Lecture 3: Tensors and representation quadrics

Nature of a tensor

There are a number of ways to introduce tensors. We shall begin by considering tensors of zero, first and second rank, before extending our discussion to tensors of third and fourth rank.

Scalar quantities are examples of tensors of zero rank; these simply have magnitude. Vectors are tensors of the first rank. These have both direction and magnitude and represent a definite physical quantity. Tensors of the second rank are quantities that relate two vectors.

Suppose we wish to know the relationship between the electric field in a crystal, represented by the vector **E**, and the current density (i.e. current per unit area of cross-section perpendicular to the current), represented by the vector **J.** In general, in a crystal the components of **J** referred to three mutually perpendicular axes (Ox_1, Ox_2, Ox_3), which we can call J_1, J_2 and J_3 will be related to the components of **E**, referred to the same set of axes in such a way that they each depend linearly on *all three of the components E_1, E_2 and E_3*. It is usual to write this in the following way:

$$J_1 = \sigma_{11}E_1 + \sigma_{12}E_2 + \sigma_{13}E_3$$
$$J_2 = \sigma_{21}E_1 + \sigma_{22}E_2 + \sigma_{23}E_3$$
$$J_3 = \sigma_{31}E_1 + \sigma_{32}E_2 + \sigma_{33}E_3$$

The nine quantities $\sigma_{11}, \sigma_{12}, \sigma_{13}, \sigma_{21}, \sigma_{22}, \sigma_{23}, \sigma_{31}, \sigma_{32}, \sigma_{33}$ are called the components of the conductivity tensor. The electrical conductivity tensor relates the vectors **J** and **E**. If we write all of the above relations in the shorthand form

$$\mathbf{J} = \sigma\,\mathbf{E}$$

we see that σ is a quantity that multiplies the vector **E** in order to obtain the vector **J**. When a tensor relates two vectors in this way it is called a tensor of the second rank or second order.

Many physical properties are represented by tensors like the electrical conductivity tensor. Such tensors are called *matter tensors*. Some examples are given in the table below.

In addition there are *field tensors* of which two second-rank tensors are very important, namely stress and strain. The stress tensor relates the vector traction (force per unit area) and the orientation of an element of area in a stressed body. The strain tensor relates the displacement of a point in a strained body and the position of the point.

Properties represented by second-rank tensors

Tensor	Vectors related	
Electrical conductivity	Electric field	Current density
Thermal conductivity	Thermal gradient (negative)	Thermal current density
Diffusivity	Concentration gradient (negative)	Flux of atoms
Permittivity	Electric field	Dielectric displacement
Dielectric susceptibility	Electric field	Dielectric polarization
Permeability	Magnetic field	Magnetic induction
Magnetic susceptibility	Magnetic field	Intensity of magnetization

Transformation of components of a vector

If we know the components of a vector, say **p**, referred to a set of orthogonal axes (Ox_1, Ox_2, Ox_3), each of unit length, i.e. orthonormal axes, it is often necessary to know the components of the same vector referred to a different set of axes (Ox_1', Ox_2', Ox_3') which are again orthonormal and have the same origin as Ox_1, Ox_2 and Ox_3, as in the figure below. We must first define how the two sets of axes are related to one another.
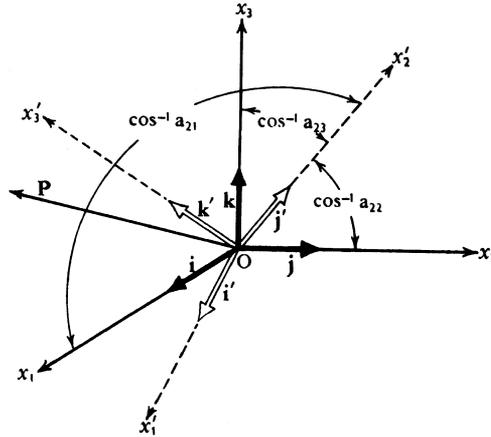
We do this by setting down a table of the cosines of the angles between each new axis and the three of the old set. The table will appear as:

<div align="center">

Old

		x_1	x_2	x_3
	x_1'	a_{11}	a_{12}	a_{13}
New	x_2'	a_{21}	a_{22}	a_{23}
	x_3'	a_{31}	a_{32}	a_{33}

</div>

Here a_{32}, for example, is the cosine of the angle between the new axis 3 and the old axis 2, i.e. the angle $x_3'Ox_2$ in the above figure. Similarly, a_{11} is the cosine of the angle between Ox_1' and Ox_1, etc. In an array of the type here, it should be noted that the sum of the squares of any row or column of the array is equal to one, because both sets of axes are orthonormal. Therefore, for example, $a_{11}^2 + a_{21}^2 + a_{31}^2 = 1$ and $a_{21}^2 + a_{22}^2 + a_{23}^2 = 1$, etc. It is evident that the elements a_{ij} constitute the elements of a rotation matrix. If we call this matrix **A**, then the inverse of this matrix, $\mathbf{A}^{-1}$, is equal to its transpose, $\tilde{\mathbf{A}}$.

Now let **p** have components p_1, p_2, p_3 along the 'old' axes so that

$$\mathbf{p} = p_1\mathbf{i} + p_2\mathbf{j} + p_3\mathbf{k}$$

where **i, j, k** are unit vectors along Ox_1, Ox_2, Ox_3 respectively. The components of **p** along the new axes Ox_1', Ox_2', Ox_3' are then

$$p_i' = a_{ij}p_j$$

using dummy suffix notation. Inverting this equation, we have

$$p_j = (a_{ij})^{-1} p'_i = (\tilde{a}_{ij})_{ij} p'_i = a_{ji} p'_i$$

since the inverse of the a_{ij} matrix is its transpose.

Suppose that

$$p_i = T_{ij} q_j$$

where the tensor T relates the vector $\mathbf{p}$ with components p_1, p_2 and p_3 to the vector $\mathbf{q}$ with components q_1, q_2 and q_3.

