The tensors useful for geophysics and estimation of anisotropic polycrystalline physical properties

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PART I : The tensors useful for geophysics

A) Tensors of physical properties of crystals

Thermal conductivity and diffusivity (2\textsuperscript{nd} rank tensor) \(\rightarrow\) can be calculated from CPO
Thermal expansion (2\textsuperscript{nd} rank tensor) \(\rightarrow\) can be calculated from CPO

Electrical conductivity, electrical polarization and dielectric properties) \(\rightarrow\) can be calculated from CPO, BUT may not be relevant if conductivity controlled by high conductivity phases in the grain boundaries (e.g. water or carbon)

Piezoelectricity (3\textsuperscript{rd} rank tensor) \(\rightarrow\) can be calculated from CPO
Elasticity (4\textsuperscript{th} rank tensor) \(\rightarrow\) seismic properties, can be calculated from CPO (crystal preferred orientation)

B) Field tensors

Stress tensor (2\textsuperscript{nd} rank tensor)

Strain tensor (2\textsuperscript{nd} rank tensor)
C) Cartesian Reference Frames

Measurement of anisotropic physical properties are reported in the literature as components of tensors, typically as tabulated values. The reference frame most commonly used is a right-handed Cartesian (also called orthonormal) system, although theoretically any type of reference frame could be used (e.g. cylindrical…). The orientation of the Cartesian reference has to be defined for the tensors components to have any meaning. In the case of crystal properties the orientation of the Cartesian reference has to be defined with respect to the crystal axes. For cubic, tetragonal and orthorhombic the obvious choice is to use the orthogonal lattice basis vectors $a[100]$, $b[010]$ and $c[001]$ crystal axes. However, for most general case of triclinic crystal symmetry where $a$, $b$, and $c$ are not orthogonal, there are many possible choices and no general convention. The choice of a specific reference frame is often guided by presence of cleavage or well developed crystal faces that allow for an easy determination of the crystal orientation.

Here I will mention 3 common choices, for the tensor Cartesian reference frame $(e_1,e_2,e_3)$:

a) $e_3 = c[001]$, $e_2 = b^* \perp (010)$ and hence for a right-handed system $e_1 = e_2 \times e_3$

b) $e_3 = c[001]$, $e_1 = a^* \perp (100)$ and $e_2 = e_3 \times e_1$

c) $e_3 = c^* \perp (001)$, $e_1 = a[100]$ and $e_2 = e_3 \times e_1$

Reference Frames a), b) and c) for triclinic plagioclase Labradorite An66 ($a=0.81747$ nm $b=1.28708$ nm $c=1.42030$ nm $\alpha=93.461^\circ$ $\beta=116.086^\circ$ $\gamma=90.514^\circ$)

Many crystallographic calculations are more easily performed in a Cartesian reference frame and you will find discussions on basis transformations in most texts on crystallography. You should also be aware that the tensor Cartesian reference frame may not be the same as the reference frame with respect to the crystal axes used for the Euler angles used to define your orientation data. For example the commonly used BearTex Texture package uses (a) and the EBSD software from HKLtechnologies uses (b). In general a transformation matrix will be needed to bring the tensor into the correct orientation for a specific Euler angle frame.
D) Tensors of crystal physical properties – represented by matrices

<table>
<thead>
<tr>
<th>Physical Property (rank)</th>
<th>Driving Force (rank)</th>
<th>Response (rank)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (0)</td>
<td>Mass (0)</td>
<td>Volume (0)</td>
</tr>
<tr>
<td>Pyroelectricity (1)</td>
<td>Temperature (0)</td>
<td>Electric Field (1)</td>
</tr>
<tr>
<td>Electric conductivity (2)</td>
<td>Electric Field (1)</td>
<td>Electric Current Density (1)</td>
</tr>
<tr>
<td>Electric Permittivity (2)</td>
<td>Electric Field (1)</td>
<td>Dielectric Displacement (1)</td>
</tr>
<tr>
<td>Dielectric Susceptibility (2)</td>
<td>Electric Field (1)</td>
<td>Polarization (1)</td>
</tr>
<tr>
<td>Chemical Diffusivity (2)</td>
<td>Potential Gradient –ve (1)</td>
<td>Chemical Flux (1)</td>
</tr>
<tr>
<td>Thermal Conductivity (2)</td>
<td>Temperature Gradient -ve (1)</td>
<td>Heat Flux (1)</td>
</tr>
<tr>
<td>Thermal Expansion (2)</td>
<td>Temperature (0)</td>
<td>Strain (2)</td>
</tr>
<tr>
<td>Magnetic Susceptibility (2)</td>
<td>Magnetic Field (1)</td>
<td>Magnetisation Intensity (1)</td>
</tr>
<tr>
<td>Magnetic Permeability (2)</td>
<td>Magnetic Field (1)</td>
<td>Magnetic Induction (1)</td>
</tr>
<tr>
<td>Piezoelectricity (3)</td>
<td>Electric Field (1)</td>
<td>Strain (2)</td>
</tr>
<tr>
<td>Elastic Compliance (4)</td>
<td>Stress (2)</td>
<td>Strain (2)</td>
</tr>
<tr>
<td>Elastic Stiffness (4)</td>
<td>Strain (2)</td>
<td>Stress (2)</td>
</tr>
</tbody>
</table>

