CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 57: Transformation of Second Rank Tensor

In this lecture, we examine how a second-rank tensor transforms when a transformation of the coordinate axes is performed. Before proceeding, it is useful to briefly review the discussion from the previous lecture and then continue from that point.

Previously, we identified a cause vector $\overline{p}$ and a response vector $\overline{q}$, where $\overline{p}$ may be interpreted as a generalized force and q as a generalized displacement. These quantities are related through a second-rank property tensor T. Depending on the physical context, this tensor may represent electrical conductivity, thermal conductivity, or other material properties. In tensor notation, this relation is written as

$$q_i = T_{ij} p_j.$$

The same relation can be expressed in matrix form, where $\overline{q}$ and $\overline{p}$ are vectors with three components, and T is a 3×3 matrix with components $T_{11}, T_{12}, T_{13}, T_{21}, T_{22}, T_{23}, T_{31}, T_{32}, T_{33}$. The cause vector has components p_1, p_2, p_3. In abbreviated matrix notation, this relation is written as

$$\overline{q} = T\overline{p}.$$

$$\begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}.$$

To determine how the tensor T transforms under a change of axes, we must first understand how a vector transforms. Throughout the discussion, we restrict ourselves to orthogonal coordinate systems, specifically Cartesian axes x_1, x_2, and x_3, which are mutually perpendicular.

Consider a vector $\overline{p}$ expressed in the original coordinate system with components p_1 along x_1, p_2 along x_2, and p_3 along x_3. Thus, the vector is written as (p_1, p_2, p_3). We now introduce a new orthogonal coordinate system with axes x'_1, x'_2, and x'_3. The vector $\overline{p}$ remains the same physical quantity, but its components with respect to the new axes, denoted by p'_1, p'_2, and p'_3, will generally be different.

The new axes are related to the old axes through angles between them. For example, the direction of x'_1 with respect to the old axes can be described by the angles it makes with x_1, x_2, and x_3. The cosines of these angles are referred to as direction cosines. Let the cosine of the angle between x'_1 and x_1 be denoted by a_{11}, between x'_1 and x_2 by a_{12}, and between x'_1 and x_3 by a_{13}.

The component of $\overline{p}$ along x'_1 is obtained by summing the projections of p_1, p_2, and p_3 onto x'_1. Thus,

$$p'_1 = a_{11}p_1 + a_{12}p_2 + a_{13}p_3.$$

Similarly, the component of p along x'_2 is given by

$$p'_2 = a_{21}p_1 + a_{22}p_2 + a_{23}p_3,$$

where a_{21}, a_{22}, and a_{23} are the direction cosines of the axis x'_2 with respect to x_1, x_2, and x_3, respectively. The third component is

$$p'_3 = a_{31}p_1 + a_{32}p_2 + a_{33}p_3,$$

where a_{31}, a_{32}, and a_{33} are the direction cosines of x'_3 with respect to x_1, x_2, and x_3.

In this manner, all three components of the vector p in the new coordinate system are obtained. In tensor notation, these three equations can be written compactly as

$$p'_i = a_{ij} p_j,$$

where j is a dummy index implying summation from 1 to 3, and i is a free index that also takes values from 1 to 3.

In matrix form, this transformation is written as

$$p' = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} p$$

$$p' = Ap,$$

where A is the direction cosine matrix with elements a_{ij}.