The *components* of the two vectors depend upon the choice of axes, because this choice determines the values $[p_1 \; p_2 \; p_3]$ and $[q_1 \; q_2 \; q_3]$. The vectors $\mathbf{p}$ and $\mathbf{q}$ themselves do not change. When the axes are changed, and hence the components of $\mathbf{p}$ and $\mathbf{q}$ change, the components T_{ij} will also change.

If now we choose new axes $\mathbf{i}'$, $\mathbf{j}'$, $\mathbf{k}'$ so that

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

we then wish to find the relation between the nine components T'_{ij} and the nine components T_{ij}.

To establish the relationship between T'_{ij} and T_{ij}, we can perform the following mathematical operations with suitable dummy suffices to determine the nine components of T'_{ij}:

(1) Write p' in terms of p: $p'_i = a_{ik} p_k$
(2) Write p in terms of q: $p_k = T_{kl} q_l$
(3) Write q in terms of q': $q_l = a_{jl} q'_j$

When we combine these three operations we have

$$p'_i = a_{ik} p_k = a_{ik} T_{kl} q_l = a_{ik} T_{kl} a_{jl} q'_j$$

or

$$p'_i = a_{ik} T_{kl} a_{jl} q'_j$$

Therefore, we have the important result

$$T'_{ij} = a_{ik} T_{kl} a_{jl} = a_{ik} a_{jl} T_{kl}$$

because the order in which a product is written on the right-hand side of this equation does not matter when the dummy suffix notation is used. This defines a tensor of the second rank, in the sense that if an operator T relates two vectors $\mathbf{p}$ and $\mathbf{q}$ through $p_i = T_{ij} q_j$, it must transform to new axes according to this transformation.

Tensors of the second rank

A tensor of the second rank, T_{ij}, is said to be symmetric if $T_{ij} = T_{ji}$, and to be skew symmetric or antisymmetric if $T_{ij} = -T_{ji}$. For our purposes, all *matter tensors* we are likely to encounter in materials science are symmetric. This is also true for stress and strain *field tensors*.

Any *symmetric* tensor S_{ij} can be transformed by a suitable choice of orthonormal axes so that it takes on the simple form

$$\begin{bmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{bmatrix}$$

i.e. all $S_{ij} = 0$ unless $i = j$. Such a tensor when expressed in this form is said to be referred to its *principal axes*. When referred to its principal axes, the components S_{11}, S_{22}, S_{33} are called the *principal components* and are often written simply as S_1, S_2, S_3 respectively.

Limitations imposed by crystal symmetry for second rank tensors

The discussion in this section applies to tensors used to represent *physical properties* of crystals, and strictly only to perfect single crystals, i.e. ones without defects.

The fact that physical properties of crystals should remain the same when the system of coordinates to which the properties are referred are rotated to a new set of coordinates by a symmetry operation was first appreciated by Franz Neumann (1798–1895), a student of Christian Samuel Weiss of the Weiss Zone Law, who applied this principle to elastic coefficients of crystals in a course in elasticity at the University of Königsberg in 1873/4. While this is one way of defining what has now come to be known as *Neumann's principle*, it is nowadays more usual to state the principle in the form:

'The symmetry elements of a physical property of a crystal must include the symmetry elements of the point group of the crystal'

It is important to appreciate that the principle does not state that the symmetry of the physical property is the same as that of the point group: the symmetry of physical properties is often higher than that of the corresponding point group.

Physical properties characterized by a second-order tensor are necessarily invariant with respect to the operation of a centre of symmetry. This is implicit in the linear relations

$$p_i = T_{ij} q_j$$

because if we substitute $-p_i$ for p_i and $-q_j$ for q_j (i.e. we reverse the directions of **p** and of **q**), the relation is still satisfied by the same values of T_{ij}. In terms of applying Neumann's principle, this means that physical properties represented by second-order tensors for all crystals must include the symmetry of $\bar{1}$; this will be true even for crystals belonging to non-centrosymmetric point groups.

It will assist in understanding what follows if we look at the centre of symmetry statement in another way. Suppose that for one set of axes (Ox_1, Ox_2, Ox_3) the relations between the p_i and the q_j are given by T_{ij}. If we now reverse the axes of reference, leaving **p** and **q** the same as before, this corresponds to choosing a new set of axes such that the array of the a_{ij} relating the axes is

<div align="center">

Old

		x_1	x_2	x_3
	x_1'	-1	0	0
New	x_2'	0	-1	0
	x_3'	0	0	-1

</div>

Here, all a_{ij} are equal to zero unless $i = j$. We now apply the transformation formula:

$$T_{ij}' = a_{ik} a_{jl} T_{kl}$$

Therefore,

$$T_{ij}' = a_{ii} a_{jj} T_{ij} = T_{ij} \text{ since } a_{11} = a_{22} = a_{33} = -1$$

What we have done here is to leave the measured quantities **p** and **q** the same and to imagine the crystal inverted through a centre of symmetry operation. We have obtained the same result as if we had reversed the directions of **p** and **q.**

Now suppose the crystal contains a diad axis of symmetry. If we measure a certain property along a certain direction with respect to this axis, and then rotate the crystal 180° about this axis and remeasure the property, we will get the same value as before by Neumann's principle. This imposes restrictions on the values of the components of any *symmetric* second-rank tensor S_{ij} which represents this property. In this context, it is relevant that the tensors of the second rank in which we will be interested will all be symmetric.