For example, the elastic, thermal, electric and magnetic effects on strain \( \varepsilon_{ij} \), to first order can be written as a function of the independent variables (stress \( \sigma_{kl} \), electric field \( E_k \), magnetic field \( H_l \) and temperature \( \Delta T \)) and their corresponding tensors as

\[
\varepsilon_{ij} = S_{ijkl} \sigma_{kl} + d_{kij} E_k + q_{lij} H_l + \alpha_{ij} \Delta T
\]

where \( S_{ijkl} \) are the elastic compliance, \( d_{kij} \) piezo-electric, \( q_{lij} \) piezo-magnetic and \( \alpha_{ij} \) thermal expansion tensors.
Zero Rank Tensor (1 component)
Scalars – example density (kg/m³)

1st Rank Tensor (3 components)
Vectors – example electric field  \( E = [E_1, E_2, E_3] = E_i \)

2nd Rank Tensor (9 components)
Relates 2 vectors – example thermal conductivity: applied vector temperature gradient and resulting vector heat flow density.

\[
T_{ij} = \begin{bmatrix}
T_{11} & T_{12} & T_{13} \\
T_{21} & T_{22} & T_{23} \\
T_{31} & T_{32} & T_{33}
\end{bmatrix}
\]

The generic 2nd rank tensor \( T \) is the relation between an applied vector \( p \) and resultant vector \( q \). We can write relation between \( p \) and \( q \) as a tensor equation

\( q = T \cdot p \) or \( p_i = T_{ij} q_j \)

In general the vectors \( p \) and \( q \) are not parallel.

The representation quadric for 2nd Rank Tensors

Illustrating the properties of the representation ellipsoid for conductivity:
\( \sigma_{ij} x_i x_j = 1 \).
Geometrical representation of symmetrical second-rank tensors as a second-degree surface (called a quadric) with its origin at the surface. The quadric may be an ellipsoid or a hyperloid. Most common second-rank tensors are symmetric (Tij = Tji) and when the 3 principal coefficients are all positive then the property is represented by an ellipsoid with axes 1/√T1, 1/√T2 and 1/√T3, which is the case for electric polarization, electrical and thermal conductivity and optical properties. If one of the principal coefficients is negative then surface is a hyperboloid of one sheet (e.g. thermal expansion of plagioclase feldspar). If two of the principal coefficients are negative then surface is a hyperboloid of two sheets or caps, this the case for the thermal expansion of calcite with contraction the basal plane. If all three of the principal coefficients are negative then surface is an imaginary ellipsoid (see below), this is the case for many susceptibilities of paramagnetic and diamagnetic minerals, such as quartz, calcite and aragonite.

The representation quadrics for a tensor, (a) an ellipsoid when all the principle axes of the tensor are positive, (b) a hyperboloid of one sheet when one the principle axes is negative and (c) a hyperboloid of two sheets when two of the principle axes are negative.

**FIGURE 11-16**
(A) Values of the thermal coefficient of expansion α, as measured along the c and a axis, at different temperatures for calcite.
(B) Change with temperature of the volume occupied by 1 kg of quartz. Note sharp inflection at the inversion temperature of 573°C. (After Austin, 1952.)
Fig 11.12 Thermal expansion of calcite, which has $\alpha_z = -3 \times 10^{-5} \, (^{\circ}{C})^{-1}$ and $\alpha_x = 23.6 \times 10^{-5} \, (^{\circ}{C})^{-1}$. (a) shows the deformation of a sphere drawn in a calcite crystal. The diagram is exaggerated about 100 times for a 100°C temperature increase. (b) is a plot of $a_z$ with the positive and negative loops of the figure marked. (c) is the representation quasicr: the hyperboloid $a_x^2 + a_y^2 + a_z^2 = 1$ (labelled +) cuts the Z axis (the triad) and the hyperboloid $a_x^2 - a_y^2 + a_z^2 = 1$ (labelled -) cuts the Y axis. In (b) and (c) the directions of zero expansion are shown as dash-dot lines. All three diagrams are sections in the Z-Y plane; the figures shown are cylindrically symmetrical about the Z axis.

Single crystal and calculated polycrystal (GRAN133)
Radius-normal property and melting wax experiment

As an example of the visualization of a quadric and a confirmation that a quadric is a real physical representation of symmetrical 2nd rank tensor we will describe the melting wax experiment. This experiment is given in Putnis (1992 p25), except we will use the example of quartz. Consider a red hot arrow touching the second order prism plane of a single crystal of quartz and creating a point heat source. A (negative) thermal gradient will result in heat flow away from the hot heat source (arrow tip) to the colder regions of the crystal. As the thermal resistivity (reciprocal of thermal conductivity) varies with direction the heat flow will not be equal in all radial directions, i.e. heat flow is anisotropic.

The melting wax (gray) experiment

When the temperature of wax on the surface of the crystal reaches it’s melting temperature, the melting front marks an isotherm corresponding to this temperature. On the (10-10) plane an elliptical isotherm forms with its long axis parallel to the c[0001] axis and the short axis in the (0001) plane reflecting perfectly the principal values of $1/\sqrt{r_{33}}$ and $1/\sqrt{r_{11}}$ of the resistivity tensor or equivalently the $\sqrt{k_{33}}$ and $\sqrt{k_{11}}$ of the symmetrical thermal conductivity tensor. On the basal (0001) plane the isotherm is circular because $r_{11} = r_{22}$.

In general the applied (or stimulus) vector (e.g. heat flux vector ($q$)) is NOT parallel the response vector (e.g. thermal gradient vector ($\Delta T$)), a situation that is common for 2nd order tensor properties of anisotropic crystals. The angle between the stimulus and can be used in to calculate the 2nd rank tensor property from a vector sum (see above). For certain directions, even in anisotropic crystals, the stimulus and response vectors are parallel (e.g. the principal axes for the example above) and the 2nd rank tensor property for that direction is simply the ratio of the two vectors as $\cos \theta = 1$. For isotropic crystals, for example all cubic symmetry crystals for 2nd rank tensors, the stimulus and response vectors are always parallel as the representative quadric is a sphere. N.B.
cubic crystals are NOT necessarily isotropic of tensors of higher rank, for example 4th rank tensors such as elasticity.

