CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 56: Tensor Properties, Symmetry and Neumann's Principle

Continuing from the previous lecture, we had discussed physical properties in general and the manner in which these properties are represented. We had then narrowed the discussion to those physical properties that can be represented by a tensor of rank two, and from that point we continue the analysis.

Here, $\overline{p}$ represents the cause vector, $\overline{q}$ represents the response vector, and T is the property tensor of rank two. Since the rank of T is two, it contains nine components. This relation can therefore be expanded to express the three components of the response vector in terms of the three components of the cause vector. The first component of the response vector can be written as

$$q_1 = T_{11}p_1 + T_{12}p_2 + T_{13}p_3,$$

the second component as

$$q_2 = T_{21}p_1 + T_{22}p_2 + T_{23}p_3,$$

and the third component as

$$q_3 = T_{31}p_1 + T_{32}p_2 + T_{33}p_3.$$

Thus, we obtain three equations corresponding to the three components of the response vector.

It is important to note a key feature of these relations. Consider the first equation for q_1. Suppose the cause vector is directed along the x_1 direction. Throughout the discussion, we adopt a Cartesian coordinate system with axes x_1, x_2, and x_3. Any vector $\overline{p}$ therefore has three components: p_1 along x_1, p_2 along x_2, and p_3 along x_3. From the first equation,

it is clear that q_1 does not depend solely on p_1; it also depends on p_2 and p_3, which are perpendicular to x_1. Only if T_{12} and T_{13} are zero would q_1 depend exclusively on p_1. This leads to an important observation: the force or cause may act in one direction, while the resulting displacement or response may occur along a different direction.

This distinction highlights the difference between isotropic and anisotropic materials. For isotropic materials, if $\overline{p}$ is the applied force, the resulting displacement $\overline{q}$ is parallel to it. For anisotropic materials, this need not be the case, and $\overline{q}$ may not be parallel to $\overline{p}$. To clarify this idea, consider a simple mechanical analogue. Suppose two springs meet at a point O, and a load P is suspended from this point. Let the two springs make equal angles with the vertical, and let their spring constants be k_1 and k_2. Let d_0 denote the displacement vector of point O.

If the first spring extends by d_1 and the second by d_2, their extensions depend on the respective spring constants. Performing a vertical force balance, the applied load P must equal the sum of the vertical components of the forces exerted by the springs. This can be written as

$$P = k_1 d_1 cos\theta + k_2 d_2 cos\theta = (k_1 d_1 + k_2 d_2) cos\theta.$$

If $k_1 = k_2$, then both springs extend by the same amount, implying $d_1 = d_2$, and the displacement vector d_0 is parallel to the applied force vector P. However, if $k_1 \neq k_2$, for instance if $k_1 < k_2$, then $d_1 > d_2$. In this case, the point O does not move vertically downward, and the displacement vector is inclined at some angle. This example illustrates that the response vector need not be parallel to the cause vector.

Returning to the three equations relating the response to the cause, it is convenient to adopt a more compact notation, as such relations will appear frequently. The first component can be written as

$$q_1 = \sum_{j=1}^{3} T_{1j} p_j,$$

the second as

$$q_2 = \sum_{j=1}^{3} T_{2j} p_j,$$

and the third as

$$q_3 = \sum_{j=1}^{3} T_{3j} p_j.$$

This can be further abbreviated by omitting the summation symbol and writing, for example, $q_1 = T_{1j} p_j$, where summation over the repeated index j is implied. In this notation, whenever an index appears twice in a single term, summation over that index from 1 to 3 is understood. The same applies to $q_2 = T_{2j} p_j$ and $q_3 = T_{3j} p_j$.

An even more compact representation avoids writing separate equations for each component. The relation can be written as

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

Here, j is the repeated index and hence a summation over j is implied, while i is a free index. Both indices are understood to vary from 1 to 3, and this range need not be explicitly stated. The repeated index j is referred to as a dummy index, since it can be replaced by any other symbol, such as m, without changing the meaning of the expression:

$$q_i = T_{im} p_m.$$

This notation is commonly known as Einstein notation, or simply tensor notation.