To see what these restrictions are, take axes (Ox_1, Ox_2, Ox_3) and suppose there is a diad axis along Ox_2, such as might arise in a material with monoclinic symmetry. Initially, we assume the tensor S_{ij} is symmetric, so that it has six independent components. Now, if we take new axes related to the old by a rotation of 180° about Ox_2, the physical property must remain the same as before. The new axes are related to the old by the array of a_{ij} as

<div align="center">

Old

		x_1	x_2	x_3
	x_1'	-1	0	0
New	x_2'	0	1	0
	x_3'	0	0	-1

</div>

The components of the tensor with respect to the new axes, S'_{ij} , are given in terms of the old components, S_{ij} , by

$$S'_{ij} = a_{ik} a_{jl} S_{kl}$$

and we must have $S'_{ij} = S_{ij}$ for all i and j. If we work out the components S'_{ij} one by one we find

$$S'_{11} = a_{11}a_{11}S_{11} = S_{11}, \qquad S'_{22} = a_{22}a_{22}S_{22} = S_{22},$$
$$S'_{33} = a_{33}a_{33}S_{33} = S_{33}, \qquad S'_{13} = a_{11}a_{33}S_{13} = S_{13}$$

but

$$S'_{23} = a_{22}a_{33}S_{23} = -S_{23} \qquad \text{and} \qquad S'_{12} = a_{11}a_{22}S_{12} = -S_{12}$$

However, we must also have $S'_{23} = S_{23}$ and $S'_{12} = S_{12}$. Therefore, $S_{23} = S_{12} = 0$. Hence, a symmetrical second-rank tensor representing a physical property of a crystal with a two-fold axis of rotational symmetry must have the components S_{23} and S_{12} equal to zero when referred to axes so that Ox_2 corresponds to the diad axis.

The limitations on the components of a symmetrical second-rank tensor representing a physical property of a crystal can therefore be summarized for each of the seven crystal systems:

Number of independent components of physical properties
represented by second-rank (order) tensors

Crystal system	Orientation of principal axes with respect to the crystal axes	Form of tensor	Number of independent components
Cubic	Any	$\begin{bmatrix} S & 0 & 0 \\ 0 & S & 0 \\ 0 & 0 & S \end{bmatrix}$	1
Tetragonal Hexagonal Trigonal[a]	x_3 parallel to 4, 6, 3 or $\bar{3}$	$\begin{bmatrix} S_1 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_3 \end{bmatrix}$	2
Orthorhombic	x_1, x_2, x_3 parallel to the diads along the x, y and z-axes	$\begin{bmatrix} S_1 & 0 & 0 \\ 0 & S_2 & 0 \\ 0 & 0 & S_3 \end{bmatrix}$	3
Monoclinic	x_2 parallel to the diad along the y-axis	$\begin{bmatrix} S_{11} & 0 & S_{13} \\ 0 & S_{22} & 0 \\ S_{13} & 0 & S_{33} \end{bmatrix}$	4
Triclinic	Not fixed	$\begin{bmatrix} S_{11} & S_{12} & S_{13} \\ S_{12} & S_{22} & S_{23} \\ S_{13} & S_{23} & S_{33} \end{bmatrix}$	6

[a]A hexagonal cell is used here for trigonal crystals.

Tensors of the second rank referred to principal axes

As we have see, when referred to its principal axes, the symmetric tensor S_{ij} relating vectors **p** and **q** only has its diagonal components S_{11}, S_{22} and S_{33} as possible non-zero components. Under these circumstances, the equations

$$p_i = S_{ij}q_j$$

reduce to

$$p_1 = S_{11}q_1, \qquad p_2 = S_{22}q_2, \qquad p_3 = S_{33}q_3.$$

Now let us return to the simple example of electrical conductivity. The conductivity tensor σ_{ij} is symmetric. When referred to its principal axes, all the σ_{ij} are zero except σ_{11}, σ_{22} and σ_{33}. If the crystal under consideration is orthorhombic, monoclinic or triclinic, there is no symmetry requirement that two or more of σ_{11}, σ_{22} and σ_{33} have to be equal. For our purposes here we shall assume that none of σ_{11}, σ_{22} and σ_{33} are equal.

Suppose we apply an electrical field **E** in the x_1-x_2 plane with components $[E_1, E_2, 0]$ along these principal axes. Then

$$J_1 = \sigma_{11}E_1 + \sigma_{12}E_2 + \sigma_{13}E_3 = \sigma_{11}E_1$$

because σ_{12} and σ_{13} are both zero.

Similarly, $J_2 = \sigma_{22}E_2$. However, $J_3 = 0$ because $E_3 = 0$. We can represent this relationship between **J** and **E** on a diagram such as the one below. This diagram can be constructed by drawing **E**, finding E_1 and E_2 and multiplying E_1 by σ_{11} to get J_1 and E_2 by σ_{22} to get J_2. We then construct **J** from its components along the axes, i.e. J_1 and J_2.

It should be noted carefully that, in general, **J** and **E** are not parallel. If **E** were directed along Ox_1, we would have $J_1 = \sigma_{11}E_1$ because then both J_2 and J_3 are zero. Likewise, if **E** were directed along Ox_2, **J** would be parallel to **E**; **J** will only be parallel to **E** if **E** is directed along a principal axis.
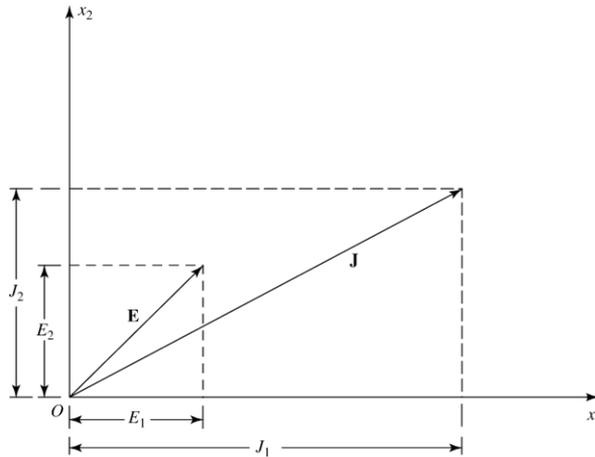
When we speak of the conductivity in a particular direction, what we actually mean in practice is that if $\mathbf{E}$ is applied in that direction and the current density is measured *in the same direction*, to give a value $J_{\parallel}$, then the conductivity in this direction is $J_{\parallel}$ divided by the magnitude of $\mathbf{E}$, i.e. $J_{\parallel}/|\mathbf{E}|$. We can find an expression for this by resolving $\mathbf{J}$ parallel to $\mathbf{E}$.