**Transformation of axes**

<table>
<thead>
<tr>
<th>“old” axes</th>
<th>x1</th>
<th>x2</th>
<th>x3</th>
</tr>
</thead>
<tbody>
<tr>
<td>x’1</td>
<td>a11</td>
<td>a12</td>
<td>a13</td>
</tr>
<tr>
<td>“new” x’2</td>
<td>a21</td>
<td>a22</td>
<td>a23</td>
</tr>
<tr>
<td>x’3</td>
<td>a31</td>
<td>a32</td>
<td>a33</td>
</tr>
</tbody>
</table>

Note in general the matrix is NOT symmetric $a_{ij} \neq a_{ji}$

**Transformation of components of a vector**

A vector $\mathbf{P}$ with components $(p_1, p_2, p_3)$ with respect to reference axes $x_1, x_2, x_3$ is transformed to $\mathbf{P’} = (p’1, p’2, p’3)$ with respect to reference axes $x’1, x’2, x’3$ using the cosines of the angles between the reference frames.

$p’1 = p1\cos(x1^x’1) + p2\cos(x2^x’1) + p3\cos(x3^x’1)$ etc.

or

$p’1 = p1*a_{11} + p2*a_{12} + p3*a_{13}$

$p’2 = p1*a_{21} + p2*a_{22} + p3*a_{23}$

$p’3 = p1*a_{31} + p2*a_{32} + p3*a_{33}$
or in dummy suffix notation
\[ p'i = p'j*aij \]

And the reverse transformation can be written as
\[ p1 = p'1*a11 + p'2*a21 + p'3*a31 \]
\[ p2 = p'1*a12 + p'2*a22 + p'3*a32 \]
\[ p3 = p'1*a13 + p'2*a23 + p'3*a33 \]
or in dummy suffix notation
\[ pi = p'j*aji \]

<table>
<thead>
<tr>
<th>Transformation laws for tensors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rank of</td>
</tr>
<tr>
<td>---------</td>
</tr>
<tr>
<td>0</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
</tbody>
</table>

Difference between a transformation matrix \((a_{ij})\) and a Tensor \((T_{ij})\)

\(a_{ij}\) is an 3 by 3 array relating two axes. \(T_{ij}\) is a physical quantity that for a given set of reference axes is represented by 9 numbers.
The effect of symmetry on symmetric 2\textsuperscript{nd} rank tensors

<table>
<thead>
<tr>
<th>Cubic</th>
<th>Tetragonal, Hexagonal, Trigonal</th>
<th>Orthorhombic</th>
<th>Monoclinic</th>
<th>Triclinic</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Sphere)</td>
<td>(Uniaxial Ellipsoid)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Effect of symmetry on Physical Properties – Neumann’s Principle

F.E. Neumann’s principle (1885) states that “symmetry elements of any physical property of a crystal must include ALL the symmetry elements of the point group of the crystal”. This implies that that a given physical property may possess a higher symmetry than that possessed by the crystal and it cannot be of a lower symmetry than that of the crystal. The physical property must have the symmetry AT LEAST as high as the one of 32 conventional point group symmetry or one of 90 magnetic points groups to which the crystal belongs. Some physical properties are inherently centrosymmetric (all symmetric second order tensors and elasticity) which will add a center of symmetry in many cases (e.g. quartz) and result in a higher symmetry than the possessed by the crystal.

Table 4.2 Number of independent components of physical properties represented by second rank (order) tensors

<table>
<thead>
<tr>
<th>Crystal system</th>
<th>Orientation of principal axes with respect to the crystal axes</th>
<th>Form of tensor</th>
<th>Number of independent components</th>
</tr>
</thead>
</table>
| Cubic          | Any. Representation quadric is a sphere                      | \[
\begin{bmatrix}
S & 0 & 0 \\
0 & S & 0 \\
0 & 0 & S \\
\end{bmatrix}
\] | 1                |
| Tetragonal     | \(x_3\) parallel to 4, 6, 3 or 3                             | \[
\begin{bmatrix}
S_1 & 0 & 0 \\
0 & S_1 & 0 \\
0 & 0 & S_3 \\
\end{bmatrix}
\] | 2                |
| Hexagonal      | \(x_1, x_2, x_3\) parallel to the diads along \(x, y, z\)-axes | \[
\begin{bmatrix}
S_1 & 0 & 0 \\
0 & S_2 & 0 \\
0 & 0 & S_3 \\
\end{bmatrix}
\] | 3                |
| Orthorhombic   | \(x_2\) parallel to the diad along \(y\)-axis               | \[
\begin{bmatrix}
S_{11} & 0 & S_{13} \\
0 & S_{22} & 0 \\
S_{13} & 0 & S_{33} \\
\end{bmatrix}
\] | 4                |
| Monoclinic     | 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 hexagonal cell is used.*
The magnitude of a 2\textsuperscript{nd} rank property in a given direction

Let a given direction (x) be specified by the direction cosines (A1,A2,A3).

