Crystals, Symmetry and Tensors Professor Rajesh Prasad Department of Materials Science and Engineering Indian Institute of Technology, Delhi Lecture 85 Coordinate Transformation of Vectors

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Let us review and revisit coordinate transformation of vectors. We have done this topic in another video, but let us have a re-look at it.

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 $(\underline{a}, \underline{b}, \underline{c}) = (\underline{a}, \underline{b}, \underline{c}) P$

new old basis matrix

basis vectors vectors = $(\underline{a} \underline{b} \underline{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$

By coordinate transformation, we mean that we now introduce two bases for the same crystal. So, this is the old basis vector, the old basis; and there is the new basis vectors. And of course, the new basis vectors if you want to have a coordinate transform, the same vector will have different coordinates in the two bases. So, we need to have a relationship between the two bases. The relationship between the two bases can be expressed because in a linear relationship, because each vector each new basis vector can be expressed as a linear combination of the old basis vector.

So, because of this linear relationship, this relationship can be expressed as multiplying a row of basis vector, the old basis vector a, b, c by a matrix P. So, this P is a matrix, which expresses that relationship. We can call P as a coordinate as a basis transformation matrix, such that it relates the old basis to the new basis. So, let us look at what is involved in this matrix P. So, if we open, if we write this explicitly, so we will have this row a, b, c; and this P is 3 by 3 matrix. So, P11, P12, P13; so these 9 components are there.

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So, if we open up this relationship, if we multiply these products; then, we get a prime as P11 a, plus P21 b plus P31 c. So, the old, the new basis vector a prime as you can see is being expressed as a linear combination of the old basis vector a, b and c. Similarly, we do it for b prime and c prime. So, the matrix P the components of this decomposition, components of a prime in terms of a, b and c are P11, P21 and P31; and these are the components of the matrix P.

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 $\frac{1}{\begin{pmatrix} x' \\ y' \\ \overline{0} \end{pmatrix}} = \frac{x \underline{a} + y \underline{b} + \overline{y} \underline{c}}{\sqrt{\frac{x'}{x}}} = \frac{x' \underline{a'} + y' \underline{b'} + \overline{y'} \underline{c'}}{\sqrt{\frac{x'}{x}} + \underline{b'}}$ \circledast $(\underline{a} \underline{b} \underline{c}) = (\underline{a} \underline{b} \underline{c}) P$ = $(\underbrace{a}_{b} \underbrace{b}_{c})$ $\begin{pmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{pmatrix}$ $a' = P_1$, $a + P_2$, $b + P_3$, c
 $b' = P_2$, $a + P_2$, $b + P_3$, c
 $c' = P_3$, $a + P_3$, $b + P_3$, c

 $-$ (\underline{a} \underline{c} \underline{c}) $\begin{pmatrix} P_{21} & P_{22} & P_{23} \ P_{31} & P_{32} & P_{33} \end{pmatrix}$ $a' = P_1 a + P_2 b + P_3 c$ $\underline{b}' = P_{12} \underline{a} + P_{22} \underline{b} + P_{32} \underline{c}$ $C' = P_{31} q + P_{32} b + P_{33} C$ $1 - 2\sqrt{2}$

Now, if we look at what we really want to relate is the old coordinates; so, there is a vector r. So, let us say an old basis vector a, b, c; and then the new basis vectors let us say a prime, b prime and c prime. So, then a given vector, let me say this given vector r will have two different representations. It will, it can be represented as xa plus yb plus zc in the old basis a, b, c; or it can be expressed as x prime a prime, y prime b prime, and z prime c prime in the new basis. So, and our goal is to relate x prime, y prime, z prime to x, y, z. So, this is again another linear relationship which is being expressed here. But in this case here, we were relating the two sets of basis vectors.

Here, we are now relating the coordinates of a given vector in two different bases. So, I have written this matrix as Q. Is this matrix Q related to P? It has to be, because P has all the information of the coordinate transformation. So, Q should also be expressible in terms of P. How can we do that, let us see. So, let us write this relationship here as a matrix, as a product of row and column matrix. So, I write it as a, b and c as a row matrix; and multiply it by a column x y and z. So, if we apply the matrix multiplication rule, we will get the expression for r in terms of a, b and c.

But, since it is the same vector, and it is being expressed in a different coordinate system; so we can now write the second term here, the second equality as a prime, b prime, c prime as my row vector; and x prime, y prime, z prime as the column. So, it is exactly the same relationship; this relationship has been recast in the as product of row and column.