Suppose $\mathbf{E}$ is applied in a direction so that its direction cosines with respect to the principal axes of the conductivity tensor are $\cos\alpha$, $\cos\beta$ and $\cos\gamma$. Then we have

$$J_1 = \sigma_{11}E_1 = \sigma_{11}E\cos\alpha$$

$$J_2 = \sigma_{22}E_2 = \sigma_{22}E\cos\beta$$

$$J_3 = \sigma_{33}E_3 = \sigma_{33}E\cos\gamma$$

where E is the magnitude of $\mathbf{E}$ (i.e. $|\mathbf{E}|$). Then, a unit vector $\hat{\mathbf{n}}$ parallel to $\mathbf{E}$ is simply the vector $[\cos\alpha, \cos\beta, \cos\gamma]$ since $\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$. Resolving $\mathbf{J}$ parallel to $\mathbf{E}$ produces a vector parallel to $\mathbf{E}$ of magnitude $J_{\parallel} = \mathbf{J}.\hat{\mathbf{n}}$. Hence,

$$J_{\parallel} = J_1\cos\alpha + J_2\cos\beta + J_3\cos\gamma = E(\sigma_{11}\cos^2\alpha + \sigma_{22}\cos^2\beta + \sigma_{33}\cos^2\gamma)$$

Therefore the conductivity in the direction parallel to $\mathbf{E}$ is

$$\boxed{\sigma = J_{\parallel}/E = \sigma_{11}\cos^2\alpha + \sigma_{22}\cos^2\beta + \sigma_{33}\cos^2\gamma}$$

The steps in deriving this equation are illustrated diagrammatically in the diagram below for the simple case where $\mathbf{E}$ is normal to the principal axis Ox_3 of the conductivity tensor, so that $\cos\gamma = 0$.
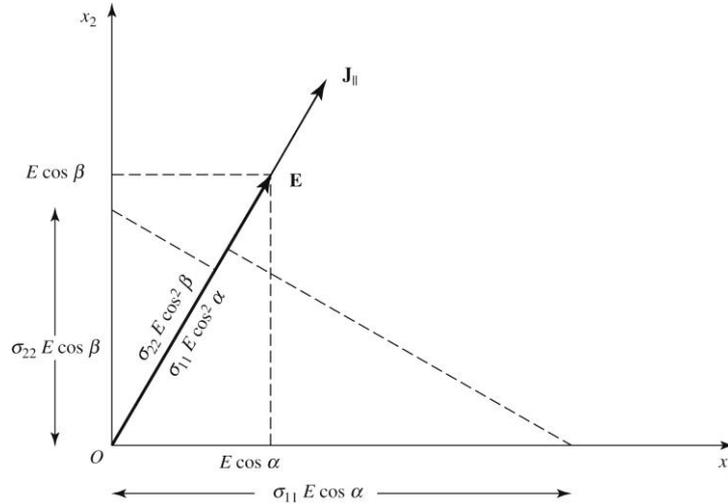
Derivation of the magnitude of the conductivity in a particular direction.
The figure is drawn for $\sigma_{11} = 250$ and $\sigma_{22} = 75$ ohm^{-1} m^{-1}, so that $\sigma_{22} = 0.3\,\sigma_{11}$.

It is instructive to derive the result given in the box on the previous page in a different way. Suppose we consider the meaning of the component σ'_{11} of the conductivity tensor irrespective of whether it is referred to principal axes.

The component σ'_{11} relates the electric field along axis Ox'_1 to the component of the current along the same axis Ox'_1. If, therefore, we wish to find the value of the conductivity in a particular direction, having been given the components of the conductivity tensor referred to its principal axes, we can proceed as follows:

Choose a new set of axes such that Ox'_1 is along the direction of interest. Then the component σ'_{11} of the conductivity tensor referred to this new set of axes gives us the conductivity along this particular direction – the $J_\parallel / E$. We are only interested in σ'_{11}, so in writing out the array of the a_{ij} for this transformation we only need to know the values of the cosines of the angles between Ox'_1 and the principal axes of the conductivity tensor, Ox_1, Ox_2 and Ox_3.

Following the scheme of the expressions in the matrix of direction cosines we therefore only need to know a_{11}, a_{12} and a_{13}. These quantities are $\cos\alpha$, $\cos\beta$ and $\cos\gamma$ respectively. Using the transformation formula, we have

$$\sigma'_{ij} = a_{ik} a_{jl} \sigma_{kl}$$

and so when $i = 1$ and $j = 1$,

$$\sigma'_{11} = a_{1k} a_{1l} \sigma_{kl}$$

Since σ_{ij} is defined relative to its principal axes, the only non-zero terms within this conductivity tensor are σ_{11}, σ_{22} and σ_{33}. Therefore,

$$\sigma'_{11} = a_{11}a_{11}\sigma_{11} + a_{12}a_{12}\sigma_{22} + a_{13}a_{13}\sigma_{33}$$

Substituting for a_{11}, a_{12}, a_{13}, we obtain

$$\boxed{\sigma'_{11} = \sigma_{11} \cos^2\alpha + \sigma_{22} \cos^2\beta + \sigma_{33} \cos^2\gamma}$$

once again.

It is clear that we could have proceeded in exactly the same way to find the conductivity in a particular direction, even if the values of the components of σ_{ij}, the conductivity tensor, had not been given to us referred to principal axes. In this case there would have been, in general, nine terms in the expansion of $\sigma'_{ij} = a_{ik} a_{jl} \sigma_{kl}$. This transformation formula clearly holds irrespective of whether the σ_{ij} are referred to principal axes.

