CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 55: Tensor Representation of Physical Properties

From this lecture onwards, we move to the final part of this course, which deals with the physical properties of crystals. To begin with, we will discuss what kinds of physical properties will be considered and how these physical properties are related to symmetry.

Before proceeding further, it is useful to mention a few references that are relevant for this part of the course and that have already been suggested earlier. One important reference is the book *Physical Properties of Crystals* authored by J. F. Nye. This is a comprehensive, though relatively old, text. A more recent reference is *Tensor Properties of Solids* by Richard F. Tinder. These books may be consulted for a deeper understanding of the topics discussed in this part of the course.

We first consider how a physical property is defined. Any physical property must be defined through a relation between measurable quantities. Let us examine a few examples. One example is density. The density of a crystal or a solid is defined as a function of its mass and its volume. A second example is electrical conductivity. Electrical conductivity is defined through a relation between the electric field and the current flux. If the electric field is denoted by E and the current flux by j, then conductivity relates these two quantities. Other examples include thermal conductivity, which relates heat flow to the temperature gradient, polarization induced in a crystal due to the application of mechanical stress, where the relevant property is piezoelectricity, and deformation of a solid under applied mechanical stress, where the property of interest is elasticity.

Most of these terms are likely familiar. However, it is important to distinguish between these examples. Consider density. Density does not depend on direction within the crystal and can be represented by a single number. In contrast, electrical conductivity in a crystal can depend on the crystallographic direction. In such a case, both magnitude and direction are relevant. When a physical property varies with direction in a crystal, the crystal is said to be anisotropic with respect to that property. The same consideration applies to the other examples mentioned above, where the specification of direction is essential.

This leads us to the question of how physical properties are specified. To address this, we introduce the concept of a tensor. Many physical properties are therefore referred to as tensor properties. The notion of a tensor will be developed gradually, but it is useful to begin with an example that is commonly encountered in mechanics, namely the stress tensor.

To specify the state of stress at a point in a solid, one uses a stress tensor. At any point, we may imagine a small cube and assign Cartesian coordinates to it. Instead of the usual x, y, and z axes, we label the axes as x_1, x_2, and x_3, where x_1 corresponds to the x-axis, x_2 to the y-axis, and x_3 to the z-axis. This coordinate system will be used consistently in subsequent lectures.

On the plane normal to the x_3 direction, a normal stress σ_{33} can be defined. On the same plane, shear stresses σ_{31} and σ_{32} act in the x_1 and x_2 directions, respectively. Similarly, on the plane normal to x_2, one can define σ_{22}, σ_{23}, and σ_{21}, and on the plane normal to x_1, one can define σ_{11}, σ_{12}, and σ_{13}. In total, there are nine components describing the state of stress at a point.

These components can be arranged in matrix form as

$$\begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix}.$$

This object is a tensor, more specifically a tensor of second rank. Although its representation resembles a matrix, a tensor is fundamentally different because its components obey a specific transformation law when the coordinate system is changed.

In general, if a tensor has rank r and we are working in three dimensions, the number of components of the tensor is 3^r. Since the stress tensor has nine components, its rank must be $r = 2$, which is why it is referred to as a second-rank tensor. As we proceed, we will encounter tensors of lower as well as higher ranks.