\(a)\) Referred to principal axes (T1,T2,T3) of the tensor

\[ T(x) = A_1^2T_1 + A_2^2T_2 + A_3^2T_3 \]

For uniaxial symmetries

\[ T(x) = T_1\sin^2\theta + T_3\cos^2\theta \]

where \(\theta\) is the angle between direction x and x3 axis (= c-axis of the crystal)

\(b)\) Referred to general axes

\[ T(x) = T_{ij}A_iA_j \]

The representation quadric radius vector

From the magnitude \(T(x)\) in a given direction one can calculate the radius vector \(r(x)\) of the representation quadric. When \(T(x)\) is negative, which occurs for example for thermal expansion in calcite, radius vector \(1/\sqrt{T(x)}\), being an imaginary value.

\[ R(x) = 1/\sqrt{T(x)} \]

Although the quadric representation is complex when one or more principal axes are negative, the representation is quite straight forward as a contoured stereogram.
Piezoelectricity – third rank tensor

Piezoelectricity is the ability of certain crystals to generate a voltage in response to applied mechanical stress. The word is derived from the Greek piezein, which means to squeeze or press. The effect is reversible; piezoelectric crystals, subject to an externally applied voltage, can change shape by a small amount. The effect is of the order of nanometres, but nevertheless finds useful applications such as the production and detection of sound, generation of high voltages, electronic frequency generation, ultrasonic transducers, and ultrafine focusing of optical assemblies. Note that Fukada and Yasuda (1957) first demonstrated that dry bone is piezoelectric, mind the step! (Fukada, E. and Yasuda, I. On the piezoelectric effect of bone, J. Phys. Soc. Japan, 12, 1158-1162, 1957)

Jacques and Pierre Curie first observed piezoelectricity in 1880. Piezoelectricity is a polarization of the crystalline medium due to the displacement of ions (e.g. O\(^2^-\) and Si\(^4+\) in quartz) from equilibrium positions, by the action of an external stress field (or electric field). Piezoelectricity only occurs in crystal that do not possess a center of symmetry (inversion center). The direct piezoelectric effect is the development of an electric dipole moment vector (per unit volume) \(P\) in a crystal when a mechanical stress \(\sigma\) (symmetric tensor of 2\(^{nd}\) rank) is applied to the crystal. Quartz and Tourmaline are the earliest known examples of piezoelectric minerals, today there over one hundred reported examples, these include Rochelle salt (potassium sodium tartrate), lead titanate zirconate ceramics (e.g. PZT-4, PZT-5A, etc.), quartz-homeotypic crystals such as Gallium phosphate (GaPO\(_4\)), AlPO\(_4\) (berlinite) and FePO\(_4\), barium titanate, and polyvinylidene flouride (a polymer film). The magnitude of the electric moment is linearly proportional to the stress, so we can write

\[
P = d \sigma \quad \text{or} \quad P_i = d_{ijk} \sigma_{jk} \quad (i,j,k \text{ 1 to 3})
\]

Where \(d_{ijk}\) are the piezoelectric constants or moduli. The converse effect also occurs when an electric field \(E\) (vector 1\(^{st}\) rank) is applied the crystal changes shape producing a strain \(\varepsilon\) (symmetric tensor of 2\(^{nd}\) rank).

\[
\varepsilon = d E \quad \text{and} \quad \varepsilon_{ij} = d_{ijk} E_k
\]

A general 3\(^{rd}\) rank tensor would require 27 components, taking into account of the symmetric nature of the stress and strain tensors (e.g. \(\sigma_{jk} = \sigma_{kj}\)) it can be shown that \(d_{ijk} = d_{ikj}\) so that only 18 out of the 27 components of the tensor \(d\) are independent.
Using the Voigt’s notation the piezoelectric tensor can represented by 3 x 6 matrix with two-subscripts $d_{mn}$ (m=1 to 3 n=1 to 6), the data in the literature are presented in this form.

$$P_m = d_{mn} \sigma_n \quad (m=1 \text{ to } 3 \quad n=1 \text{ to } 6)$$

and

$$\varepsilon_n = d_{mn} E_m$$

Where correspondence between Voigt’s 2 index notation $d_{mn}$ and the tensor 3 index notation $d_{ijk}$ is

$$d_{i11} = d_{11}, \quad d_{i22} = d_{22}, \quad d_{i33} = d_{33}, \quad d_{i44} = 2d_{123}, \quad d_{i55} = 2d_{135}, \quad d_{i66} = 2d_{112}$$

Which we can write more compactly as

$$d_{ijk} = d_{mn} \quad \text{for } n=1,2,3 \text{ and } m=1,2,3$$

$$2d_{ijk} = d_{mn} \quad \text{for } n=4,5,6 \text{ and } m=1,2,3$$

It is the converse effect that has it is application to quartz in the electronics industry by applying an oscillating electric field the crystal vibrates at fixed frequency. The direct effect is used gas and cigarette lighters where a mechanical force is applied to a crystal to generate a high potential difference and produces a spark.

Alpha-quartz belongs to the crystal class 32 (or $D_3$) is the best know example of a piezoelectric mineral.