Therefore, we can state that to find the value of a property of a crystal in a particular direction we proceed as follows:

Let the components of the tensor representing this property be given as T_{ij} referred to axes (Ox_1, Ox_2, Ox_3). Choose an axis along the direction of interest and call this Ox_1'. Let this axis have direction cosines referred to (Ox_1, Ox_2, Ox_3) of a_{11}, a_{12}, a_{13} respectively. Then the value of the property T_{11}' in the direction we are interested in is given by

$$T_{11}' = a_{1i}a_{1j}T_{ij}$$

This relation holds for all second-rank tensors whether or not they are symmetrical. This equation can be written in a convenient shorthand notation by removing the dash and the '1' subscripts in this equation, so that the property T along the direction of interest is

$$T = l_i l_j T_{ij}$$

where the relevant direction cosines are now defined as l_1, l_2 and l_3 to conform to the notation used by Nye.

Representation quadric

The equation

$$\sigma_{11}' = \sigma_{11} \cos^2\alpha + \sigma_{22} \cos^2\beta + \sigma_{33} \cos^2\gamma$$

is that of a general surface of the second degree referred to its principal axes, taking in general the form

$$\frac{1}{r^2} = A \cos^2\alpha + B \cos^2\beta + C \cos^2\gamma$$

which is of the same form as the equation for σ_{11}'. As a consequence, the variation of a given *property* of a crystal with direction, can be represented by a suitable figure in three-dimensional space. When all the values of the property are positive, as in the case of electrical conductivity, this second-degree surface, or representation quadric, is an ellipsoid.

If in general we construct an ellipsoid of semi-principal axes $1/\sqrt{S_1}, 1/\sqrt{S_2}, 1/\sqrt{S_3}$, as in the figure on the next page, so that a general point on the ellipsoid satisfies the equation

$$S_1 x_1^2 + S_2 x_2^2 + S_3 x_3^2 = 1$$

then the length r of any radius vector of the ellipsoid (representation quadric) is equal to the reciprocal of the square root of the magnitude of the property S in that direction.

Returning to the example of electrical conductivity, and we know the values σ_1, σ_2 and σ_3 of the components of the electrical conductivity referred to principal axes, then we can construct the ellipsoid defining the conductivity quadric.

If now a field $\mathbf{E}$ is applied in any direction, the magnitude of the conductivity in that direction can be found by drawing a radius vector r in the direction of $\mathbf{E}$, measuring the value of r and taking the reciprocal of the square root of r to find the conductivity in that direction.
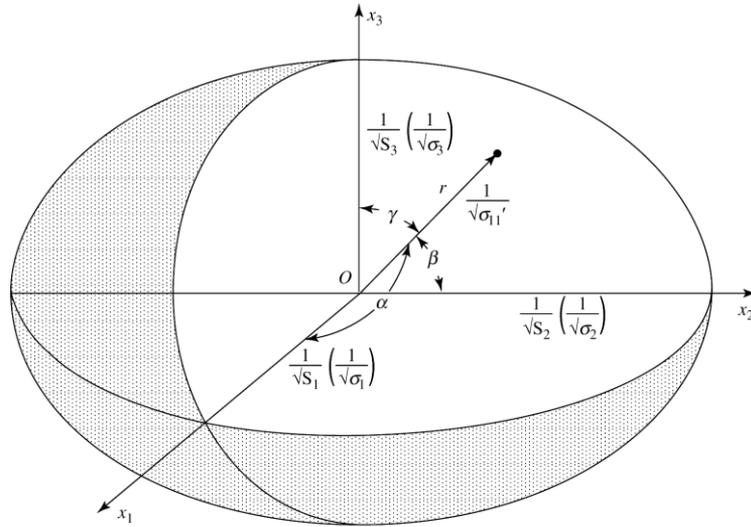
Radius–normal property of the representation quadric

The representation ellipsoid has a further very useful property known as the *radius–normal* property. It can be stated as follows: if S_{ij} are the components of a symmetrical second-rank tensor relating the vectors $\mathbf{p}$ and $\mathbf{q}$ so that $p_i = S_{ij}q_j$, then the direction of $\mathbf{p}$ for a given $\mathbf{q}$ can be found by drawing a radius vector OQ of the representation quadric parallel to $\mathbf{q}$ and finding the normal to the quadric at Q. This is shown in two dimensions in the figure below.
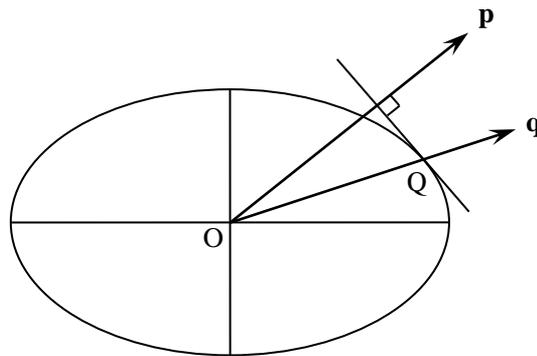
The radius-normal property of a representation ellipsoid

A proof of this property is given in Section 5.9 of Kelly and Knowles.

Third and fourth-rank tensors

Just as a second-rank tensor relates two vectors, so a third-rank tensor relates a second-rank tensor and a vector, and a fourth-rank tensor relates two second-rank tensors, and so on. Thus, for a tensor of the third rank T_{ijk}, such as the piezoelectric tensor, we can envisage a relationship between a second rank tensor σ_{jk} and a vector p_i so that, for example,

$$p_i = T_{ijk}\sigma_{jk}$$

Equally, relationships could be of the general form

$$\sigma_{ij} = T_{ijk}\,p_k$$

where we require the tensor of the third rank to transform as

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

generalising the result for a tensor of the second rank. Likewise, a tensor of the fourth rank T_{ijkl} such as the stiffness tensor c_{ijkl} and the compliance tensors s_{ijkl}, can relate two tensors of the second rank, σ_{ij} and g_{kl} through an equation of the form

$$\sigma_{ij} = T_{ijkl}\,g_{kl}$$

where T_{ijkl} transforms as

$$T'_{ijkl} = a_{im}a_{jn}a_{kp}a_{lq}T_{mnpq}$$

We are now in a position to examine the relationship between the stress and strain field tensors. Further aspects not considered here considering the effects of crystal symmetry on third and fourth rank tensors are discussed in the book by Kelly and Knowles.

