Crystals, Symmetry and Tensors

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Lecture 6a

Review

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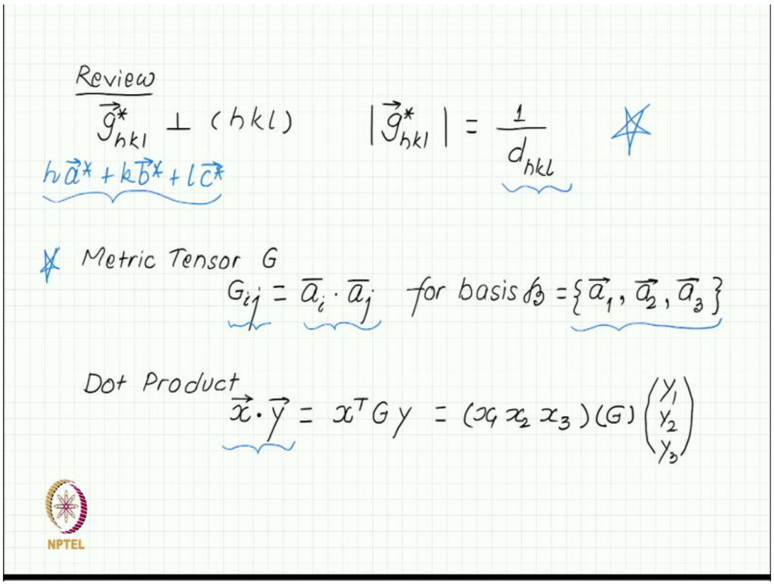

Now, just a little bit of Review of what we have established till the previous lecture. So, for example, in the last lecture we showed in fact last to last lecture, we had shown g star hkl is perpendicular to the plane hkl, which means a reciprocal lattice vector with components hkl in reciprocal space, which means, this is a short form for a vector which should be written fully as ha star plus kb star plus lc star that is what we is meant by a reciprocal lattice vector g star hkl, the components are hkl, but components are always with respect to some basis and when we are seeing a reciprocal vector.

So, the components are with respect to the reciprocal basis and the reciprocal basis is a star, b star, c star. So, a reciprocal lattice vector hkl is perpendicular or is normal to the real lattice plane hkl. So, real lattice plane hkl you know the miller indices hkl. So, its intercepts are a by h, b by k and c by l on the x, y and z axis of the real space on the a, b and c axis. So, this was one of the relationships we established. The other relationship which we established in the last class is that the length of this vector length of the same vector is exactly the reciprocal of interplanar spacing dh kl.

So, the length of g star hkl is the reciprocal of the interplanar is spacing dhkl, these I told you these two are the most important relationship. In fact, this is the reason for existence of reciprocal space. If these two properties were not there, reciprocal space would not have been defined at all and would have been no use for us. So, these two are the two critical properties then, we defined a quantity called metric tensor, because we found that if we only know the component, then component wise product and their sum is not the dot product unless and until the basis is orthonormal.

Unless and until basis is orthonormal, then component wise product and there sum is not the dot product, so dot product requires a little bit more involved formula which is shown here for you. So, that x dot y becomes x transpose Gy where G is the reciprocal G is the metric tensor defined by the dot products ai and aj, where ai is are the basis vectors of the space. So, for every basis, you will have a corresponding metric tensor and then you can find the dot product in that basis.

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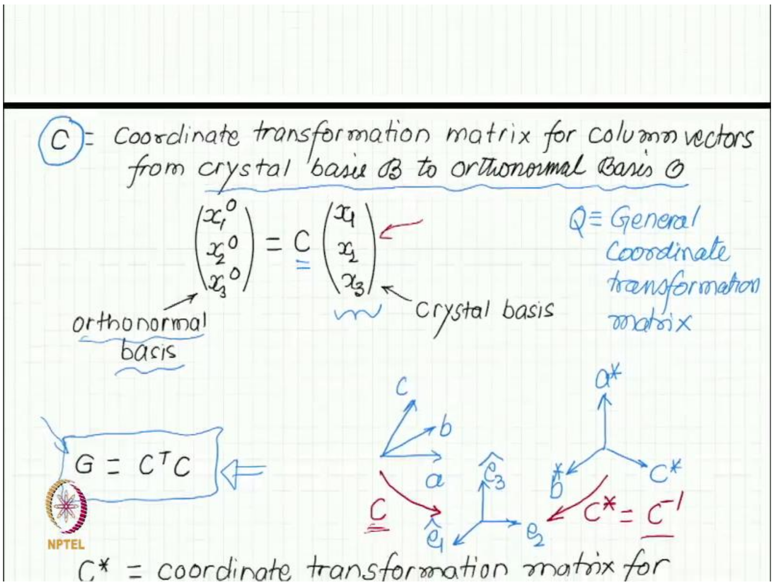
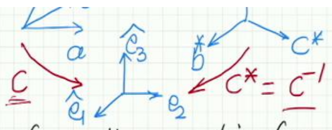


$$G = C^T C \Leftarrow$$



C^* = coordinate transformation matrix for row vectors in reciprocal basis $\mathcal{B}^*$ to row vectors in orthonormal basis

✓ $C^* = C^{-1}$

$$(h_0\, k_0\, l_0) = (h\, k\, l)\, C^{-1}$$

$$\rightarrow \begin{pmatrix} h_0 \\ k_0 \\ l_0 \end{pmatrix} = (C^{-1})^T \begin{pmatrix} h \\ k \\ l \end{pmatrix}$$

Det(C) = V = Volume of the unit cell defined

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New Results for this lecture

(1) Volume V^* of the unit cell defined by Reciprocal basis $\mathcal{B}^* = \{\vec{a}_1^*, \vec{a}_2^*, \vec{a}_3^*\}$

$C^* = C^{-1}$

We also introduced a useful coordinate transfer we introduced coordinate transformation in general and the general coordinate transformation we called Q. So, that symbol we will stick to in this core you can call it is only a matrix. So, you can call it anything p, q, r or whatever, but we have decided to call a general coordinate transformation matrix as Q. So, Q is a general coordinate transformation matrix whereas, for the special case of a transformation matrix from crystal bases to orthonormal bases for that we have used the symbol C.

