Carnegie Mellon

Anisotropic Elasticity

27-750

Texture, Microstructure & Anisotropy

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MSE

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Notation

F Stimulus (field)

R Response

P Property

j electric current

E electric field

D electric polarization

ε Strain (also, permutation tensor)

σ Stress (or conductivity)

ρ Resistivity

d piezoelectric tensor

C elastic stiffness

S elastic compliance

a transformation matrix

W work done (energy)

dW work increment

I identity matrix

O symmetry operator (matrix)

Y Young's modulus

δ Kronecker delta

e axis (unit) vector

T tensor

α direction cosine

Objective

- The objective of this lecture is to provide a mathematical framework for the description of properties, especially when they vary with direction.
- A basic property that occurs in almost applications is *elasticity*. Although elastic response is *linear* for all practical purposes, it is often *anisotropic* (composites, textured polycrystals etc.).
- Why do we care about elastic anisotropy? In composites, especially fibre composites, it is easy to design in substantial anisotropy by varying the lay-up of the fibres. See, for example: **http://www.jwave.vt.edu/crcd/kriz/lectures/Geom_3.html**
- Geologists are very familiar with elastic anisotropy and exploit it for understanding seismic results; see, e.g., **https://en.wikipedia.org/wiki/Seismic_anisotropy** .

In Class Questions

1. Why is plastic yielding a non-linear property, in contrast to elastic deformation?
2. What is the definition of a tensor?
3. Why is stress is 2nd-rank tensor?
4. Why is elastic stiffness a 4th-rank tensor?
5. What is "matrix notation" (in the context of elasticity)?
6. What are the relationships between tensor and matrix coefficients for stress? Strain? Stiffness? Compliance?
7. Why do we need factors of 2 and 4 in some of these conversion factors?
8. How do we use crystal symmetry to decrease the number of coefficients needed to describe stiffness and compliance?
9. How many independent coefficients are needed for stiffness (and compliance) in cubic crystals? In isotropic materials?
10. How do we express the directional dependence of Young's modulus?
11. What is Zener's anisotropy factor?

Q&A

1. How do we write the relationship between (tensor) stress and (tensor) strain? $\sigma=C:\varepsilon$. How about the other way around? $\varepsilon=S:\sigma$. What are "stiffness" and "compliance" in this context? The stiffness tensor is the collection of coefficients that connect all the different stress coefficients/components to all the different strain coefficients/components. How do we express this in Voigt or vector-matrix notation? The only difference is that the stress and strain are vectors and the stiffness and compliance are matrices. If indices are used then stress and strain each have two indices and the stiffness and compliance each have four.
2. What are the relationships between the coefficients of the (4^{th} rank) stiffness tensor and the stiffness matrix (6x6)? See the notes for details but, e.g., $\{11,22,33\}_{tensor}$ correspond to $\{1,2,3\}_{matrix}$. E.g. C_{12}(matrix)=C_{1122}(tensor). What about the compliance tensor and matrix? Here, more care is required because certain coefficients have factors of 2 or 4.
3. What does work conjugacy mean? The energy stored in a body when elastic strains and stresses are present is calculated as the product of the stress and strain, which means that the work done makes the strain and stress conjugate (joined) variables. What does this mean for the relationships between (2^{nd} rank) tensor stress and its vector form? What about strain? Answering these two together, we note that work conjugacy means that whatever notation is used to express stress and strain, the product of the two must be the same because of conservation of energy. This then explains why factors of two are used in the conversion to/from matrix to tensor representations of the shear components of strain (but not the normal strain components). These factors of two could have been applied to stress, but by convention we do this for strain.
4. How do we write the tensor transformation rule in vector-matrix notation? See the notes for details but the basic idea is that a 6x6 matrix (that can be applied to a stiffness or compliance tensor) is formed from the coefficients of the transformation matrix.
5. How do we apply crystal symmetry to elastic moduli (e.g. the stiffness tensor)? We apply a symmetry operator to the (stiffness) tensor and set the new and old versions of the tensor equal to each other, coefficient by coefficient. What net effect does it have on the stiffness matrix for cubic materials? Applying the cubic crystal symmetry to the stiffness tensor reduces most of the coefficients to zero and there are only 3 independent coefficients that remain.