The piezoelectric tensor for quartz is

<table>
<thead>
<tr>
<th>Crystal</th>
<th>$P_{mn}$ Piezoelectric Tensor</th>
<th>Components of vector $P$ along a,m,c</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frame</td>
<td>$d_{1m}$ $d_{2m}$ $d_{3m}$ $d_{4m}$ $d_{5m}$ $d_{6m}$</td>
<td>Components of vector $P$ along a,m,c</td>
</tr>
<tr>
<td>a-axis</td>
<td>$d_{11}$ $-d_{11}$ $0$ $d_{14}$ $0$ $0$</td>
<td>$P_1=d_{11}\sigma_1 - d_{11}\sigma_2 + d_{14}\sigma_4$</td>
</tr>
<tr>
<td>m-axis</td>
<td>$0$ $0$ $0$ $0$ $-d_{14}$ $-2d_{11}$</td>
<td>$P_2=-d_{14}\sigma_1 - 2d_{11}\sigma_6$</td>
</tr>
<tr>
<td>c-axis</td>
<td>$0$ $0$ $0$ $0$ $0$ $0$</td>
<td>$P_3=0$</td>
</tr>
</tbody>
</table>

It is obvious that not component of stress along the c-axis can cause a piezoelectric polarization as $P_3=0$. Similarly one cannot induce a piezoelectric polarization by the application of a tensile (or compressive) stress along the c-axis as $\sigma_1$ is not present in the components of $P_1$ and $P_2$. The piezoelectric polarization can only be activated in basal plane (0001) containing the a- and m-axes. Only the tensile (or compressive) stresses along the a-axis ($\sigma_1$ ) and m-axes ($\sigma_2$ ) plus the shear stresses in the basal plane in the direction of the m-axis ($\sigma_4$,$\sigma_23$) and in the m(01-10) plane in the direction of the a-axis ($\sigma_6$,$\sigma_{12}$).
The actual d tensor for quartz (values are $10^{-12}$ coulombs/Newton or m/V)

\[
d_{11} = 2.3 \times 10^{-12} \text{ m/V} \quad d_{14} = -0.67 \times 10^{-12} \text{ m/V}
\]

(and for converse effect $e_{11} = 0.173 \text{ c/m}^2$ $e_{14} = 0.040 \text{ c/m}^2$)

$$d = \begin{bmatrix}
-2.3 & 2.3 & 0 & -0.67 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.67 & 4.6 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$ for right-handed quartz (Cady 1946)

By convection for a right-handed crystal the +a-axis (diad axis) develops a positive electrical change on the application of mechanical compression. A left-handed crystal develops a negative charge along the +a-axis under compression. Hence $d_{11}$ is negative for a right-handed crystal and positive for left-handed crystal, $d_{14}$ also changes sign. In beta-quartz (hexagonal symmetry class 622) $d_{11}$ vanishes leaving $d_{14}$ as the only piezoelectric constant with a very much weaker overall piezoelectric effect.
Symmetry Properties of the Piezoelectric Tensor

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Number of Constants</th>
<th>Matrix Form</th>
</tr>
</thead>
</table>
| Triclinic (18 constants) | 1 | \[
\begin{pmatrix}
    d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\
    d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\
    d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36}
\end{pmatrix}
\] |
| Monoclinic (8 constants) | 2 | \[
\begin{pmatrix}
    0 & 0 & 0 & 0 & d_{14} & 0 & d_{16} \\
    d_{21} & d_{22} & d_{23} & d_{24} & 0 & d_{26} \\
    0 & 0 & 0 & 0 & d_{44} & 0 & d_{46}
\end{pmatrix}
\] |
| Monoclinic (10 constants) | m | \[
\begin{pmatrix}
    d_{11} & d_{12} & d_{13} & 0 & 0 & d_{55} & 0 \\
    0 & 0 & 0 & d_{34} & 0 & 0 & d_{56} \\
    d_{31} & d_{32} & d_{33} & 0 & 0 & 0 & 0
\end{pmatrix}
\] |
| Orthorhombic (3 constants) | 222 | \[
\begin{pmatrix}
    0 & 0 & 0 & 0 & 0 & d_{44} & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\] |
| Orthorhombic (5 constants) | mm2 | \[
\begin{pmatrix}
    0 & 0 & 0 & 0 & 0 & d_{55} & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    d_{31} & d_{32} & d_{33} & 0 & 0 & 0 & 0
\end{pmatrix}
\] |
| Trigonal (6 constants) | 3 | \[
\begin{pmatrix}
    d_{11} & -d_{11} & 0 & d_{14} & d_{15} & -2d_{22} \\
    -d_{22} & d_{22} & 0 & d_{15} & -d_{14} & -2d_{33} \\
    d_{31} & d_{32} & d_{33} & 0 & 0 & 0
\end{pmatrix}
\] |
| Trigonal (2 constants) | 32 | \[
\begin{pmatrix}
    d_{11} & -d_{11} & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\] |
| Trigonal (4 constants) | 3m | \[
\begin{pmatrix}
    0 & 0 & 0 & 0 & d_{55} & -2d_{22} \\
    -d_{22} & d_{22} & 0 & 0 & 0 & 0 \\
    d_{31} & d_{31} & d_{33} & 0 & 0 & 0
\end{pmatrix}
\] |
| Hexagonal & Tetragonal (4) | 6, 4 | \[
\begin{pmatrix}
    0 & 0 & 0 & d_{14} & d_{15} & 0 \\
    0 & 0 & 0 & d_{14} & -d_{14} & 0 \\
    d_{31} & d_{31} & d_{33} & 0 & 0 & 0
\end{pmatrix}
\] |
| Hexagonal & Tetragonal (1) | 622, 422 | \[
\begin{pmatrix}
    0 & 0 & 0 & 0 & d_{44} & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\] |
| Hexagonal & Tetragonal (3) | 6mm, 4mm | \[
\begin{pmatrix}
    0 & 0 & 0 & 0 & d_{15} & 0 \\
    0 & 0 & 0 & 0 & d_{15} & 0 \\
    d_{31} & d_{31} & d_{33} & 0 & 0 & 0
\end{pmatrix}
\] |
| Hexagonal (2 constants) | 6 | \[
\begin{pmatrix}
    d_{11} & -d_{11} & 0 & 0 & 0 & 0 \\
    -d_{22} & d_{22} & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\] |
| Hexagonal (1 constant) | 6m2 | \[
\begin{pmatrix}
    0 & 0 & 0 & 0 & -2d_{22} \\
    -d_{22} & d_{22} & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0
\end{pmatrix}
\] |
| Tetragonal (4 constants) | 4 | \[
\begin{pmatrix}
    0 & 0 & 0 & d_{14} & d_{15} & 0 \\
    0 & 0 & 0 & -d_{15} & d_{14} & 0 \\
    d_{31} & -d_{31} & 0 & 0 & 0 & d_{36}
\end{pmatrix}
\] |
| Tetragonal (2 constants) | 42m | \[
\begin{pmatrix}
    0 & 0 & 0 & 0 & d_{14} & 0 \\
    0 & 0 & 0 & d_{14} & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & d_{16}
\end{pmatrix}
\] |
| Cubic (1 constant) | 23, 43m | \[
\begin{pmatrix}
    0 & 0 & 0 & d_{14} & 0 & 0 \\
    0 & 0 & 0 & 0 & d_{14} & 0 \\
    0 & 0 & 0 & 0 & 0 & d_{16}
\end{pmatrix}
\] |
Elasticity – fourth rank tensor