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 $r = x a + y b + z c = x'a' + y' b' + z' c'$ $\begin{pmatrix} x' \\ y' \\ \overline{0} \end{pmatrix} = Q \begin{pmatrix} x \\ y \\ \overline{0} \end{pmatrix}$ $r = (a \underline{b} \underline{c}) \begin{pmatrix} x \\ y \\ \overline{y} \end{pmatrix} = (a' \underline{b'} \underline{c'}) \begin{pmatrix} x' \\ y' \\ \overline{z'} \end{pmatrix}$ \circledast $\begin{pmatrix} x' \\ y' \\ \overline{g}' \end{pmatrix} = \mathbb{Q} \begin{pmatrix} x \\ y \\ \overline{g} \end{pmatrix}$
 $r = (\underline{a} \underline{b} \underline{c}) \begin{pmatrix} x \\ y \\ \overline{g} \end{pmatrix} = (\underline{a}' \underline{b}' \underline{c}') \begin{pmatrix} x' \\ y' \\ \overline{g}' \end{pmatrix}$
 $r = (\underline{a} \underline{b} \underline{c}) (\underline{g}) = (\underline{a}' \underline{b}' \underline{c}') (\underline{g})$ $=(a \underline{b} \underline{c})(p)$ \circledast

Now, what we can do here is we want to see what this will give us in terms of its relationship. So, we got this relation. Now, we use in this relation we use what we have already established for a prime, b prime, c prime. So, we saw that a prime, b prime, c prime was a, b, c times the matrix P; so, for this I have written. So, I have written the new basis vector a prime, b prime, c prime in terms of the old basis vector a, b, c P, using the relationship with which we started this relationship.

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 $\frac{(a \underline{b} \underline{c})}{(a \underline{c})}$ $\begin{pmatrix} 2 \\ y \\ z \end{pmatrix} = \underbrace{(a \underline{b} \underline{c}) P}$ $\begin{pmatrix} x \\ y \\ z \end{pmatrix} = P \begin{pmatrix} x \\ y \\ z \end{pmatrix}$

So, if this is the case now, we can see that in both LHS and RHS, we have the same row a, b and c. And since this is a general reduction true for any x, y, z; so, we can conclude that the column x, y, z which is being multiplied by a, b, c. And the column P times x prime, y prime, z prime which is being multiplied by the same a, b, c should be equal. So, we have almost found our desired relation, we have expressed the old components in terms of the new component. However, we wanted the new components in terms of the old one; so, if that is the case, we simply invert this relation. The new components can be written in terms of old as P inverse x, y, z.

So, we have established the relationship that if P was the matrix which was relating the two bases, then P inverse is the matrix which will relate the two components. Of course, one has to take care here that when we are writing the basis vectors, then we are writing the matrix; we are writing them as a row, row vectors. So, basis vectors are written as row, whereas components are written as column; so, we are using that convention. And if that is the case, then the inverse of matrix P which was relating the two bases, relates now the two components. So, sometimes instead of writing using the inverse of the matrix, we call that inverse as another matrix Q. So, we get the relation x, y, z, where Q is nothing but inverse of P.

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 $\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = Q \begin{pmatrix} x \\ y \\ z \end{pmatrix}$
bonents
ponents $=\left(\begin{array}{ccc} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \end{array}\right)\left(\begin{array}{c} 2 \\ y \\ z \end{array}\right)$

So, Q is P inverse, and the relationship between the two set of coordinates; the new coordinates or a new components of a vector, and this is the old components of the vector. So, if we expand this matrix Q in terms of its components; so, 3 by 3 matrix having nine components. Of course, we saw that Q was P inverse, so if we know P, we can find Q as inverse of P; but Q can directly be found without finding P also. So, let us look at that interpretation that how can we find Q directly by looking at the relationships between different bases.

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 $= \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$ Consider $\frac{a}{a} = 1 \frac{a}{a} + 0 \frac{b}{a} + 0 \frac{c}{a}$ of the old basis Components

So, let us start with this relation that the new coordinates are expressed as Q times the old coordinate. And as our old vector to begin with, let us consider the first basis vector of the old coordinate system; first vector of the old basis. So, this vector if I express it in the old basis will simply be 1a plus 0b plus 0c; that is it will be represented by a column $1\ 0\ 0$. So, $1\ 0\ 0$ is components of a in old basis. We would like to know what is the component or what are the components of a in the new basis?