So, C we will use for a basis transformation matrix from crystal basis to orthonormal basis or Cartesian basis and what is the definition or what is the property of C, the property of C is that if it multiplies a column vector the components, the components of any vector written as column. So, what is written as x1, x2, x3 is a components of a given vector written as column and you multiply it with the coordinate transformation matrix, then it will give you the components of the same vector in the orthonormal system the corresponding orthonormal basis.

So, from a general basis, the vector is being transformed or its component is being transformed to orthonormal basis. Then, we ended the last lecture with an interesting result that this metric tensor and this coordinate transformation matrix from crystal to orthonormal basis are related by this interesting relation that if you know C, you can calculate G, C transpose C, of course G is much easier to calculate than C.

So, this equation really is not a recommendation for calculating G because once you know the lattice parameter, you can directly calculate G in terms of the lattice parameter, because it is simple dot product a dot b and things like that.

So, a dot b is ab cos gamma. Similarly, all nine terms are written very simply for G. So, you will not use this equation really to find determine G from C if it so, accidentally happens that you know C and you are not knowing the lattice parameter, then you may use this in that case, but otherwise, it is not calculational recommendation, but it is an important relation which simplifies many algebraic calculations and can be used for establishing many properties, which we will see soon.

Then, similarly, the corresponding coordinate transformation matrix in the reciprocal space we are calling C star. So, we are having three coordinate systems now, we have the crystal coordinate system a, b, and c then correspondingly we find the reciprocal coordinate system a star, b star, and c star and we have then the orthonormal basis e1, e2 and e3.

So, what we are doing is that we are setting up a matrix which takes us from crystal basis to orthonormal basis that is being called C and the corresponding reciprocal basis if it is being taken to the same orthonormal basis orthonormal saying orthonormal basis also does not uniquely define it, it can have many different orientations in a space, you have to choose one so there is a lot of freedom in choosing your orthonormal basis.

For example, we did a when we introduced the C matrix, we tried to calculate by taking e1 I have not drawn it that way you can see here, but we took it e1 as parallel to a or a parallel to e1. That was one of our choices. But, whatever choice you make, that is not necessary some people may even make parallel e3 to c or as I have drawn, none of the axis may be parallel. All that is required is that there is a fixed orthonormal coordinate system which has a fixed orientation relationship to the a, b, c system, then c is defined and any such C will work.

And once C is defined the corresponding c star is automatically defined one c is defined because once a, b, c is defined a star, b star, c star is calculated in terms of a, b, c. So, c star and c are not independent, they are related. And one of the exercise of the last lecture was also to establish that relation, where we showed that c star was nothing but c inverse. So, the name reciprocal is very much justified, everything turns out to be reciprocal in this space.

So, the corresponding coordinate transformation matrix c star you will find is nothing but inverse of the C matrix only care which has to be taken that when we use this C, when we use C matrix as we have shown here C matrix, we write the vectors as a column matrix. Whereas when we go to the star space, when we go to the reciprocal space, and we start using C star matrices, we start writing our vector as hkl is a row.

We start writing them as row and if you write them as row then you are made matrix multiplication by the rule of matrix multiplication matrix multiplies it from the right instead of multiplying it from the left, some people do not like this change from row to column they say that once and for all we have decided that all vectors whether in real or in reciprocal, we will always write it in column if you decide that you can do that, then you can take the transpose and then you will find that h naught, k naught, l naught, if you take the transpose of the above equation transposition changes the sequence of the matrix as you know and you will get hkl.

Then you will say that the corresponding transformation these things keep means make a lot of confusion. And even I keep getting confused. When I go from one book to the other one has to keep care be careful. What is that books convention? Whether it is C inverse or C transverse transpose? Because C inverse need not be a symmetric matrix. So, its transpose will be a different matrix. So, you whenever you come up with a new paper or a new textbook, or a new document on crystallography, or this kind of transformation, you should make sure what is the convention.

So, if the convention is to write the reciprocal vector also as columns, then one transposition comes. So it is a question of choice. Some people say that this is more neater that everything is column, but then they have to live with an additional transposition over inverse. Some people say why transpose just start writing the reciprocal basis reciprocal vectors as row then it is simply inverse and inverse. In a way, it is easier to remember because you are working in a reciprocal space.

So, everything is inverse of the real space. Now, we also have established one relation in the very beginning that determinant of this coordinate transformation matrix, the matrix which transforms the crystal basis to orthonormal basis has this important property, determinant is volume of the crystal basis, volume of the unit cell defined by the crystal basis. So, a, b, c will always define a parallel pipping. They will have a volume and that volume will be determinant of the C matrix. These are all established. We have done this.