5 Tensors and physical properties

In this chapter we introduce the tensor description of physical properties along with Neumann's Principle relating symmetry to physical properties.

5.1 Physical properties

As pointed out in the introduction, many different types of anisotropic properties are described in this book, but all have one thing in common: a physical property is a relationship between two measured quantities. Four examples are illustrated in Fig. 5.1.

Elasticity is one of the standard equilibrium properties treated in crystal physics courses. The elastic compliance coefficients relate mechanical strain, the dependent variable, to mechanical stress, the independent variable. For small stresses and strains, the relationship is linear, but higher order elastic constants are needed to describe the departures from Hooke's Law.

Thermal conductivity is typical of the many transport properties in which a gradient leads to flow. Here the dependent variable is heat flow and the independent variable is a temperature gradient. Again the relationship is linear for small temperature gradients.

Hysteretic materials such as ferromagnetic iron exhibit more complex physical properties involving domain wall motion. In this case magnetization is the dependent variable responsive to an applied magnetic field. The resulting magnetic susceptibility depends on the past history of the material. If the sample is initially unmagnetized, the magnetization will often involve only

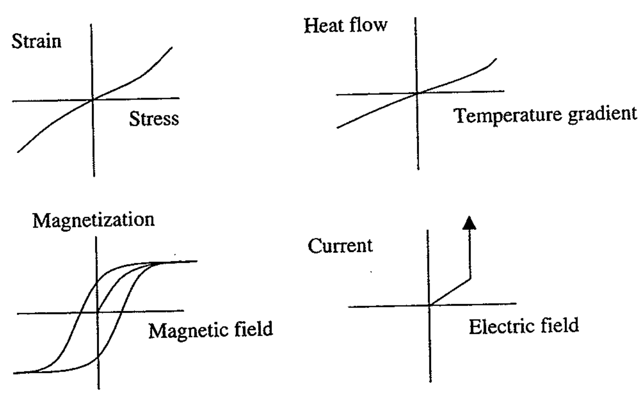

Fig. 5.1 Four types of physical properties. Elasticity is a typical equilibrium property relating stress and strain. Thermal conductivity is representative of the transport properties. Ferromagnetism is hysteretic in nature while electric breakdown is an irreversible property in which the material is permanently altered.

reversible domain wall motion for small magnetic fields. In this case the susceptibility is anhysteretic, but for large fields the wall motion is only partly reversible leading to hysteresis.

The fourth class of properties leads to permanent changes involving irreversible processes. Under very high electric fields, dielectric materials undergo an electric breakdown process with catastrophic current flow. Under small fields Ohm's Law governs the relationship between current density and electric field with a well-defined resistivity, but high fields lead to chemical, thermal, and mechanical changes that permanently alter the sample. Irreversible processes are sometimes anisotropic but they will not be discussed in this book.

5.2 Polar tensors and tensor properties

Measured quantities such as stress and strain can be represented by tensors, and so can physical properties like elastic compliance that relate these measurements. This is why tensors are so useful in describing anisotropy.

All tensors are defined by the way in which they transform from one coordinate system to another. As explained in Chapter 2, all these transformations involve a set of direction cosines a_{ij}, where i, $j = 1, 2, 3$.

In this book we deal mainly with two kinds of tensors: polar tensors and axial tensors. Axial tensors change sign when the handedness changes, whereas polar tensors do not. Their transformation laws are slightly different.

For a polar tensor, the general transformation law for a tensor of rank N is

$$T'_{ijk\ldots} = a_{il}a_{jm}a_{kn}\ldots T_{lmn\ldots},$$

where $T'_{ijk\ldots}$ is the tensor component in the new axial system, $T_{lmn}\ldots$ is a tensor component in the old system, and $a_{il}, a_{jm}, a_{kn}\ldots$ are the direction cosines relating the two coordinate systems. In this expression, each tensor component has N subscripts and there are N direction cosines involved in the product $a_{il}\,a_{jm}\,a_{kn}\ldots$. The tensor rank N has a very simple meaning. It is simply the number of directions involved in measuring the property. As an example, the thermal conductivity k relates the heat flow h to the temperature gradient $\mathrm{d}T/\mathrm{d}Z$:

$$h = -k\frac{\mathrm{d}T}{\mathrm{d}Z}.$$

There are two directions involved in measuring k: the direction in which we set up the temperature gradient, and the direction that the heat flow is measured. In general the two directions will not be the same. In tensor form this equation becomes

$$h_i = -k_{ij}\frac{\mathrm{d}T}{\mathrm{d}Z_j}.$$

The minus sign in these two expressions remind us that heat always flows down the temperature gradient from hot to cold. Here there are three tensors: h_i and $\mathrm{d}T/\mathrm{d}Z_j$ are first rank polar tensor *quantities* that transform as

$$h'_i = a_{ij}h_j$$

and

$$\frac{dT'}{dZ_i} = a_{ij}\frac{dT}{dZ_j}$$

while the thermal conductivity, that depends on both measurement directions, is a second rank tensor *property*.

$$k'_{ij} = a_{il}a_{jm}k_{lm}.$$

There are two important points to remember here. First, repeated subscripts always imply summation so there will be nine terms on the right side of the last equation. Second, h_i and dT/dZ_j are *not* properties of the material. We are at liberty to choose these experimental conditions in any way we wish, but the thermal conductivity is a property that belongs to the material. It therefore depends on the symmetry of the material, whereas the heat flow and temperature gradient do not.

The tensor rank of other physical properties is determined in a similar way. Pyroelectricity describes a relationship between thermal and electrical variables: a change in temperature ΔT creates a change in the electric polarization P. Polarization is a vector (= first rank tensor) and temperature is a scalar (= zero rank tensor). Therefore the pyroelectric coefficient, defined by $P_i = p_i\Delta T$, is a first rank tensor property.

Four directions are involved in the measurement of elastic constants. There are two directions for mechanical force and two for mechanical strain. Stress is force per unit area, and one direction is needed for the force, and another for the normal to the face on which the force acts. Strain is change in length per unit length, and directions are needed for both the reference line and the direction of the change. Therefore two subscripts are needed for stress X_{ij} and two for strain x_{ij}. Elastic compliance, that relates the two through Hooke's Law, will therefore require four subscripts:

$$x_{ij} = s_{ijkl}X_{kl}.$$

The elastic constants, s_{ijkl}, are represented by a fourth rank tensor.

5.3 Axial tensor properties

Later in the book we will deal with several properties that change sign when the axial system changes from right-handed to left-handed. Properties such as pyromagnetism, optical activity, and the Hall Effect are axial tensors that depend on the handedness. Axial tensors transform in the following manner:

$$T'_{ijk\ldots} = |a|a_{il}a_{jm}a_{kn}\ldots T_{lmn\ldots}$$

which is almost identical to that of a polar tensor. The difference is $|a|$, the determinant of the direction cosine matrix. As explained previously, $|a| = \pm 1$, depending on whether or not the handedness of the axial system changes during the transformation. For symmetry operations involving mirror planes or inversion centers, $|a| = -1$ and the sign of the tensor coefficient changes. No change occurs for rotation axes.

Magnetoelectricity is a good example of an axial tensor property. The magnetoelectric coefficients relate a change in magnetization (a first rank axial tensor) to a change in electric field (a first rank polar tensor). Since two directions are involved in the measurement, magnetoelectricity is a second rank axial tensor property.

5.4 Geometric representations

Tensor properties involve the product of direction cosines, as listed in Table 5.1. A second rank polar tensor will include terms like $\cos^2\phi$, for example, and can therefore be represented by a quadric surface.

Representative geometries are shown in Fig. 5.2. Scalar properties such as density and specific heat are independent of sample orientation and therefore the property can be visualized as a sphere. A vector property like pyroelectricity will have its maximum value along the polar axis and then fall to zero for directions perpendicular to the polar axis. The pyroelectric coefficients will change sign for opposing directions creating a negative lobe. Other odd-rank polar tensors will also show positive and negative lobes.