In any crystalline material there is balance between Coulomb attractive forces between oppositely charge ions and Born repulsive forces due to the overlap of electron shells. At any given thermodynamic state the crystal will tend toward an equilibrium structure. For example changing the temperature will result in thermal expansion or contraction depending on sign of the temperature change. A similar situation will result for a change in hydrostatic pressure, the crystal structure will adjust at the atomic level to the new thermodynamic state, this is also true for general change in the state of stress (non-hydrostatic).

The elastic constants relate applied external forces, described by the stress tensor, to the resulting deformation, described by the strain tensor. In the present case a crystal is considered as a homogeneous, anisotropic medium and that both stress and strain are homogeneous. The elastic tensor can also be defined in terms of the change upon elastic deformation of an appropriate thermodynamic potential. This definition, which will also lead to the expression for the elastic constants, places elasticity within the same framework of other thermodynamic properties of the crystal, such as the equation of state and the entropy. These may all be expressed in terms of the derivatives of the potential with respect to its natural variables. For example, the stress produced by a deformation under isothermal conditions is

\[ \sigma_{ij} = \rho \frac{dA}{d\varepsilon_{ij}} \]

while the stress produced at constant entropy (isentropic) conditions is

\[ \sigma_{ij} = \rho \frac{dE}{d\varepsilon_{ij}} \]

where \( \rho \) is crystal density, \( \varepsilon_{ij} \) is Lagrangian crystal strain tensor, \( A \) is Helmholtz free energy, \( E \) is the internal energy and the subscripts on the derivatives indicate that temperature (T) or entropy (S) is held constant.
The elastic constants are defined in terms of the Hooke's law relation between stress and strain. The isothermal and adiabatic elastic constants are given by:

\[ c^{T}_{ijkl} = \left( \frac{d\sigma_{ij}}{d\varepsilon_{kl}} \right)_T \]
\[ c^{S}_{ijkl} = \left( \frac{d\sigma_{ij}}{d\varepsilon_{kl}} \right)_S \]

respectively. The adiabatic elastic constants \( c^{S}_{ijkl} \) are most relevant to seismology, where the timescale of deformation is much shorter than that of thermal diffusion over relevant length scales. Isothermal elastic constants are relevant, for example, in static compression experiments. In the limit of zero temperature and in the absence of zero point motion, the conditions corresponding to most first-principles theoretical calculations, the adiabatic and isothermal elastic constants are identical to each other and are referred to as athermal elastic constants. It is worth pointing out that other definitions of the elastic constants are possible. In order to distinguish them, the \( c_{ijkl} \) may be referred to as the stress-strain coefficients. We may alternatively define the elastic constants as the second derivatives of the crystal energy with respect to the strain components.

\[ c^{T}_{ijkl} = \rho \left( \frac{d^2A}{d\varepsilon_{ij} d\varepsilon_{kl}} \right)_T \]

which is identical to \( c_{ijkl} \) only in the absence of hydrostatic prestress.

There are 81 independent elastic constants, in general; however, this number is reduced to 21 by the requirement of the Voigt symmetry that \( c_{ijkl} \) are symmetric with respect to the interchanges \((i, j), (k, l)\), and \((ij, kl)\). This allows replacement of a pair of Cartesian indices \( ij \) by single index \(\alpha\), according to the scheme:

\[
\begin{align*}
\text{ij} & \quad \alpha \\
11 & \quad 1 \\
22 & \quad 2 \\
33 & \quad 3 \\
32 \text{ or } 23 & \quad 4 \\
31 \text{ or } 13 & \quad 5 \\
21 \text{ or } 12 & \quad 6
\end{align*}
\]

In Voigt notation the elastic constants thus form a symmetric matrix:

\[
\begin{pmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\
c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\
& c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\
& & c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\
& & & c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\
& & & & c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66}
\end{pmatrix}
\]

The diagonal constants \( c_{ii} \) with \( i <= 3 \) may be referred to as the longitudinal (compressive) elastic constants; \( c_{ii} \) with \( i >= 4 \) may be called the shear elastic constants. Those \( c_{ij} \) with \( i \) not equal to \( j < 3 \) are referred to as the off-diagonal constants, and finally, \( c_{ij} \) with \( i =< 3 \) and \( j > 3 \), which measure the shear strain produced by a longitudinal stress, may be called the mixed elastic constants.