Infinitesimal strain

This is relevant for a description of how elastic strains affect perfect crystals when considering both piezoelectricity and elasticity

The distortion of a body can be described by giving the displacement of each point from its location in the undistorted state. Any displacements which do *not* correspond to a translation or rotation of the body as a whole will produce a strain.

If we confine ourselves to two dimensions, we can choose an origin fixed in space such as O in the diagram below. Let P be a point with coordinates (x_1, x_2) in the unstrained state, which after distortion of the body moves to the point P'. (Then the displacement of the point P is the vector PP'.) Let the coordinates of P' be $(x_1 + u_1, x_2 + u_2)$.
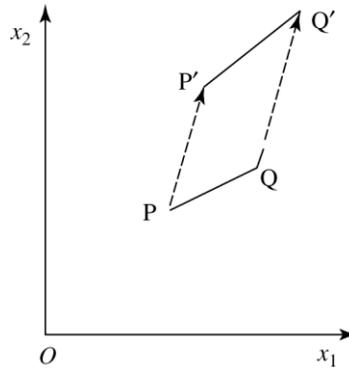
Now consider a point Q with coordinates $(x_1 + dx_1, x_2 + dx_2)$ lying infinitesimally close to P in the unstrained state. After deformation Q moves to Q'. Now, in a strained body the displacement of Q will not be exactly the same as that of P. The displacement of Q to Q' has components $(u_1 + du_1, u_2 + du_2)$. We can write

$$du_1 = \frac{\partial u_1}{\partial x_1} dx_1 + \frac{\partial u_1}{\partial x_2} dx_2$$

and

$$du_2 = \frac{\partial u_2}{\partial x_1} dx_1 + \frac{\partial u_2}{\partial x_2} dx_2$$

Defining the four quantities at the point P,

$$e_{11} = \frac{\partial u_1}{\partial x_1}, \quad e_{12} = \frac{\partial u_1}{\partial x_2}, \quad e_{22} = \frac{\partial u_2}{\partial x_2}, \quad e_{21} = \frac{\partial u_2}{\partial x_1},$$

all of which can be compactly written as

$$du_i = e_{ij} \, dx_j \quad (j = 1, 2)$$

Since du_i and dx_j are vectors, then e_{ij} is a tensor, which we can term the relative displacement tensor. We shall now demonstrate the physical meaning of the various e_{ij} when each is very small compared to unity.

Let us take two special positions of the vector PQ: first parallel to Ox_1 (PQ_1), and then parallel to Ox_2 (PQ_2), and find out how a rectangular element at P is distorted:
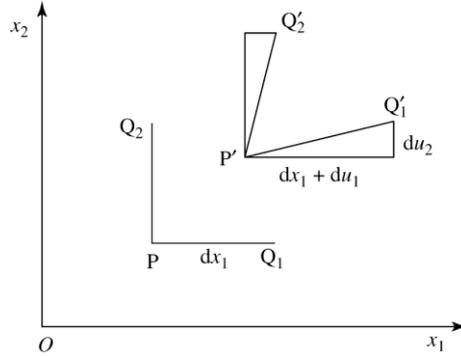

For PQ_1 we put $dx_2 = 0$ and obtain

$$du_1 = \frac{\partial u_1}{\partial x_1} dx_1 = e_{11} \, dx_1$$

$$du_2 = \frac{\partial u_2}{\partial x_1} dx_1 = e_{21} \, dx_1$$

It is clear that e_{11} measures the extension per unit length of PQ_1 resolved along Ox_1, while e_{21} measures the anticlockwise rotation of PQ_1, provided that e_{11} and e_{21} are small. Similarly, e_{22} measures the change in length per unit length of PQ_2, resolved along Ox_2 and e_{12} measures the small clockwise rotation of PQ_2.

This relative displacement tensor e_{ij} is not completely satisfactory as a measure of strain, because it is possible to have non-zero components of e_{ij} without there being any distortion of the body. Thus, consider a rigid-body rotation through a small angle ω, illustrated below. Evidently we have $e_{11} = e_{22} = 0$, but $e_{12} = -\omega$ and $e_{21} = \omega$ (since for small angles, $\tan \omega = \omega - O(\omega^3) \cong \omega$, neglecting the higher order terms since we are considering infinitesimal relative displacements).
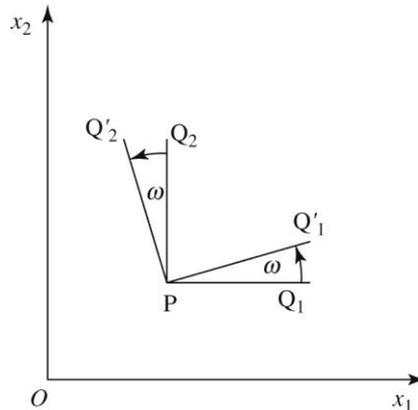
To remove the component of rotation from a general e_{ij} we express it as the sum of a symmetrical tensor, ε_{ij}, and an antisymmetrical tensor, ω_{ij}, so that

$$e_{ij} = \varepsilon_{ij} + \omega_{ij} = \frac{1}{2}\left(e_{ij} + e_{ji}\right) + \frac{1}{2}\left(e_{ij} - e_{ji}\right)$$

Then $\varepsilon_{ij} = \frac{1}{2}\left(e_{ij} + e_{ji}\right)$ is defined as the *pure strain* and $\omega_{ij} = \frac{1}{2}\left(e_{ij} - e_{ji}\right)$ measures the rotation. The shear component of the pure strain tensor ε_{12} is half the engineering shear strain γ (see Kelly and Knowles for further details).