Q&A, part 2

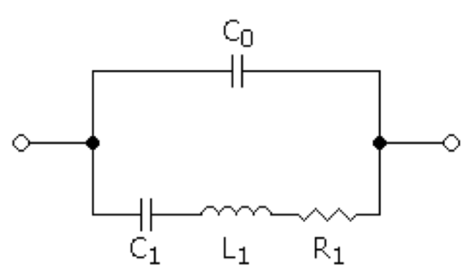
6. How do we convert from stiffness to compliance (and *vice versa*)? The detailed mathematics is out of scope for this course. It is sufficient to know that the two tensors combine to form a 4^{th} rank identity tensor, from which one can obtain algebraic relationships as given in the notes. Be aware that these formulae depend on the crystal symmetry (as do the compliance & stiffness tensors themselves).
7. How do we apply symmetry (and transformations of axes in general) to the property of anisotropic elasticity? There are two answers. The first answer is that one can apply the tensor transformation rule, just as explained in previous lectures. Generate the transformation matrix with any the methods described (i.e. dot products between old and new axes, or using the combination of axis and angle). Then write out the transformation with 4 copies of the matrix taking care to specify the indices correctly. The alternative answer is to generate a 6x6 transformation matrix that can be used with vector-matrix (Voigt) notation for either the stress, strain (6x1) vectors or the modulus (6x6) matrix.
8. How do we show that symmetry reduces the number of independent coefficients in an anisotropic elasticity modulus tensor? Given a symmetry matrix, one proceeds just as in the previous examples i.e. apply symmetry and then equate individual coefficients to find the cases of either zero or equality(between different coefficients).
9. How do we calculate the (anisotropic) elastic (Young's) modulus in an arbitrary direction? This looks ahead to the next lecture. The idea is to realize that a tensile test is such that there is only one non-zero coefficient in the stress tensor (or vector); the strain tensor, however, has to have more than one non-zero coefficient (because of the Poisson effect). Therefore one uses the relationship that strain = compliance x stress. By rotating the compliance tensor such that one axis (usually x) is parallel to the desired direction, one obtains the Young's modulus in that direction as $1/S_{11}$.

Anisotropy: Practical Applications

- The practical applications of anisotropy of composites, especially fiber-reinforced composites are numerous.
- The stiffness of fiber composites varies tremendously with direction. Torsional rigidity is very important in car bodies, boats, aeroplanes etc.
- Even in monolithic polymers (e.g. drawn polyethylene) there exists large anisotropy because of the alignment of the long-chain molecules.

Application example: quartz oscillators

- Piezoelectric quartz crystals are commonly used for frequency control in watches and clocks. Despite having small values of the piezoelectric coefficients, quartz has positive aspects of low losses and the availability of orientations with negligible temperature sensitivity. The property of piezoelectricity relates strain to electric field, or polarization to stress.
- $\varepsilon_{ij} = d_{ijk}E_k$
- PZT, lead zirconium titanate $PbZr_{1-x}Ti_xO_3$, is another commonly used piezoelectric material.