The presence of crystallographic symmetry further reduces the number of independent elastic constants. The highest possible symmetry is that of an isotropic material such as a glass or a randomly oriented polycrystalline aggregate, which is fully characterized by two elastic
constants. These can be defined as the bulk and shear modulus, \( K \) and \( G \), respectively, or in terms of alternative moduli such as the Young's modulus or Lamé parameter, or ratios of moduli, such as the Poisson's ratio. Relationships among these measures are given in a number of sources. A cubic crystal is characterized by three constants, \( c_{11}, c_{12}, \) and \( c_{44} \). Crystals with lower symmetry will possess a larger number of independent constants, for example, nine for orthorhombic crystals \( (c_{11}, c_{22}, c_{33}, c_{12}, c_{13}, c_{23}, c_{44}, c_{55}, \) and \( c_{66} ) \) and 21 for triclinic crystals (the largest number possible).

**Hooke's Law**

\[
\begin{align*}
\sigma & = c \varepsilon \\
\varepsilon & = s \sigma
\end{align*}
\]

where  
\( c = \) stiffness coefficients (dimensions of stress)  
\( s = \) compliance coefficients (dimensions of 1/stress)  
\( \sigma = \) stress tensor (second order tensor)  
\( \varepsilon = \) deformation tensor (second order tensor)

\[
\sigma_{ij} = c_{ijkl} \varepsilon_{kl}
\]

or

\[
\varepsilon_{ij} = s_{ijkl} \sigma_{kl}
\]

\( i,j,k,l \) can have the values \( 1,2 \) or \( 3 \)

so \( 3 \times 3 \times 3 \times 3 = 3^4 = 81 \) coefficients.

But due to the symmetry of the deformation and stress tensors the 81 coefficients are not independent.

\[
\sigma_{ij} = \begin{bmatrix}
\sigma_{11} & \sigma_{12} & \sigma_{13} \\
\sigma_{12} & \sigma_{22} & \sigma_{23} \\
\sigma_{13} & \sigma_{23} & \sigma_{33}
\end{bmatrix}
\]

The diagonal components of the stress tensor \( (i=j ; \sigma_{11},\sigma_{22} & \sigma_{33}) \) are the components normal stress. The off-diagonal components \( (i\neq j ; \sigma_{12},\sigma_{13} \text{ etc.}) \) are shear stresses (denoted \( \tau \) by some authors) and they are symmetric (\( \sigma_{ij}=\sigma_{ji} \)).

\[
\varepsilon_{ij} = \begin{bmatrix}
\varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\
\varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\
\varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33}
\end{bmatrix}
\]

The diagonal components of the of the deformation tensor \( (i=j ; \varepsilon_{11},\varepsilon_{22} \text{ et } \varepsilon_{33}) \) are axial extensions or contractions. The off-diagonal components \( (i\neq j ; \varepsilon_{12},\varepsilon_{13} \text{ etc.}) \) shear deformations are (\( \varepsilon_{ij}=\varepsilon_{ji} \)).

Therefore the number of independent coefficients \( c_{ijkl} \text{ et } s_{ijkl} \) is reduced to 36.

\( c_{ijkl} = c_{jikl} = c_{ijlk} = c_{jilk} \)
The Matrix notation

Matrices                                     Tensors
p,q = 1to 6                                 i,j,k,l = 1to 3
\( \sigma_{pq} = c_{pq} \varepsilon_{q} \)         \( \sigma_{ij} = c_{ijkl} \varepsilon_{kl} \)
\( \varepsilon_{p} = S_{pq} \sigma_{q} \)         \( \varepsilon_{ij} = S_{ijkl} \sigma_{kl} \)

Matrix   \((p,q)\)           1       2       3       4       5       6
Tensor   \((ij\ or\ kl)\)     11      22      33      23 or 32   31 or 13   12 or 21

\[
\sigma_{ij} = \begin{bmatrix}
\sigma_{11} & \sigma_{12} & \sigma_{13} \\
\sigma_{12} & \sigma_{22} & \sigma_{23} \\
\sigma_{13} & \sigma_{23} & \sigma_{33}
\end{bmatrix}
\quad \rightarrow \quad \sigma_{i} = \begin{bmatrix}
\sigma_{1} & \sigma_{6} & \sigma_{5} \\
\sigma_{6} & \sigma_{2} & \sigma_{4} \\
\sigma_{5} & \sigma_{4} & \sigma_{3}
\end{bmatrix}
\]

\[
\varepsilon_{ij} = \begin{bmatrix}
\varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\
\varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\
\varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33}
\end{bmatrix}
\quad \rightarrow \quad \varepsilon_{i} = \begin{bmatrix}
\varepsilon_{1} & \varepsilon_{2} & \varepsilon_{3} \\
\varepsilon_{2} & \varepsilon_{2} & \varepsilon_{2} \\
\varepsilon_{3} & \varepsilon_{3} & \varepsilon_{3}
\end{bmatrix}
\]

In addition we need to introduce factors of 2 and 4 into the equations relating compliance in
tensor and matrix notations

\( S_{ijkl} = S_{pq} \) for \( p=1,2,3 \) and \( q = 1,2,3 \)
\( 2S_{ijkl} = S_{pq} \) for either \( p= \) or \( q = 4,5,6 \)
\( 4S_{ijkl} = S_{pq} \) for either \( p= \) and \( q = 4,5,6 \)
However
\( C_{ijkl} = C_{pq} \) for all \( i,j,k,l \) and all \( p \) and \( q \) (for \( i,j,k,l = 1,2,3 \) and \( p,q = 1 \) to \( 6 \))