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what is the components of $\frac{a}{\omega}$ in new basis
new components of $\frac{a}{\omega}$ ι $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ Q_{21} a in the a in ola basis

So, all we have to do is to multiply our coordinate transformation matrix Q with the column vector representing a, which is 1 0 0. If we do this multiplication using the matrix multiplication rule, we see that the output will come as Q11, Q21 and Q31. So, this is a in the new basis; same vector a but its component in the new basis. But, this column is nothing but the first column of the matrix, you can see this.

By multiplying by 1 0 0, what we have done is essentially picked out the first column of the matrix. So, which means first column of the matrix is nothing but the first basis vector, first old basis vector expressed in terms of its new components; so, new components of a. Similarly, the second column will be if we multiply by 0 1 0 will be new components of b; and the third column will be new components of c.

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So, we have found an algorithm by which we can write the matrix Q by looking at what are the components of a, b and c in terms of the newer basis vectors, a prime, b prime and c prime. So, this becomes our coordinate transformation matrix. A way to remember is that, on the top we have the old basis vectors; and on the left, we have the new basis vectors. So, which means old basis vectors are being expressed as components in terms of the new basis vectors as; and they are written as columns. In the mnemonic to remember this is that in any hierarchy, old people are on top and new people usually have leftist leanings.

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Now, let us look at the transformation we specialize. So, we have done this all this in another video also; but I just wanted to review it to connect it with what we are going to do now. So, now, we need transformation between two orthonormal bases that is what is important. And this is because, most tensor properties when we express tensor property or properties of crystalline materials as tensors, then we express them in orthonormal basis. Although crystal may have its own crystallographic basis; so, we might be talking about a hexagonal crystal. We may be expressing let us say electrical conductivity of zinc, zinc is hexagonal.

However, we will not use the basis the natural crystallographic basis of hexagonal crystal, which is a not equal to B, not equal to c; and alpha, beta 90 degree, and gamma equal to 120 degree. You know that hexagonal basis. But, even for hexagonal crystal or even for any crystal if we are expressing its electrical conductivity as the second rank tensor, we are using orthonormal basis.

However, while handling the tensors, it is quite often important to use or transfer, use more than one orthonormal basis; and transform the components from one basis to another. So, that is important. So, now instead of a, b, c just to remind us that we are in the Cartesian coordinate system, or orthonormal basis; I am using instead of a, b, c which gives us a hint that we are working in crystallographic system.

I am using e1, e2, e3 as unit vectors of the Cartesian system; so, I am using now. But, we have two basis vectors again, two coordinate systems again; one is the old one e1, e1 cap, e2 cap and e3 cap. And the new one e1 prime cap, e2 prime cap, and e3 prime cap. So, how do we right now the coordinate transformation or the basis transformation for this case? Well, it is exactly the same; because what we have handled is a much more general case when we said that the transformation is from a, b, c to a prime, b prime, c prime. We were not putting any constraints on the lengths of a, b and c or angles between them. So, only in now orthonormal system, a, b and c are unit vectors; and the angles between them is 90 degree.

So, the general procedure is still applicable to them, but it is a specialized case. And we want to look at the special property of this transformation, that from one orthonormal basis to another orthonormal basis. So, in this case, using our general procedure which we had developed, we can again write the old basis vectors on top; so, e1 cap, e2 cap and e3 cap come on the top. And I express e1 the components of e1 in the new basis e1 prime, e2 prime and e3 prime as the first column. And again, just to remind that we are in the special case of orthonormal to orthonormal transformation. I am using the symbol A instead of Q for this case.

Then, A11, I can write the matrix component the nine-matrix component; and these components I have the same meaning as we developed in the for the general case. So, A11, A21 and A31 are the components of e1 in terms of the new basis e1 prime, e2 prime and e3 prime. So, the first column are components of e1, second column is components of e2, and third column is components of e3 in the new basis.

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 $= 1$ cos θ
= $\cos \theta = \cos(\hat{\theta}_j, \hat{\theta}'_i)$ $cos(\hat{q}, \hat{q}')$ $cos(\hat{e}_1, \hat{e}_1')$ $(\widehat{e}_1, \widehat{e}_2, \widehat{e}_3) \rightarrow (\widehat{e}_1, \widehat{e}_2, \widehat{e}_3)$ O^d new A_{21} A_{22} \hat{e} $\frac{1}{\sqrt{2}}$

If we now look at the component have a simple interpretation in case of orthonormal basis; because if you want to take component of ej, let say we are taking components. So, in this matrix any component Aij component is component of ej along ei prime. So, let us say that this is ej and this is ei prime. So, if I want to find component of ej in ei prime, I simply drop perpendicular that is find its projection. And you know that if this angle is theta, the length of ej is a unit vector. So, this projection, this component is nothing but 1 cos theta, which is simply cos theta.