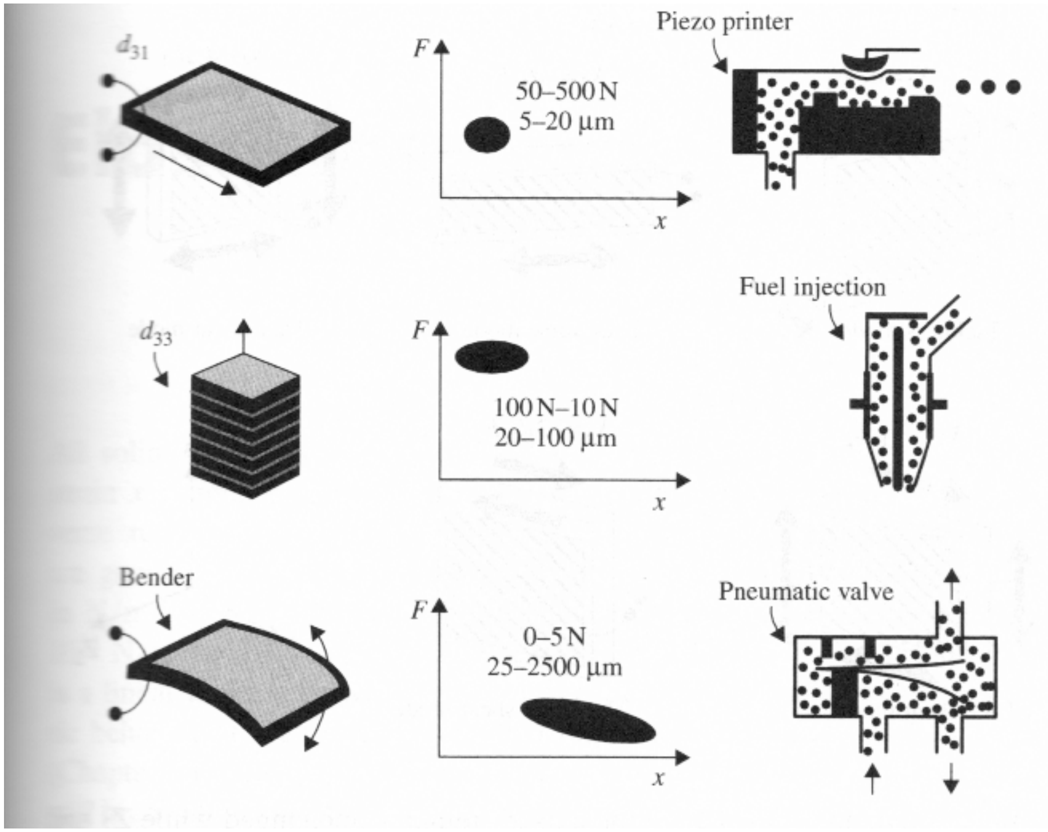
Examinable

Piezoelectric Devices

• The property of piezoelectricity relates strain to electric field, or polarization to stress.

$\varepsilon_{ij} = d_{ijk}E_k$

• PZT, lead zirconium titanate $PbZr_{1-x}Ti_xO_3$, is another commonly used piezoelectric material.



Note: Newnham consistently uses vector-matrix notation, rather than tensor notation. We will explain how this works later on.

Fig. 12.12 Ceramic multilayer actuators consist of thin layers of piezoelectric ceramic and metal electrodes. In contrast to traditional piezoelectrics, even low voltages produce large forces and substantial displacements. A tradeoff exists between force and displacement. The multilayer stack utilizing the d_{33} coefficient give kilonewton forces capable of pushing heavy weights through small distances. Bimorph benders make use of the smaller transverse of d_{31} coefficients to give larger displacements in the millimeter range, but only small forces.

[Newnham]

Piezoelectric Crystals

- How is it that crystals can be piezoelectric?
- The answer is that the bonding must be ionic to some degree (i.e. there is a net charge on the different elements) and the arrangement of the atoms must be non-centrosymmetric.
- PZT is a standard piezoelectric material. It has Pb atoms at the cell corners ($a \sim 4Å$), O on face centers, and a Ti or Zr atom near the body center. Below a certain temperature (*Curie T*), the cell transforms from cubic (high T) to tetragonal (low T). Applying stress distorts the cell, which changes the electric displacement in different ways (see figure).
- Although we can understand the effect at the single crystal level, real devices (e.g. sonar transducers) are polycrystalline. The operation is much complicated than discussed here, and involves "poling" to maximize the response, which in turns involves motion of domain walls.

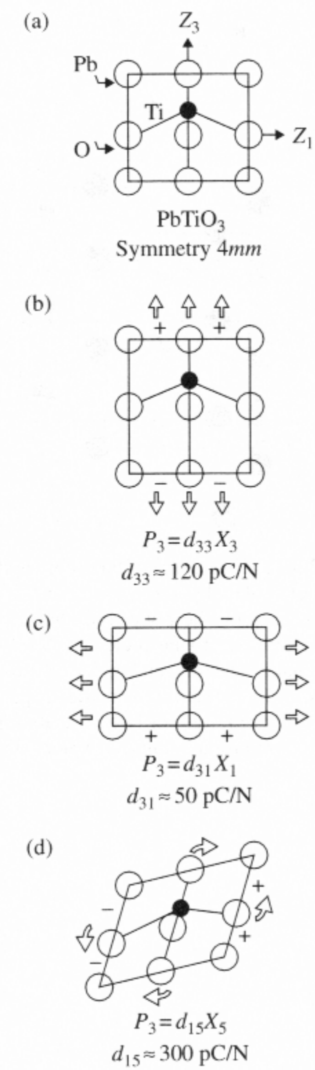


Fig. 12.11 Structure–property relations for the intrinsic piezoelectric effect in $PbTiO_3$. In the unstressed state there is an electric dipole associated with the off-center shift of the titanium atom. Under stress, this dipole can be increased (d_{33}), decreased (d_{31}), or tilted (d_{15}).