In specifying infinitesimal strain in three dimensions, the result is

$$\begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{bmatrix} = \begin{bmatrix} e_{11} & \frac{1}{2}\left(e_{12} + e_{21}\right) & \frac{1}{2}\left(e_{13} + e_{31}\right) \\ \frac{1}{2}\left(e_{21} + e_{12}\right) & e_{22} & \frac{1}{2}\left(e_{23} + e_{32}\right) \\ \frac{1}{2}\left(e_{31} + e_{13}\right) & \frac{1}{2}\left(e_{32} + e_{23}\right) & e_{33} \end{bmatrix}$$

The diagonal components of ε_{ij} are the changes in length per unit length of lines parallel to the axes and are called the tensile strains. The off-diagonal components measure shear strains so that, for instance, ε_{13} is one-half the change in angle between two lines originally parallel to the Ox_1 and Ox_3 axes.

Since pure strain is a symmetrical second-rank tensor, it can be referred to principal axes. Under these circumstances, the shear components vanish and we then have

$$\varepsilon = \begin{bmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 & 0 \\ 0 & 0 & \varepsilon_3 \end{bmatrix}$$

The components of a given strain transform according to the general transformation law

$$\varepsilon_{ij} = a_{ik} a_{jl} \varepsilon_{kl}$$

Stress

The stress tensor is also a symmetric tensor when a material in equilibrium, and so in general it can be represented in the form

$$\sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{bmatrix}$$

Therefore, when the axes of reference are rotated, the components of a given stress transform according to the general transformation law

$$\sigma_{ij} = a_{ik} a_{jl} \sigma_{kl}$$

Since the stress tensor is symmetrical ($\sigma_{ij} = \sigma_{ji}$), it is always possible to find a set of axes, the principal axes, so that a cube with its edges parallel to them has no shear stresses acting upon its faces. Referred to the principal axes, the stress takes the form

$$\begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{pmatrix}$$

where σ_1, σ_2 and σ_3 are called the principal stresses.

Elasticity of crystals

The most general linear dependence of stress on strain has the form

$$\sigma_{ij} = c_{ijkl} \varepsilon_{kl}$$

The constants c_{ijkl} are called stiffness constants. The existence of non-zero values of certain of the c_{ijkl} has rather surprising consequences. For example, if c_{1112} is not zero, the occurrence of a finite shear strain ε_{12} implies the existence of a proportional tensile stress σ_{11}. By symmetry arguments, it can be shown that constants of the type c_{1112} are zero in an isotropic medium, but they are in general not zero in a single crystal. The existence of a single strain component in a crystal may require that there be non-zero values of all the stress components.

Similarly,

$$\varepsilon_{ij} = s_{ijkl} \sigma_{kl}$$

where the constants s_{ijkl} are called compliances.

As these two formulae both consist of nine equations, each containing nine terms on the right-hand side, it might appear that 81 compliances or stiffness constants must be specified. However, the number of independent constants can always be reduced from 81 to 21.

Since $\varepsilon_{12} = \varepsilon_{21}$, the constants c_{ij12} and c_{ij21} always occur together in $\sigma_{ij} = \left(c_{ij12} + c_{ij21}\right)\varepsilon_{12}$. It is therefore permissible to set $c_{ij12} = c_{ij21}$, and, in general, $c_{ijkl} = c_{ijlk}$. Next, suppose that only the strain component ε_{11} exists. We have

$$\sigma_{12} = c_{1211}\varepsilon_{11}$$

and

$$\sigma_{21} = c_{2111}\varepsilon_{11}$$

Because $\sigma_{12} = \sigma_{21}$, $c_{1211} = c_{2111}$ and in general $c_{ijkl} = c_{jikl}$. Similar arguments apply to the s_{ijkl}.

The number of independent constants is now reduced to 36, and so we can use the contracted notation for stress and a contracted notation for strain where

$$\begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{pmatrix} \rightarrow \begin{pmatrix} \varepsilon_1 & \frac{1}{2}\varepsilon_6 & \frac{1}{2}\varepsilon_5 \\ \frac{1}{2}\varepsilon_6 & \varepsilon_2 & \frac{1}{2}\varepsilon_4 \\ \frac{1}{2}\varepsilon_5 & \frac{1}{2}\varepsilon_4 & \varepsilon_3 \end{pmatrix}$$

(note the factors of $\frac{1}{2}$, explained in Kelly and Knowles).

A corresponding contraction is applied to c_{ijkl}, so that, for example, $c_{1233} \rightarrow c_{63}$, $c_{2323} \rightarrow c_{44}$, $c_{2332} \rightarrow c_{44}$, etc. Hence the formulae $\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$ can now be written in the contracted form

$$\sigma_i = c_{ij}\varepsilon_j$$

Factors of 2 and 4 must also be introduced into the definition of s_{ij}, as follows:

$$s_{mn} = 2s_{ijkl} \quad \text{when one only of either } m \text{ or } n \text{ is 4, 5 or 6}$$

$$s_{mn} = 4s_{ijkl} \quad \text{when both } m \text{ and } n \text{ are 4, 5 or 6}$$

For example, $s_{13} = s_{1133}$, $s_{14} = 2s_{1123}$ and $s_{46} = 4s_{2312}$. With these definitions, the formulae $\varepsilon_{ij} = s_{ijkl}\sigma_{kl}$ can be written as

$$\varepsilon_i = s_{ij}\sigma_j$$

The fact that the energy stored in an elastically strained crystal depends on the strain, and not on the path by which the strained state is reached, makes $c_{ij} = c_{ji}$ and $s_{ij} = s_{ji}$, reducing to 21 the maximum number of non-zero c_{ij} and s_{ij} (see for example, Section 6.5 of Kelly and Knowles).

The most general stiffness and compliance constants for crystals of class 1 can now be written in the form of matrices with 21 independent terms; the 6×6 stiffness matrices can be represented in the form

$$
\begin{pmatrix}
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet
\end{pmatrix}
\quad \text{, or, since } c_{ij} = c_{ji} \text{, and } s_{ij} = s_{ji} \text{,}
\quad
\begin{pmatrix}
\bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
 & \bullet & \bullet & \bullet & \bullet & \bullet \\
 & & \bullet & \bullet & \bullet & \bullet \\
 & & & \bullet & \bullet & \bullet \\
 & & & & \bullet & \bullet \\
 & & & & & \bullet
\end{pmatrix}
$$

When arbitrary axes of references are chosen, any crystal has 21 different elastic constants although, because of crystal symmetry, there may be some relations between the constants.