The same relation can also be expressed using matrix notation. In this form, the relation is written as

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

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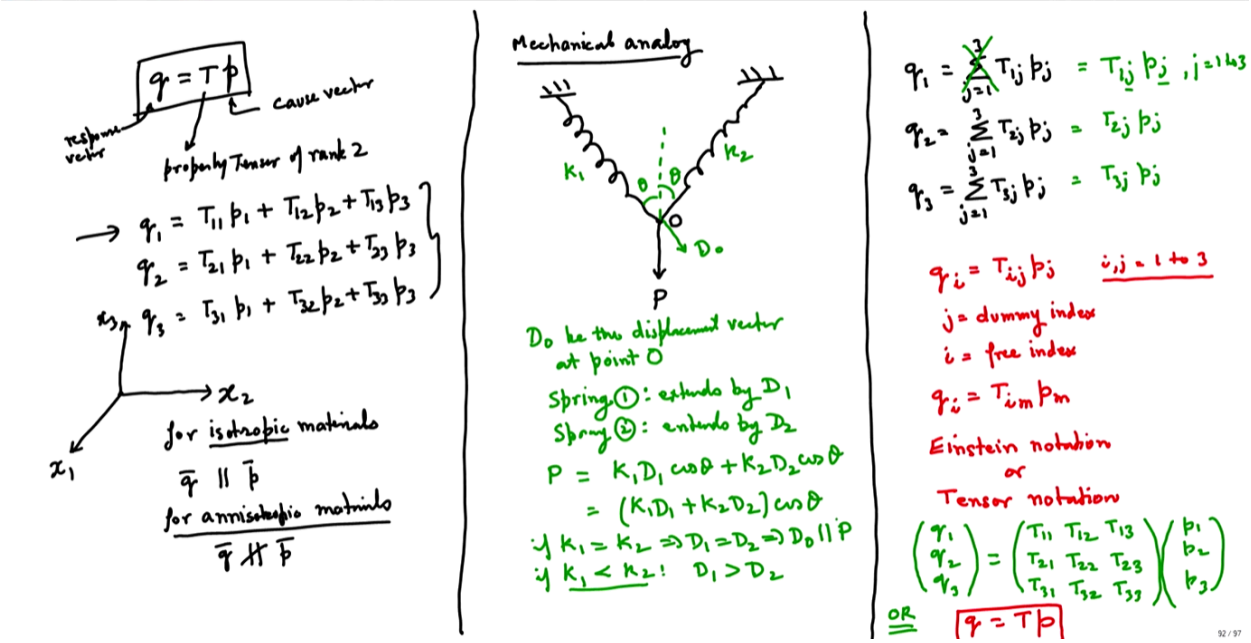


More briefly, this can be written as $\overline{q} = T\overline{p}$, where $\overline{q}$ and $\overline{p}$ are column vectors and T is a 3×3 matrix. Both tensor notation and matrix notation will be used to describe the relationship between the cause vector and the response vector.

Before proceeding further, it is necessary to discuss the effect of crystal symmetry on physical properties. In this context, the point group of a crystal becomes important, and a key principle known as Neumann's principle must be carefully considered. Neumann's principle states that the symmetry elements of a physical property of a crystal must include the symmetry elements of the point group of the crystal. Thus, all symmetry elements present in the point group, such as rotational symmetry, inversion, and reflection symmetry, must also be present in the symmetry of the physical property. However, this statement also implies that a physical property may possess additional symmetry of its

own. In other words, the symmetry of a physical property may be greater than or equal to that of the crystal's point group.