The same transformation rule applies to the vector q. Thus,

$$q'_i = a_{ij} q_j,$$

or, in matrix notation,

$$q' = Aq.$$

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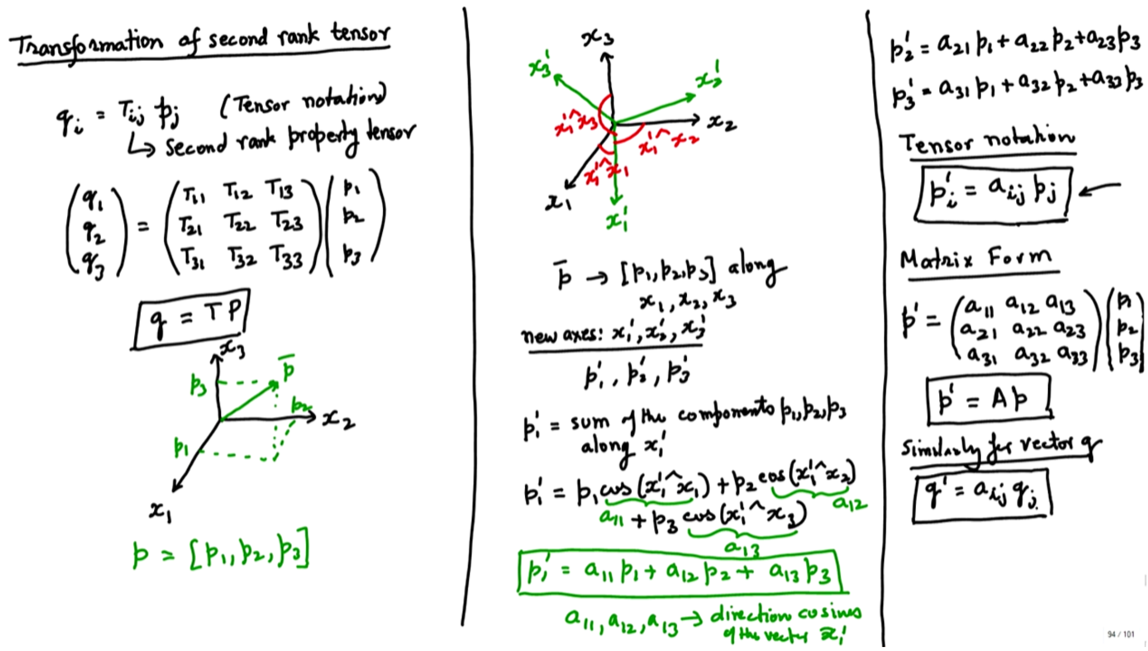

It is also useful to consider the reverse transformation, that is, expressing the components of a vector in the original coordinate system in terms of its components in the transformed system. For the vector $\bar{p}$, the reverse transformation can be written as

$$p_1 = a_{11}p'_1 + a_{21}p'_2 + a_{31}p'_3,$$

$$p_2 = a_{12}p'_1 + a_{22}p'_2 + a_{32}p'_3,$$

$$p_3 = a_{13}p'_1 + a_{23}p'_2 + a_{33}p'_3.$$

In tensor notation, this becomes

$$p_i = a_{ji}p'_j,$$

and in matrix form,

$$p = A^T p',$$

where A^T denotes the transpose of the direction cosine matrix. An analogous relation holds for the vector $\overline{q}$:

$$q_i = a_{ji}q'_j,$$

or

$$q = A^T q' .$$

Having established how the vectors $\overline{p}$ and $\overline{q}$ transform under a change of coordinate axes, we now turn to the transformation of the property tensor itself. In the original coordinate system, the relation between the response and the cause is

$$q_i = T_{ij}p_j.$$

After transformation to the new coordinate system, the corresponding relation is

$$q'_i = T'_{ij}p'_j,$$

where T'_{ij} denotes the components of the transformed tensor. The problem now is to determine how T_{ij} transforms to T'_{ij}.

To derive this transformation, we begin by writing the transformed response vector in terms of the original one:

$$q'_i = a_{im}q_m.$$

Here, the dummy index j has been replaced by m without changing the meaning of the expression. Substituting for q_m using the original relation $q_m = T_{mn}p_n$, we obtain

$$q'_i = a_{im}T_{mn}p_n.$$

At this stage, we will further substitute for p_n in terms of the transformed components, using the inverse transformation of the vector $\overline{p}$. This procedure leads to the transformation law for the second-rank tensor T_{ij}, which will be completed and discussed in detail in the continuation of this derivation.