[Newnham]

Mathematical Descriptions

- Mathematical descriptions of properties are available.
- Mathematics, or a type of mathematics provides a *quantitative framework*. It is always necessary, however, to make a correspondence between mathematical variables and physical quantities.
- In group theory one might say that there is a set of mathematical operations & parameters, and a set of physical quantities and processes: if the mathematics is a good description, then the two sets are isomorphous.
- This lecture makes extensive use of *tensors*. A tensor is a quantity that can be transformed from one set of axes to another via the *tensor transformation rule* (next slide).

Tensor: definition, contd.

- In order for a quantity to "qualify" as a *tensor* it has to obey the *axis transformation rule*, as discussed in the previous slides.
- The *transformation rule* defines relationships between transformed and untransformed tensors of various ranks.
- It says that any tensor quantity can be transformed from one reference frame to another; this *transformation of axes* is sometimes called a *passive rotation*.

Vector: $V'_i = a_{ij} V_j$

2nd rank $T'_{ij} = a_{ik} a_{jl} T_{kl}$

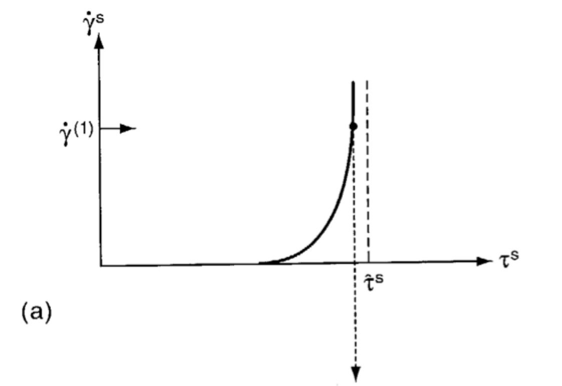
3rd rank $T'_{ijk} = a_{il} a_{jm} a_{kn} T_{lmn}$

4th rank $T'_{ijkl} = a_{im} a_{jn} a_{ko} a_{lp} T_{mnop}$

This rule is a critical piece of information, which you must know how to use.

Non-Linear properties, example

- Another important example of non-linear anisotropic properties is plasticity, i.e. the irreversible deformation of solids.
- A typical description of the response at plastic yield (what happens when you load a material to its yield stress) is elastic-perfectly plastic. In other words, the material responds elastically until the yield stress is reached, at which point the stress remains constant (strain rate unlimited).



- A more realistic description is a power-law with a large exponent, n~50. The stress is scaled by the *crss*, and be expressed as either shear stress-shear strain rate [graph], or tensile stress-tensile strain [equation].

$$\dot{\varepsilon} = \left(\frac{\sigma}{\sigma_{yield}} \right)^n$$

[Kocks]

Linear properties

- Certain properties, such as elasticity in most cases, are linear which means that we can simplify even further to obtain

$$R = R_0 + \mathbf{P}F$$

or if $R_0 = 0$,

$$R = \boldsymbol{P}F.$$

stiffness

e.g. elasticity: $\boldsymbol{\sigma} = C\, \boldsymbol{\varepsilon}$

In tension, $C \equiv$ *Young's modulus, Y or E.*

Elasticity

- *Elasticity*: example of a property that requires tensors to describe it fully.
- Even in cubic metals, a crystal is quite anisotropic. The [111] in many cubic metals is stiffer than the [100] direction.
- Even in cubic materials, 3 numbers/coefficients/moduli are required to describe elastic properties; isotropic materials only require 2.
- *Familiarity with Miller indices, suffix notation, Einstein convention, Kronecker delta, permutation tensor, and tensors is assumed.*

Elastic Anisotropy: 1

- First we restate the linear elastic relations for the properties *Compliance*, written *S*, and *Stiffness*, written *C* (admittedly not very logical choice of notation), which connect stress, $\boldsymbol{\sigma}$, and strain, $\boldsymbol{\varepsilon}$. We write it first in vector-tensor notation with *":"* signifying *inner product* (i.e. add up terms that have a common suffix or index in them):

$$\boldsymbol{\sigma} = C:\boldsymbol{\varepsilon}$$
$$\boldsymbol{\varepsilon} = S:\boldsymbol{\sigma}$$

- In *component* form (with suffixes),

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$$
$$\varepsilon_{ij} = S_{ijkl}\sigma_{kl}$$

Elastic Anisotropy: 2

The definitions of the stress and strain tensors mean that they are both symmetric (second rank) tensors. Therefore we can see that

$$\varepsilon_{23} = S_{2311}\sigma_{11}$$

$$\varepsilon_{32} = S_{3211}\sigma_{11} = \varepsilon_{23}$$

which means that,

$$S_{2311} = S_{3211}$$

and in general,

$$S_{\mathrm{ijkl}} = S_{\mathrm{jikl}}$$

We will see later on that this reduces considerably the number of different coefficients needed.

