

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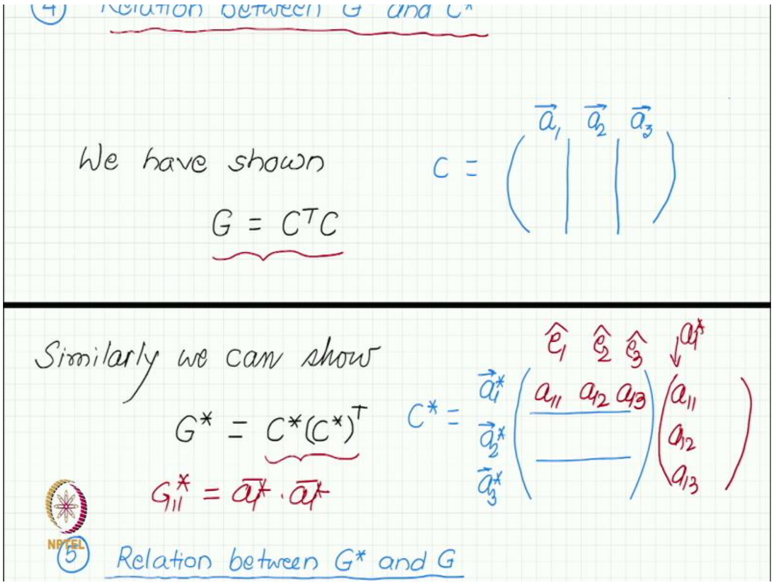

Now, let us construct metric tensor in reciprocal space, the question comes reciprocal space also is defined by three basis vector a1 star, a2 star, a3 star, there also we can take the corresponding dot products, a1 star, dot a2 star, and so on. So, we can define they are also a metric tensor Gi j star which is ai star dot aj star but then, since ai stars are defined in terms of ai's, this Gij star also must not be an independent quantity must be related somehow to the real space quantity G in this case. So, what is that relation?

So, we will let us look at that relation. First, we will establish the relation between G star and C star. Now, we have already shown that relation between G and C, C transpose C. So, what will be the relation between G star and C star you may imagine that it will be C star transpose times C star you will almost be right except for the fact that you have to change the sequence.

So, there it was C transpose c here it becomes C star C transpose and this flipping of sequence is because, again it is the same convention going back to the convention to make our matrix to make our matrix C star compatible with this row multiplication by hkl we defined it such that the rows were corresponding to this was the first component of a1 star components with respect to what components with respect to the orthonormal basis.

So, the first-row terms the first term is the component of a1 star first component of a1 star in orthonormal basis second component of a1 star in orthonormal basis and third component of a1 star in orthonormal basis maybe if you wish you can write it as a11, a12 and a13 first column of first component of a1 second component of a1 and third component of a1. So, because you write like this, then for the compatibility of matrix and you want the dot product you want the dot product like this a1 star dot aj star.

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So, a1 star is available as the first row, aj stars would be available as the second row sorry, as the columns of the second matrix, so, that is why the second matrix you take the transposition to make these as column and then you can see that if you do the matrix multiplication, so, the first row by first column is nothing but a1 dot, a1 star dot a1 star because now this one is a1 star. So, first row a11 or G11 star G11 star is a1 star dot a1 star as was desired.

So, to get that desired effect, you have to write transportation afterwards it is just a matter of definition, you see, you take the transpose nothing will happen, it will not flip because it will be transpose of transpose. So, it will again make C star as the first place. So, symmetry properties satisfied, but still it is important whether in the product we write C star first or C star transpose first.

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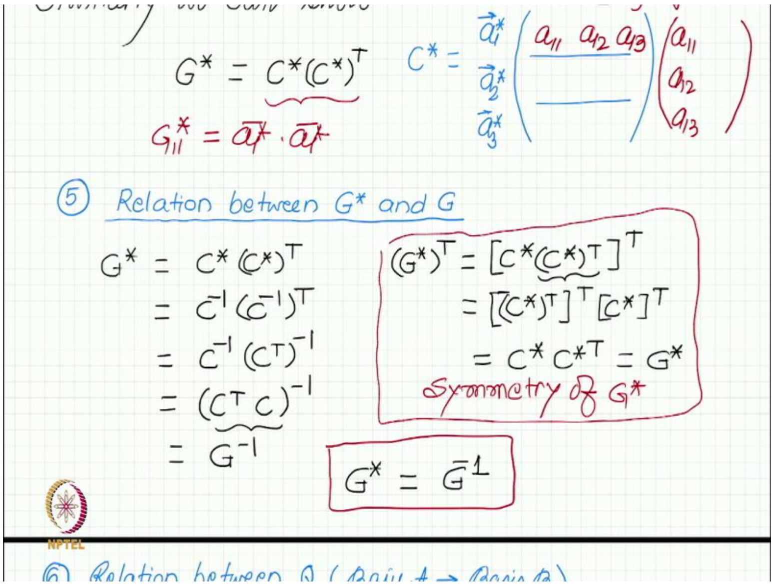

Now we can establish the relation between G star and G. So, let us try to establish that relation if you are almost done you can see with this relation, all you have to do is do a little algebra. So, G star is C star, C star transpose what I do not know whether everybody caught that discussion with Rajat. So, what we are saying that G star is symmetric means G transport should be same as G star. So, if we take G star transpose. So, C star, C star transpose transpose and in transposition, when we add the product is there then we flip the sequence.

So, the second matrix transpose will come first and the first matrix transpose will come second but the second matrix was already transpose C star transport. So, that is why we are taking C star transpose transpose. So, then again it becomes C star and this become C star transpose which was G star. So, which shows that G star is the symmetry property of G star is

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consistent with this fact, but then the sequence also is important, we cannot just throw around T transpose either in the first place or in the second place it has to be in the second place.

Now, C star is C inverse. So, we use that property we have just shown that. Now, inverse of a matrix and transpose of a matrix these are two operations which you can apply on a matrix and they are commutative with any matrix with respect to any matrix whether you take the inverse and then transpose or you take the transpose and then invert it will give you the same result can be proven easily, but we do not do it now, you can take it as an exercise. So, we just flip this and then we use again the rule for inverse of a product which changes the order of the multiplication.

So, C inverse CT inverses CT time C whole inverse direct from the matrix rules which you must have study. But C Transpose C you must be recognising it by now, C transpose C is what? Yes, Arshita the metric tensor G which is G inverse. So, once more verified that reciprocal space is reciprocal. It is metric tensor the metric tensor of the reciprocal space is the reciprocal of the metric tensor of the real space.