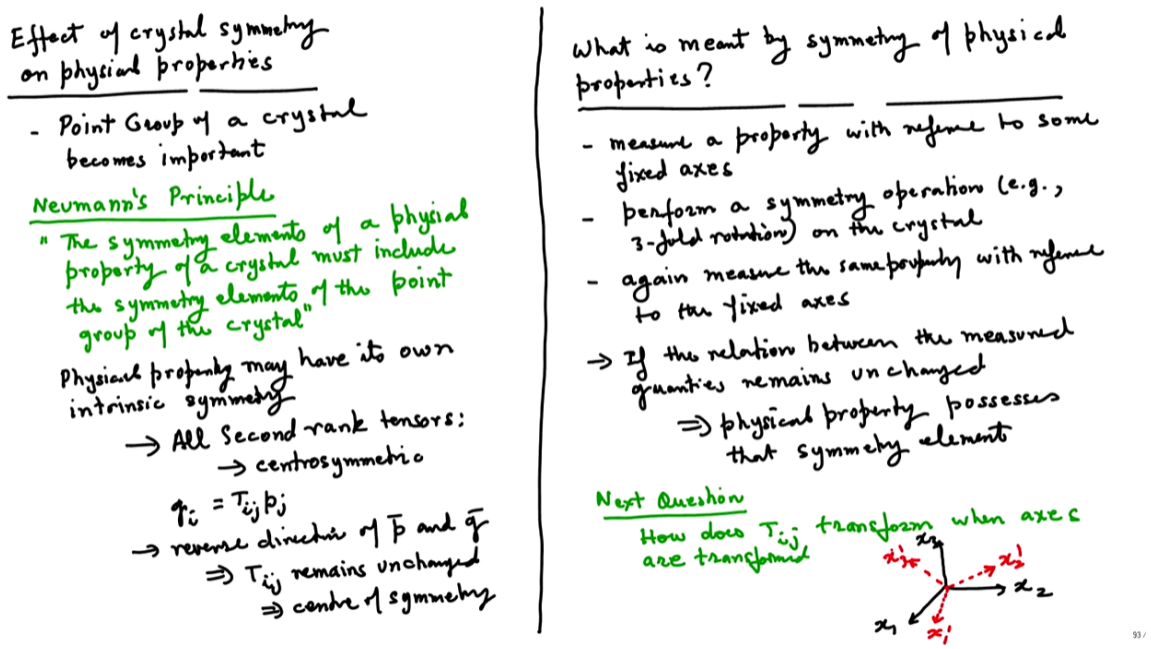
It is also necessary to clarify what is meant by the symmetry of a physical property. Suppose a physical property is measured with respect to a fixed set of axes. A symmetry operation, such as a threefold rotation, is then performed on the crystal, while the reference axes remain fixed. The physical property is measured again with respect to the same axes. Physical properties are determined through relations between measurable quantities, such as a cause vector and a response vector. If, after the symmetry operation, the relation between these measured quantities remains unchanged, then the physical property is said to possess that symmetry element. For example, if the relation remains unchanged under a threefold rotation, the physical property is said to have threefold rotational symmetry.

Physical properties may also exhibit intrinsic symmetry. As an example, all second-rank tensor properties are centrosymmetric. This means that if the directions of both $\overline{p}$ and $\overline{q}$ are reversed, the tensor T_{ij} remains unchanged:

$$q_i = T_{ij} p_j \quad implies \quad -q_i = T_{ij}(-p_j).$$

This invariance indicates the presence of a center of symmetry. This property will be examined in greater detail later, and it will be shown explicitly that all second-rank tensors possess a center of symmetry.

The next issue to be addressed concerns the transformation of the tensor components when the coordinate system is changed. Consider an initial Cartesian coordinate system with axes x_1, x_2, and x_3. If a transformation is performed to a new set of axes x'_1, x'_2, and x'_3, the components of the tensor T_{ij} must transform to a new set of components T'_{ij}. This reflects the fact that, while the physical property itself remains unchanged, its

numerical components depend on the choice of coordinate system. The relationship governing this transformation will be derived and discussed in the next lecture.

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