Stiffness in sample coords.

- Consider how to express the elastic properties of a single crystal in the sample coordinates. In this case we need to rotate the (4th rank) tensor stiffness from crystal coordinates **to** sample coordinates using the orientation (matrix), a :

$$c_{ijkl}' = a_{im} a_{jn} a_{ko} a_{lp} c_{mnop}$$

- Note how the transformation matrix appears four times because we are transforming a 4th rank tensor!
- The axis transformation matrix, a, is sometimes also written as λ, also as the **orientation matrix** g.

Young's modulus from compliance

- Young's modulus as a function of direction can be obtained from the compliance tensor as:

  $$E = 1/s'_{1111}$$

  Using compliances and a stress boundary condition (only $\sigma_{11} \neq 0$) is most straightforward. To obtain s'_{1111}, we simply apply the same transformation rule,

$$s'_{ijkl} = a_{im}\, a_{jn}\, a_{ko}\, a_{lp} s_{mnop}$$

"Voigt" or "matrix" notation

- It is useful to re-express the three quantities involved in a simpler format. The stress and strain tensors are **vectorized**, i.e. converted into a 1x6 notation and the elastic tensors are reduced to 6x6 matrices.

$$\begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix} \longleftrightarrow \begin{pmatrix} \sigma_{1} & \sigma_{6} & \sigma_{5} \\ \sigma_{6} & \sigma_{2} & \sigma_{4} \\ \sigma_{5} & \sigma_{4} & \sigma_{3} \end{pmatrix}$$

$$\longleftrightarrow \left(\sigma_1, \sigma_2, \sigma_3, \sigma_4, \sigma_5, \sigma_6\right)$$

"matrix notation", contd.

- Similarly for strain:

$$\begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{pmatrix} \longleftrightarrow \begin{pmatrix} \varepsilon_{1} & \frac{1}{2}\varepsilon_{6} & \frac{1}{2}\varepsilon_{5} \\ \frac{1}{2}\varepsilon_{6} & \varepsilon_{2} & \frac{1}{2}\varepsilon_{4} \\ \frac{1}{2}\varepsilon_{5} & \frac{1}{2}\varepsilon_{4} & \varepsilon_{3} \end{pmatrix}$$

$$\longleftrightarrow \left(\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4, \varepsilon_5, \varepsilon_6\right)$$

The particular definition of shear strain used in the reduced notation happens to correspond to that used in mechanical engineering such that ε_4 is the change in angle between direction 2 and direction 3 due to deformation.

Work conjugacy, matrix inversion

- The more important consideration is that the reason for the factors of two is so that work conjugacy is maintained.

$$dW = \sigma : d\varepsilon = \sigma_{ij} : d\varepsilon_{ij} = \sigma_k \bullet d\varepsilon_k$$

Also we can combine the expressions
$\boldsymbol{\sigma} = C\boldsymbol{\varepsilon}$ and $\boldsymbol{\varepsilon} = S\boldsymbol{\sigma}$ to give:

$\boldsymbol{\sigma} = CS\boldsymbol{\sigma}$, which shows:

$I = CS$, or, $C = S^{-1}$

Tensor conversions: stiffness

- Lastly we need a way to convert the tensor coefficients of stiffness and compliance to the matrix coefficients. For stiffness, it is very simple because one substitutes values according to the following table, such that [*vector-matrix*] C_{11} = C_{1111} [*tensor*] for example.

Tensor	11	22	33	23	32	13	31	12	21
Matrix	1	2	3	4	4	5	5	6	6

Stiffness Matrix

$$C = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix}$$

Vector-matrix notation (two indices for the moduli, one index for stress or strain); note that this matrix is symmetric, therefore there are only 21 independent coefficients, even for triclinic crystals (see later slides).