Actually, there is a small correction to be made here. Instead of writing the indices as i and j, let me rewrite the relation as

$$q_m = T_{mn}p_n.$$

Here, the subscript i has been replaced by m and the subscript j by n. Using this corrected form, I now substitute q_m into the transformation equation for the response vector. Thus,

$$q'_i = a_{im}q_m = a_{im}T_{mn}p_n.$$

The next step is to substitute for p_n. To do this, we refer to the reverse transformation of the vector $\bar{p}$. Replacing the free index i by n in the reverse transformation, we write

$$p_n = a_{jn}p'_j.$$

Substituting this expression into the previous equation gives

$$q'_i = a_{im}T_{mn}a_{jn}p'_j.$$

Now, let us compare this equation with the transformed constitutive relation

$$q'_i = T'_{ij}P'_j.$$

From this comparison, it is clear that the combination of terms $a_{im}T_{mn}a_{jn}$ must represent the transformed tensor component T'_{ij}. The indices m and n are dummy indices, and therefore they are summed over and do not appear in the final expression. Hence, the transformation law for a second-rank tensor can be written in tensor notation as

$$T'_{ij} = a_{im}a_{jn}T_{mn}.$$

All the quantities appearing in this tensor notation are scalar components, which allows us to rearrange them freely. This expression therefore gives the complete transformation rule for a second-rank tensor under a change of coordinate axes.

In matrix form, the same transformation can be written as follows. The direction cosine matrix is

$$\mathrm{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix},$$

and the tensor in the original coordinate system is

$$\mathrm{T} = \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix}.$$

The transformation involves premultiplication by A and postmultiplication by the transpose of A. The transpose of the direction cosine matrix is

$$\mathrm{A}^T = \begin{pmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{pmatrix}.$$

Unlike the scalar case, this rearrangement cannot be performed arbitrarily because these quantities are matrices. The final transformation law in matrix notation is therefore written compactly as

$$T' = ATA^T.$$

This matrix expression is entirely equivalent to the tensor notation derived earlier.

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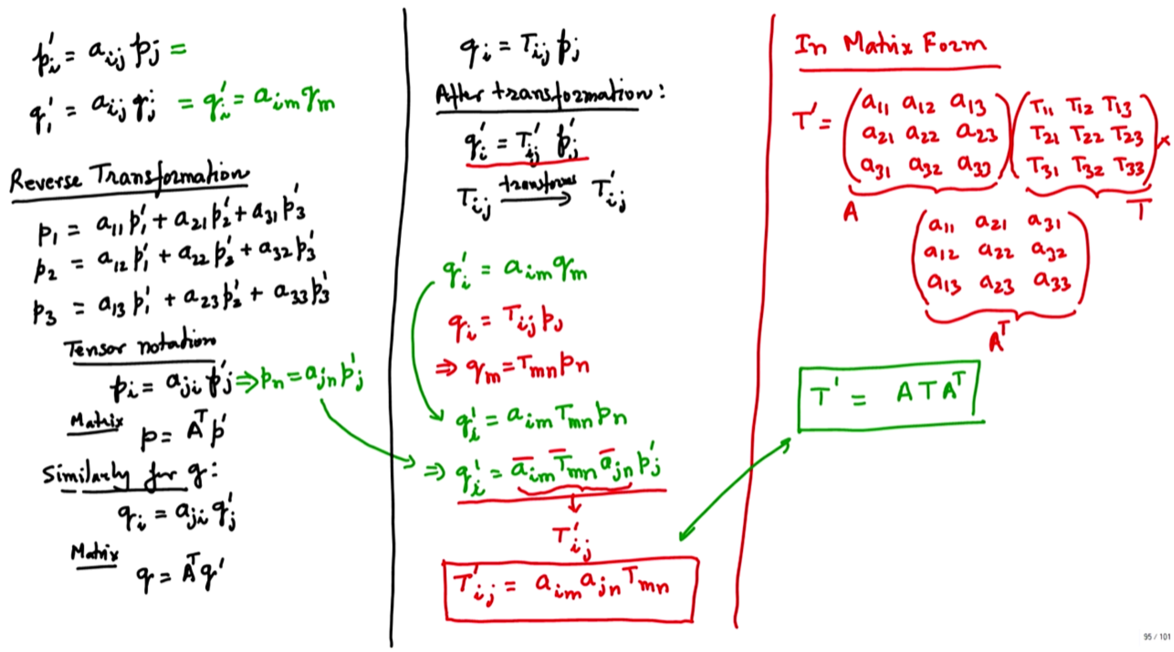