Transformation law
\( p = \delta_{ij,i} + (1 - \delta_{ij})(9-i-j) \)
\( q = \delta_{kl,k} + (1 - \delta_{kl})(9-k-l) \)

with the Kronecker delta , \( \delta_{ij} = 0 \) when \( i \neq j \) and \( \delta_{ij} = 1 \) when \( i=j \)
Compressibility

The change of an elastic crystal’s dimensions when subjected to hydrostatic pressure can be defined in any given direction by the linear compressibility $\beta(x)$ ($\beta$). The change in length ($dl/l_0$) (i.e. elastic strain) along a given direction ($x_i$) in the crystal for a given pressure ($p$) is given by $(dl/l_0) = \epsilon(x_i) = \epsilon_{ij} x_i$

$x_j = -p \beta(x)$ where $\beta(x) = S_{ijkk} x_i x_j$. The change of volume (or dilation) is an invariant of the strain tensor which for small strains is $\Delta V/V_0 = \epsilon_{ii} = -p S_{ii}$. Hence the volume compressibility $\beta = -(dV/dP)/V_0 = - (\Delta V/V_0)/p = - \epsilon_{ii}/p = S_{ii}$. The bulk modulus $K = 1/\beta$.

Young’s Modulus

No single surface can represent the elastic behaviour of a single crystal. The surface of the Young’s modulus is often used. Young’s modulus for a given direction is defined as the ratio of the longitudinal stress to the longitudinal elastic strain. Note in a triclinic elastic body a tensile or compressive stress in a longitudinal direction will also produce lateral and shear strains. Young’s modulus is given by $1/S_{ijkl}$ or $1/S_{1111}$ where $S_{ijkl} = R_{ij} R_{jn} R_{ko} R_{ip} S_{mnop}$ with $i,j,k,l = 1,1,1,1$ and $m,n,o,p = 1$ to $3$. Some examples are given for quartz, calcite, plagioclase and olivine. Note the high values of Young’s modulus are also high values of $V_p$. Plagioclase is triclinic, but it’s elastic constants have been measured in monoclinic frame because the crystal twinned on the Albite law giving a pseudo-monoclinic symmetry.
### Symmetry Properties of the Elastic Constants Tensor

#### Triclinic (21 constants)

\[
\begin{pmatrix}
1, \overline{1} \\
\end{pmatrix}
\begin{pmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\
c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\
c_{33} & c_{34} & c_{35} & c_{36} \\
c_{44} & c_{45} & c_{46} \\
c_{55} & c_{56} \\
c_{66} \\
\end{pmatrix}
\]

#### Orthorhombic

\[
\begin{pmatrix}
2, m, 2/m \\
32, 3m, 3m \\
\end{pmatrix}
\begin{pmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\
c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\
c_{33} & c_{34} & c_{35} & c_{36} \\
c_{44} & c_{45} & c_{46} \\
c_{55} & c_{56} \\
c_{66} \\
\end{pmatrix}
\]

#### Monoclinic (13 contants)

\[
\begin{pmatrix}
2, m, 2/m \\
3, \overline{3} \\
\end{pmatrix}
\begin{pmatrix}
c_{11} & c_{12} & c_{13} & 0 & c_{15} & 0 \\
c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\
c_{33} & c_{34} & c_{35} & c_{36} \\
c_{44} & c_{45} & c_{46} \\
c_{55} & c_{56} \\
c_{66} \\
\end{pmatrix}
\]

#### Trigonal (7 constants)

\[
\begin{pmatrix}
3, \overline{3} \\
\end{pmatrix}
\begin{pmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & 0 \\
c_{21} & c_{23} & c_{24} & c_{25} & c_{26} \\
c_{33} & c_{34} & c_{35} & c_{36} \\
c_{44} & c_{45} & c_{46} \\
c_{55} & c_{56} \\
c_{66} = \frac{1}{2}(c_{11} - c_{12}) \\
\end{pmatrix}
\]

#### Hexagonal (5 constants)

\[
\begin{pmatrix}
6, 6/m, 622, 6mm, 62m, 6/mmm \\
\end{pmatrix}
\begin{pmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & 0 \\
c_{21} & c_{23} & c_{24} & c_{25} & c_{26} \\
c_{33} & c_{34} & c_{35} & c_{36} \\
c_{44} & c_{45} & c_{46} \\
c_{55} & c_{56} \\
c_{66} = \frac{1}{2}(c_{11} - c_{12}) \\
\end{pmatrix}
\]

#### Tetragonal (7 constants)

\[
\begin{pmatrix}
4, 4/m \\
\end{pmatrix}
\begin{pmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\
c_{21} & c_{23} & c_{24} & c_{25} & c_{26} \\
c_{33} & c_{34} & c_{35} & c_{36} \\
c_{44} & c_{45} & c_{46} \\
c_{55} & c_{56} \\
c_{66} \\
\end{pmatrix}
\]

#### Tetragonal (6 constants)

\[
\begin{pmatrix}
422, 4mm, 42m, 4/mmm \\
\end{pmatrix}
\begin{pmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\
c_{21} & c_{23} & c_{24} & c_{25} & c_{26} \\
c_{33} & c_{34} & c_{35} & c_{36} \\
c_{44} & c_{45} & c_{46} \\
c_{55} & c_{56} \\
c_{66} \\
\end{pmatrix}
\]

#### Cubic (3 constants)

\[
\begin{pmatrix}
23, m3, 432, 43m, m3m \\
\end{pmatrix}
\begin{pmatrix}
c_{11} & c_{12} & c_{13} \\
c_{11} & c_{12} & c_{13} \\
c_{11} & c_{12} & c_{13} \\
c_{44} & c_{44} & c_{44} \\
\end{pmatrix}
\]
Putting it all together......


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