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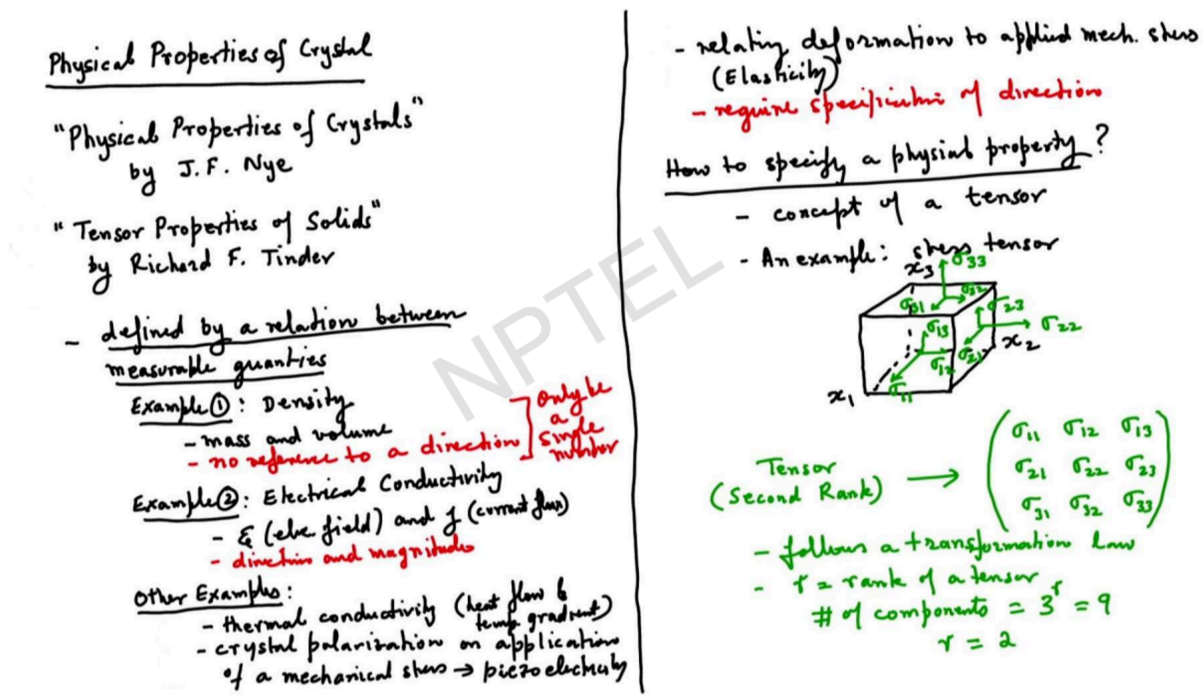

Consider now another familiar quantity, namely a vector. Examples of vectors include mechanical force, temperature gradient, and the magnetic moment of a dipole. A vector can be specified by three components. If a vector is denoted by $\overline{p}$, its components along the x_1, x_2, and x_3 axes are p_1, p_2, and p_3. From the tensor point of view, a vector is a tensor with three components in three-dimensional space, which corresponds to $3^r = 3$. Hence, the rank is $r = 1$, and a vector is a tensor of rank one.

Now consider a scalar quantity, such as density or temperature. In such cases, it is meaningless to specify a direction. Only a single value is required to describe the quantity. Since the number of components is one, we have $3^r = 1$, which implies $r = 0$. Therefore, a scalar can be regarded as a tensor of rank zero.

Thus, scalars require one value, vectors require three components, and higher-rank tensors require multiple components. We now consider how these concepts are related in describing physical properties.

A physical property can be viewed as describing how a material responds to a change in external conditions. The response of a solid to an external stimulus can be characterized by a property. Suppose the external condition is described by a vector, and the response is also described by a vector. The external stimulus may be regarded as a cause vector, such as an applied force or an electric field, which we denote by $\overline{p}$. The response of the system may be regarded as an effect vector, such as a displacement, which we denote by $\overline{q}$.

If the response is linearly related to the cause, then $\overline{q}$ is related to $\overline{p}$ through a property represented by a tensor T.

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

Since $\overline{p}$ and $\overline{q}$ are both vectors, that is, tensors of rank one, the tensor T must be of rank two. Many physical properties can be represented in this way by second-rank tensors.

Several examples illustrate this. From Ohm's law, the current flux (j) is related to the electric field through the electrical conductivity tensor σ. From Hooke's law, strain is related to applied stress (σ) through the elastic property tensor (E). Another example is magnetization (M), which develops under the application of a magnetic field and is related to it through the magnetic susceptibility tensor. In all these cases, the dependence is linear, and this linear relationship is generally valid for small values of the cause vector and correspondingly small responses.

For example, if one plots magnetization versus magnetic field (H), the response is linear for small fields, becomes nonlinear at higher fields, and eventually saturates. The tensor relations discussed here apply in the linear regime.

Thus, for physical properties represented by second-rank tensors, the relation between cause and effect can be written in component form, relating the components of the response to those of the stimulus through the tensor components. This relation will be elaborated further in the next lecture.

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