Axis Transformations

- It is still possible to perform axis transformations, as allowed for by the Tensor Rule. The coefficients can be combined [Newnham] together into a 6 by 6 matrix that can be used for 2nd rank tensors such as stress and strain, below.

- Stress (in vector notation) transforms as: $X'_i = \alpha_{ij} X_j$
- Strain (in vector notation) transforms as: $x'_i = (\alpha^{-1}_{ij})^T x_j$ where superscript "T" signifies transpose of the matrix.

Table 10.1 Transformation matrices for stresses and strains written in matrix form

(α)	(a_{11}^2)	(a_{12}^2)	(a_{13}^2)	$(2a_{12}a_{13})$	$(2a_{13}a_{11})$	$(2a_{11}a_{12})$
	(a_{21}^2)	(a_{22}^2)	(a_{23}^2)	$(2a_{22}a_{23})$	$(2a_{23}a_{21})$	$(2a_{21}a_{22})$
	(a_{31}^2)	(a_{32}^2)	(a_{33}^2)	$(2a_{32}a_{33})$	$(2a_{33}a_{31})$	$(2a_{31}a_{32})$
	$(a_{21}a_{31})$	$(a_{22}a_{32})$	$(a_{23}a_{33})$	$(a_{22}a_{33}+a_{23}a_{32})$	$(a_{21}a_{33}+a_{23}a_{31})$	$(a_{22}a_{31}+a_{21}a_{32})$
	$(a_{31}a_{11})$	$(a_{32}a_{12})$	$(a_{33}a_{13})$	$(a_{12}a_{33}+a_{13}a_{32})$	$(a_{13}a_{31}+a_{11}a_{33})$	$(a_{11}a_{32}+a_{12}a_{31})$
	$(a_{11}a_{21})$	$(a_{12}a_{22})$	$(a_{13}a_{23})$	$(a_{12}a_{23}+a_{13}a_{22})$	$(a_{13}a_{21}+a_{11}a_{23})$	$(a_{11}a_{22}+a_{12}a_{21})$
(α^{-1})	(a_{11}^2)	(a_{21}^2)	(a_{31}^2)	$(2a_{21}a_{31})$	$(2a_{31}a_{11})$	$(2a_{11}a_{21})$
	(a_{12}^2)	(a_{22}^2)	(a_{32}^2)	$(2a_{22}a_{32})$	$(2a_{32}a_{12})$	$(2a_{12}a_{22})$
	(a_{13}^2)	(a_{23}^2)	(a_{33}^2)	$(2a_{23}a_{33})$	$(2a_{33}a_{13})$	$(2a_{13}a_{23})$
	$(a_{12}a_{13})$	$(a_{22}a_{23})$	$(a_{32}a_{33})$	$(a_{22}a_{33}+a_{32}a_{23})$	$(a_{12}a_{33}+a_{32}a_{13})$	$(a_{22}a_{13}+a_{12}a_{23})$
	$(a_{13}a_{11})$	$(a_{23}a_{21})$	$(a_{33}a_{31})$	$(a_{21}a_{33}+a_{31}a_{23})$	$(a_{31}a_{13}+a_{11}a_{33})$	$(a_{11}a_{23}+a_{21}a_{13})$
	$(a_{11}a_{12})$	$(a_{21}a_{22})$	$(a_{31}a_{32})$	$(a_{21}a_{32}+a_{31}a_{22})$	$(a_{31}a_{12}+a_{11}a_{32})$	$(a_{11}a_{22}+a_{21}a_{12})$

Tensor conversions: compliance

- For compliance some factors of two are required and so the rule becomes:

$$p S_{ijkl} = S_{mn}$$

$$p = 1 \qquad m.AND.n \in [1,2,3]$$

$$p = 2 \qquad m.XOR.n \in [1,2,3]$$

$$p = 4 \qquad m.AND.n \in [4,5,6]$$

Relationships between coefficients: C in terms of S

Some additional useful relations between coefficients for cubic materials are as follows. Symmetrical relationships exist for compliances in terms of stiffnesses (next slide).

$$C_{11} = (S_{11}+S_{12})/\{(S_{11}-S_{12})(S_{11}+2S_{12})\}$$

$$C_{12} = -S_{12}/\{(S_{11}-S_{12})(S_{11}+2S_{12})\}$$

$$C_{44} = 1/S_{44}.$$

S in terms of C

The relationships for S in terms of C are symmetrical to those for stiffnesses in terms of compliances (a simple exercise in algebra).