Even rank tensor properties will occasionally have positive and negative lobes as well. As discussed later, some physical properties such as permittivity and elasticity are constrained to have positive principal coefficients, while others such as thermal expansion, may have both positive and negative values. The illustrations in Fig. 5.2 are typical for permittivity and elasticity. Numerous examples will be presented later.

Table 5.1 Transformation laws for polar tensors of various ranks. The rank of a tensor denotes the number of different directions that must be specified in carrying out the measurement of a physical property

Tensor rank	Transformation law	Geometric representation
0	$T' = T$	Sphere
1	$T'_i = a_{ij}T_j$	Vector
2	$T'_{ij} = a_{ik}a_{jl}T_{kl}$	Quadric
3	$T'_{ijk} = a_{il}a_{jm}a_{kn}T_{lmn}$	Cubic
4	$T'_{ijkl} = a_{im}a_{jn}a_{ko}a_{lp}T_{mnop}$	Quartic

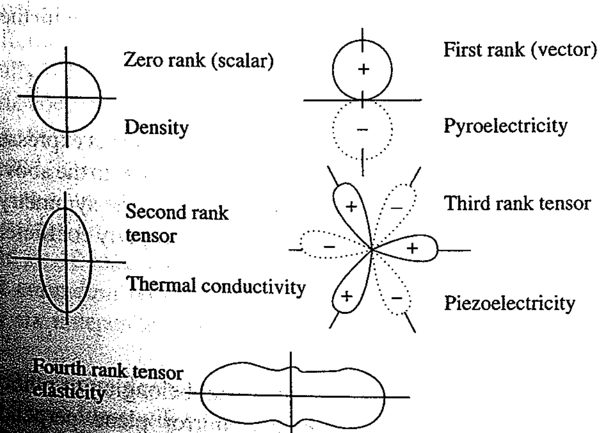

Fig. 5.2 Typical geometric surfaces of physical properties plotted as a function of measurement directions.

5.5 Neumann's Principle

The most important concept in Crystal Physics is Neumann's Principle that states: [redacted] The proof of Neumann's Principle is common sense. What it says is that measurements made in symmetry-related directions will give the same property coefficients.

Sodium chloride is a cubic crystal belonging to point group $m3m$. The [100] and [010] directions are equivalent fourfold symmetry axes (Fig. 5.3). Since these directions are physically the same, it makes sense that measurements of permittivity, elasticity, or any other physical property will be the same in these two directions. This means that when the magnitudes of the property are plotted as a function of direction, the resulting figure will show fourfold symmetry when viewed along the [100] or [010] directions. In other words the symmetry of the physical property will include the symmetry elements of the point group.

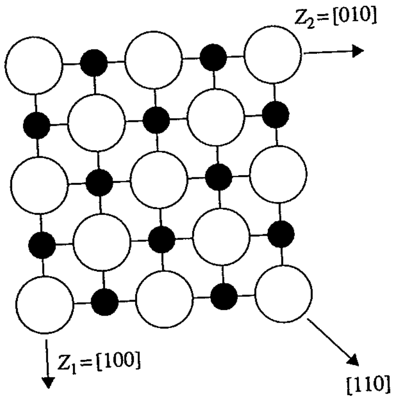

Fig. 5.3 Crystal structure of NaCl showing the equivalence of [100] and [010] directions.

But the reverse is not true, for the symmetry of the physical property may be much higher than that of the point group. This becomes obvious when we visualize a scalar property such as specific heat. Here the geometric representation is a sphere (symmetry group $\infty\infty m$) that includes the symmetry of sodium chloride (point group $m3m$) but not vice versa.

The argument just applied to [100] directions in NaCl, holds for other directions as well. In NaCl, the [110] and [$\bar{1}$10] directions are symmetry-related twofold axes, and therefore the properties will be the same when measurements are carried out in a similar way along [110] and [$\bar{1}$10].