However, if the axes of reference are related to the crystal structure, the requirements of symmetry will ensure that some constants are zero through Neumann's principle. This is discussed for various crystal systems in Section 6.5 of Kelly and Knowles. Here, as an example, we will consider only cubic materials.

Elasticity of cubic crystals

The matrix form for both c_{ij} and s_{ij} for all point groups in the cubic system is:

so that there are only three independent stiffnesses: c_{11}, c_{12} and c_{44}. Likewise, there are only three independent compliances: s_{11}, s_{12} and s_{44}. The three independent compliances are related to the three independent stiffnesses through the formulae

$$
s_{11} = \frac{c_{11} + c_{12}}{(c_{11} - c_{12})(c_{11} + 2c_{12})} \quad , s_{12} = -\frac{c_{12}}{(c_{11} - c_{12})(c_{11} + 2c_{12})} \quad \text{and } s_{44} = \frac{1}{c_{44}} \quad .
$$

In an isotropic medium, the elastic constants must be independent of the choice of coordinate axes. This requirement imposes an extra condition in addition to the conditions of cubic symmetry, which can be shown to be the condition

$$2c_{44} = c_{11} - c_{12}$$

or equivalently,

$$s_{44} = 2(s_{11} - s_{12})$$

The degree of anisotropy of a cubic single crystal can be measured by the departure from unity of the ratio A, where

$$A = \frac{2c_{44}}{c_{11} - c_{12}} = \frac{2(s_{11} - s_{12})}{s_{44}}$$

The ratio A is a measure of the relative resistance of the crystal to two types of shear strain: c_{44} is a measure of the resistance to shear on the (010) plane in the [001] direction, while $\frac{1}{2}(c_{11} - c_{12})$ is the stiffness with respect to shear on (110) in the direction [1 $\bar{1}$ 0]. Only single crystals of W and Al come close to being isotropic.

If we now look at cubic materials in a bit more detail, it is possible to drive the following very useful general results:

The C_{ijkl} transform from axes 1, 2 and 3 to the axes 1′, 2′ and 3′ so that in general

$$C'_{ijkl} = c_{12}\delta_{ij}\delta_{kl} + c_{44}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + (c_{11} - c_{12} - 2c_{44})\, a_{iu}a_{ju}a_{ku}a_{lu}$$

where the dummy suffix u takes the values 1, 2 and 3 and where δ is the Kronecker delta. Likewise, for the same change in axes,

$$S'_{ijkl} = s_{12}\delta_{ij}\delta_{kl} + \frac{s_{44}}{4}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + (s_{11} - s_{12} - \frac{1}{2}s_{44})\, a_{iu}a_{ju}a_{ku}a_{lu}$$

Thus, for example,

$$C'_{3232} = c_{44} + (c_{11} - c_{12} - 2c_{44})(a_{31}^2 a_{21}^2 + a_{32}^2 a_{22}^2 + a_{33}^2 a_{23}^2)$$

$$S'_{3232} = \frac{s_{44}}{4} + (s_{11} - s_{12} - \frac{s_{44}}{2})(a_{31}^2 a_{21}^2 + a_{32}^2 a_{22}^2 + a_{33}^2 a_{23}^2)$$

Shear elastic constants c'_{44} on the (111) plane of cubic crystals

Suppose we were interested in the variation of the elastic constants c'_{44} on the (111) plane. We might choose out '3' axis to be the normal to the (111) plane, leaving us two axes '1' and '2' to define in this plane.

Since the plane of interest is (111), it follows that $a_{31} = a_{32} = a_{33} = 1/\sqrt{3}$. Hence,

$$C'_{3232} = c'_{44} = c_{44} + \frac{1}{3}(c_{11} - c_{12} - 2c_{44})(a_{21}^2 + a_{32}^2 + a_{33}^2) = \frac{1}{3}(c_{11} - c_{12} + c_{44})$$

since $(a_{21}^2 + a_{32}^2 + a_{33}^2) = 1$ irrespective of how we define our '2' and '1' axes. Therefore, we have immediately the result that the c'_{44} shear elastic constant of cubic materials is isotropic in the (111) plane. It also follows that the s'_{44} shear elastic constant of cubic materials is also isotropic in the (111) plane, as is the shear modulus $G = 1/s'_{44}$ on this plane.

Young's modulus as a function of orientation in cubic crystals

A second useful result is the formula for Young's modulus, E, as a function of orientation. From the formula for S'_{ijkl}, we have:

$$S'_{1111} = s'_{11} = s_{12} + \frac{s_{44}}{2} + (s_{11} - s_{12} - \frac{1}{2}s_{44})(a_{11}^4 + a_{12}^4 + a_{13}^4)$$

or, equivalently,

$$s'_{11} = s_{11} - 2(s_{11} - s_{12} - \frac{1}{2}s_{44})(a_{11}^2 a_{12}^2 + a_{12}^2 a_{13}^2 + a_{13}^2 a_{11}^2)$$

so that $E = 1/s'_{11}$.

If '1' is along <111>, we have $a_{11}^2 = a_{12}^2 = a_{13}^2 = 1/3$, so that

$$s'_{11} = s_{11} - \frac{2}{3}(s_{11} - s_{12} - \frac{1}{2}s_{44}) = \frac{1}{3}(s_{11} + 2s_{12} + s_{44})$$

whence

$$E = \frac{3}{(s_{11} + 2s_{12} + s_{44})}$$

Along <100>,

$$E = \frac{1}{s_{11}}$$

Using these formulae, it is easy to show that cubic metals with $A > 1$ are most stiff along <111> directions and least stiff along <001> directions; the reverse is true for cubic metals with $A < 1$.