$S_{11} = (C_{11}+C_{12})/\{(C_{11}-C_{12})(C_{11}+2C_{12})\}$
$S_{12} = -C_{12}/\{(C_{11}-C_{12})(C_{11}+2C_{12})\}$
$S_{44} = 1/C_{44}$

$S_{11} - S_{12} = (C_{11}+2C_{12})/\{(C_{11}-C_{12})(C_{11}+2C_{12})\}$
$S_{11} - S_{12} = 1/(C_{11}-C_{12})$.

Neumann's Principle

- A fundamental natural law: *Neumann's Principle*: *the symmetry elements of any physical property of a crystal must include the symmetry elements of the point group of the crystal*. The property may have additional symmetry elements to those of the crystal (point group) symmetry. There are 32 crystal classes for the point group symmetry.
- F.E. Neumann 1885.

Neumann, extended

- If a crystal has a defect structure such as a dislocation network that is arranged in a non-uniform way then the symmetry of certain properties may be reduced from the crystal symmetry. In principle, a finite elastic strain in one direction decreases the symmetry of a cubic crystal to tetragonal or less. Therefore the modified version of *Neumann's Principle*: *the symmetry elements of any physical property of a crystal must include the symmetry elements that are common to the point group of the crystal and the defect structure contained within the crystal*.

Effect of crystal symmetry

- Consider an active rotation of the crystal, where *O* is the symmetry operator. Since the crystal is indistinguishable (looks the same) after applying the symmetry operator, the result before, $R^{(1)}$, and the result after, $R^{(2)}$, must be identical:

$$\left.\begin{array}{c} R^{(1)} = \mathbf{P}F \\ R^{(2)} = O\mathbf{P}O^{T}F \\ R^{(1)} \overset{=}{\longleftrightarrow} R^{(2)} \end{array}\right\}$$

The two results are indistinguishable and therefore equal. It is essential, however, to express the property and the operator in the same (crystal) reference frame.

Symmetry, properties, contd.

- Expressed mathematically, we can rotate, e.g. a second rank property tensor thus:

  $\mathbf{P}' = O\mathbf{P}O^{\mathrm{T}} = \mathbf{P}$, or, in coefficient notation,

  $P'_{ij} = O_{ik}O_{il}P_{kl}$

  where *O* is a symmetry operator.
- Since the rotated (property) tensor, $\mathbf{P}'$, must be the same as the original tensor, $\mathbf{P}$, then we can equate coefficients:

  $$P'_{ij} = P_{ij}$$
- If we find, for example, that $P'_{21} = -P_{21}$,then the only value of P_{21} that satisfies this equality is $P_{21} = 0$.
- Remember that you must express the property with respect to a particular set of axes in order to use the coefficient form. In everything related to single crystals, *always* use the crystal axes as the reference frame!
- Homework question: based on cubic crystal symmetry, work out why a second rank tensor property can only have *one* independent coefficient.

Effect of symmetry on stiffness matrix

- Why do we need to look at the effect of symmetry? For a cubic material, only 3 *independent* coefficients are needed as opposed to the 81 coefficients in a 4th rank tensor. The reason for this is the symmetry of the material.
- What does symmetry mean? Fundamentally, if you pick up a crystal, rotate [mirror] it and put it back down, then a symmetry operation [rotation, mirror] is such that *you cannot tell that anything happened*.
- From a mathematical point of view, this means that the property (its coefficients) *does not change*. For example, if the symmetry operator changes the sign of a coefficient, then it must be equal to zero.

2nd Rank Tensor Properties & Symmetry

TABLE 3

The effect of crystal symmetry on properties represented by symmetrical second-rank tensors