What about the properties along [100] and [110]? Will they sometimes be the same? For scalar properties the answer is, of course, yes. For higher rank tensor properties, it will depend upon the point group symmetry *and* the tensor rank. In cubic crystals, second rank tensors like permittivity and resistivity, measurements along [100] and [110] will be the identical, but not for fourth rank tensor properties like elastic compliance. The reasons will become clearer after applying Neumann's Principle to a number of different situations.

5.6 Analytical form of Neumann's Principle

In expressing Neumann's Principle mathematically, we begin with the definition of a tensor

$$T'_{ijk\ldots} = a_{il}a_{jm}a_{kn}\ldots T_{lmn\ldots}.$$

The direction cosine matrix for any symmetry operation is expressed through the (a) matrix. These (a) coefficients are then substituted into the above equation to transform the tensor coefficients under the action of the symmetry operator. If the crystal possesses this symmetry element, the property coefficient must be left unchanged.

Mathematically this means

$$T'_{ijk\ldots} = T_{ijk\ldots}.$$

As an example, consider a monoclinic crystal belonging to point group m. There is only one symmetry element, a mirror plane perpendicular to

$Z_2 = [010]$, the b crystallographic axis. The direction cosine matrix for $m \perp Z_2$ is

$$(a) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}.$$

We now apply Neumann's Principle to a third rank tensor property, beginning with tensor coefficient T'_{111},

$$T'_{111} = a_{11}^3 T_{111} + a_{11}^2 a_{12} T_{112} + \cdots + a_{13}^3 T_{333}.$$

For the mirror plane, all terms go to zero except the first term:

$$T'_{111} = T_{111}.$$

By Neumann's Law this coefficient remains unchanged. This means coefficient T_{111} is unaffected by the mirror plane.

The situation is different for T_{222}.

$$T'_{222} = a_{22}^3 T_{222} + a_{22}^2 a_{21} T_{221} + \cdots.$$

Again all terms disappear except the first, and $T'_{222} = -T_{222}$. In this case Neumann's Principle says $-T_{222} = T_{222}$ which is only possible if $T_{222} = 0$. Therefore this property coefficient must disappear for crystals belonging to point group m.

This is why Neumann's Principle is useful to an experimentalist. It greatly simplifies the description of physical properties by eliminating some coefficients and equalizing others.

To illustrate, consider two of the standard single crystal materials available to scientists and engineers: quartz (SiO_2) and corundum (Al_2O_3). Both belong to the trigonal crystal system but have different point group symmetries. Quartz is in point group 32 while corundum is somewhat higher in $\bar{3}m$.

Symmetry arguments based on Neumann's Principle tell us that neither crystal is pyroelectric since first rank polar tensors disappear for both point groups. In regard to permittivity, resistivity, thermal expansion, and other second rank tensor properties, there will be three nonzero coefficients, but only two measurements are required because two of the three coefficients are equal.

For piezoelectricity and other third rank polar tensors, quartz and corundum are very different. Quartz is an outstanding piezoelectric material while corundum is totally useless. The center of symmetry in point group $\bar{3}m$ causes all piezoelectric coefficients disappear. Quartz, on the other hand, has five nonzero coefficients, two of which are independent. A large number of piezoelectric [illegible]ators and timing devices make use of these two coefficients.

Elasticity is a fourth rank tensor property so there are many different directions to consider. For a triclinic crystal with no mirror planes or rotation axes, [illegible] would be 18 independent elastic constants, but the higher symmetry of [illegible] and corundum reduce the required number of experiments consider[illegible] only six independent elastic coefficients are present in point group 32 [illegible]

[illegible] simplifications are found for other polar and axial tensor [illegible] These ideas will be discussed throughout the book.

Problem 5.1

The cubic crystal structure of rocksalt is pictured in Figs. 5.3 and 13.4. The [100] direction is equivalent to [010], [001], [$\bar{1}$00], [0$\bar{1}$0], and [00$\bar{1}$], a total of six directions. How many directions are related to [110] by symmetry? What about [111] and [210]?

Problem 5.2

There are ten properties listed in Table 1.1. Each is represented by a different tensor. Write out the tensor transformation for each property. For pyroelectricity, a first rank polar tensor, there are three coefficients. How many for the other properties?