Before concluding the lecture, it is useful to discuss some properties of the direction cosine matrix A. Consider the product AA^T. Writing this out explicitly and multiplying the first row of A with the first column of A^T, the first term obtained is

$$a_{11}^2 + a_{12}^2 + a_{13}^2.$$

This term represents the sum of the squares of the direction cosines of the axis $\bar{x}'_1$. The sum of the squares of the direction cosines of any unit vector is equal to unity, and hence this term is equal to 1.

Now consider the second term, obtained by multiplying the first row of A with the second column of A^T:

$$a_{11}a_{21} + a_{12}a_{22} + a_{13}a_{23}.$$

To interpret this term, write the unit vectors as

$$\bar{x}'_1 = a_{11}\bar{x}_1 + a_{12}\bar{x}_2 + a_{13}\bar{x}_3,$$

$$\bar{x}'_2 = a_{21}\bar{x}_1 + a_{22}\bar{x}_2 + a_{23}\bar{x}_3.$$

The dot product $\bar{x}'_1 \cdot \bar{x}'_2$ is exactly the expression above. Since we are working with orthogonal coordinate systems, the axes $\bar{x}'_1$, $\bar{x}'_2$, and $\bar{x}'_3$ are mutually perpendicular. Therefore, the dot product of $\bar{x}'_1$ and $\bar{x}'_2$ is zero, and this term vanishes.

Proceeding in the same manner for all remaining terms, one finds that

$$\mathrm{AA}^T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

which is the identity matrix, denoted by I.

Taking the determinant of both sides, we obtain

$$det(AA^T) = det(I) = 1.$$

Using the property that the determinant of a product of matrices is the product of their determinants, this can be written as

$$det(A)det(A^T) = 1.$$

Since the determinant of a matrix is equal to the determinant of its transpose, this reduces to

$$(detA)^2 = 1.$$

Hence, the determinant of the direction cosine matrix A can take only the values $+\ 1$ or $-\ 1$. If the axis transformation preserves handedness, that is, a right-handed coordinate system transforms into another right-handed system, then $detA =+ 1$. If a right-handed system transforms into a left-handed system, then $detA =- 1$.

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Properties of Direction Cosine Matrix (A)

$$AA^T = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} a_{11} & a_{21} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{13} & a_{23} & a_{33} \end{pmatrix} = \begin{pmatrix} \overbrace{a_{11}^2 + a_{12}^2 + a_{13}^2}^{①} & \overbrace{a_{11}a_{21} + a_{12}a_{22} + a_{13}a_{23}}^{②} & * \\ * & * & * \\ * & * & * \end{pmatrix}$$

Term ①

$$a_{11}^2 + a_{12}^2 + a_{13}^2 = 1$$

Term ②

$$\bar{x}_1' = a_{11}\bar{x}_1 + a_{12}\bar{x}_2 + a_{13}\bar{x}_3$$

$$\bar{x}_2' = a_{21}\bar{x}_1 + a_{22}\bar{x}_2 + a_{23}\bar{x}_3$$

$$\bar{x}_1' \cdot \bar{x}_2' = \text{term ②} = 0$$

$$AA^T = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \text{Identity Matrix} = I$$

$$\text{Det}(AA^T) = \text{Det}(I) = 1$$

$$\text{Det}(AA^T) = \text{Det}(A)\underbrace{\text{Det}(A^T)}_{\text{Det}(A)} = 1$$

$$\text{Det}(A) \times \text{Det}(A) = 1$$

$$\text{Det}(A) = \pm 1$$