And What is theta? We can write theta more explicitly that theta is angle between ej and ei prime. So, Aij is nothing but cosine of angle between ej and ei prime; so, this is an interesting

interpretation. This will not work if the basis is not orthonormal. But, in the orthonormal case, there is a simple interpretation of the components of the transformation matrix in terms of cosines. So, we can write this over A matrix; so, notice that these are e1 prime, e3 prime; and here we have e1, e2 and E3.

So, the first term 1 1 is nothing but cosine of e1 and e1 prime. In the second row, we have cosine of e2 and e1 prime, cosine of e3 and e1 prime. Similarly, you can fill all these nine terms, each of them is a cosine term; and it is a cosine between two directions, and it can be called direction cosine of ej. So, for example, this is a direction cosine of e1 with respect to e1 prime.

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 $A = \begin{pmatrix} \hat{q}' & A_{11} & A_{12} & A_{13} \\ \hat{q}' & A_{21} & A_{22} & A_{23} \\ \hat{q}' & A_{31} & A_{32} & A_{33} \end{pmatrix}$ A as a matrix of direction casines \circledast $A = \begin{pmatrix} cos(\hat{\theta}, \hat{e}_1') & cos(\hat{e}_2, \hat{e}_1') & cos(\hat{e}_3, \hat{e}_1') \\ cos(\hat{e}_1, \hat{e}_1') & cos(\hat{e}_2, \hat{e}_2') & cos(\hat{e}_3, \hat{e}_2') \\ cos(\hat{e}_1, \hat{e}_3') & cos(\hat{e}_2, \hat{e}_3') & cos(\hat{e}_3, \hat{e}_3') \end{pmatrix}$ $=\left(\begin{array}{cccc} \widehat{C}_1\cdot \widehat{C}_1' & \widehat{C}_2\cdot \widehat{C}_1' & \widehat{C}_3\cdot \widehat{C}_1'\\ \widehat{C}_1\cdot \widehat{C}_2' & \widehat{C}_1\cdot \widehat{C}_2' & \widehat{C}_3\cdot \widehat{C}_2'\\ \widehat{C}_1\cdot \widehat{C}_2' & \widehat{C}_1\cdot \widehat{C}_2' & \widehat{C}_3\cdot \widehat{C}_2'\\ \widehat{C}_1\cdot \widehat{C}_2' & \widehat{C}_1\cdot \widehat{C}_2' & \widehat{C}_3\cdot \widehat{$

So, now we see that this whole thing becomes a matrix of direction cosines; and, we have written it, we can write it in full like this. Now, you can also see that I can express the cosine of e1 and even prime is nothing but dot product of e1 and e1 prime. This is also because, again because of the (ortho) orthonormal character; because both bases vectors are of length 1, e1 is also of length 1, e1 prime is also of length 1, and the cosine of angle theta. So, if we take the dot product e1 and e1 prime, it will be the dot product will be 1 into 1 cos theta; and that is a cos theta which we are looking for. So, instead of cosine, we can write them as dot product also. So, we can write it as dot product e2, e1 prime, e3 e1 prime and so on. So, it is a matrix of dot products that can be another interpretation.

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Transformation of a vector components
 $\begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$ $x'_i = \sum_{j=1}^{3} A_{ij} x_j$

 $x'_i = \sum_{j=1}^3 A_{ij} x_j$ $x_i = \theta_{ij} x_j$ $x_i' = A_{ij} x_j$

So, finally, you transform the components of a vector, we need this matrix of direction cosine and we have seen how to construct them. You can think of it them as either dot product or as cosines. And if we write this in index notation, so the same matrix equation can be written as, sum of Aij xj with j going from 1 to 3.

Or, if we remember Einstein, so, in his honor, we can use Einstein convention; and we simply drop the summation symbol. And assume that since j is being repeated, since j is dummy, we have the summation over j; j is equal to 1 to 3. So, this is the expression for coordinate transformation of our vector. So, exactly same thing we would have written; means, for general transformation, we are writing we would have written x prime is equal to Qij xj relationship is not any different. Only interpretation of Q and A are slightly different in the sense that A has this a special character that they are direction cosines between two sets of vectors. Q will not simply be a direction cosine in the general case. So, thank you very much.