Optical classification	*System*	*Characteristic symmetry* (see p. 280)†	*Nature of representation quadric and its orientation*	*Number of independent coefficients*	*Tensor referred to axes in the conventional orientation*‡
Isotropic (anaxial)	Cubic	4 3-fold axes	*Sphere*	1	$\begin{bmatrix} S & 0 & 0 \\ 0 & S & 0 \\ 0 & 0 & S \end{bmatrix}$
Uniaxial	Tetragonal Hexagonal Trigonal	1 4-fold axis 1 6-fold axis 1 3-fold axis	*Quadric of revolution* about the principal symmetry axis $(x_3)(z)$	2	$\begin{bmatrix} S_1 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_3 \end{bmatrix}$
Biaxial	Orthorhombic	3 mutually perpendicular 2-fold axes; no axes of higher order	*General quadric* with axes $(x_1, x_2, x_3) \parallel$ to the diad axes (x, y, z)	3	$\begin{bmatrix} S_1 & 0 & 0 \\ 0 & S_2 & 0 \\ 0 & 0 & S_3 \end{bmatrix}$
	Monoclinic	1 2-fold axis	*General quadric* with one axis $(x_2) \parallel$ to the diad axis (y)	4	$\begin{bmatrix} S_{11} & 0 & S_{31} \\ 0 & S_2 & 0 \\ S_{31} & 0 & S_{33} \end{bmatrix}$
	Triclinic	A centre of symmetry or no symmetry	*General quadric.* No fixed relation to crystallographic axes	6	$\begin{bmatrix} S_{11} & S_{12} & S_{31} \\ S_{12} & S_{22} & S_{23} \\ S_{31} & S_{23} & S_{33} \end{bmatrix}$

† Axes of symmetry may be rotation axes or inversion axes.

‡ The setting of the reference axes x_1, x_2, x_3 in column 6 in relation to the crystallographic axes x, y, z and to the symmetry elements is that shown in column 4. For further notes on axial conventions, see Appendix B.

- The table from Nye shows the number of independent, non-zero coefficients allowed in a 2nd rank tensor according to the crystal symmetry class.

Examinable

Effect of symmetry on stiffness matrix

- Following Reid, p.66 *et seq.*:
  Apply a -90° rotation about the crystal-z axis (axis 3)*,
  $C'_{ijkl} = O_{im}O_{jn}O_{ko}O_{lp}C_{mnop}$:
  $\mathbf{C}' = \mathbf{C}$

$$O_4^z = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$C' = \begin{bmatrix} C_{22} & C_{21} & C_{23} & C_{25} & -C_{24} & -C_{26} \\ C_{21} & C_{11} & C_{13} & C_{15} & -C_{14} & -C_{16} \\ C_{23} & C_{13} & C_{33} & C_{35} & -C_{34} & -C_{36} \\ C_{25} & C_{15} & C_{35} & C_{55} & -C_{54} & -C_{56} \\ -C_{24} & -C_{14} & -C_{34} & -C_{54} & C_{44} & C_{46} \\ -C_{26} & -C_{16} & -C_{36} & -C_{56} & C_{46} & C_{66} \end{bmatrix}$$

*Reid describes this as +90°, but -90° reproduces his result (because he apparently considers positive to be clockwise).

Examinable

Effect of symmetry, 2

- Using P' = P, we can equate all the coefficients in the 6x6 matrix and find that:

  $C_{11}=C_{22}$, $C_{13}=C_{23,}$ $C_{44}=C_{35}$, $C_{16}=-C_{26,}$
  $C_{14}=C_{15} = C_{24} = C_{25} = C_{34} = C_{35} = C_{36} = C_{45} = C_{46} =$
  $C_{56} = 0$.

$$C' = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\ C_{12} & C_{11} & C_{13} & 0 & 0 & -C_{16} \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & C_{46} \\ C_{16} & -C_{16} & 0 & 0 & C_{46} & C_{66} \end{bmatrix}$$

Effect of symmetry, 3

- Thus by repeated applications of the symmetry operators, one can demonstrate (for cubic crystal symmetry) that one can reduce the 81 coefficients down to only 3 independent quantities. These become two in the case of isotropy.

$$\begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}$$

Cubic crystals: anisotropy factor

- If one applies the symmetry elements of the cubic system, it turns out that only three independent coefficients remain: C_{11}, C_{12} and C_{44}, (similar set for compliance). From these three, a useful combination of the first two is

$$C' = (C_{11} - C_{12})/2$$

- See Nye, *Physical Properties of Crystals*

Zener's anisotropy factor

- C' = $(C_{11}$ - $C_{12})/2$ turns out to be the stiffness associated with a shear in a <110> direction on a plane. In certain martensitic transformations, this modulus can approach zero which corresponds to a structural instability.
- Zener (Physics, Carnegie Tech. Inst.) proposed a measure of elastic anisotropy based on the ratio C_{44}/C'. This turns out to be a useful criterion for identifying materials that are elastically anisotropic, i.e., via the extent to which C_{44}/C' varies from unity.
- Note that this provides a way to convert an anisotropic elastic stiffness into an isotropic one. One can, e.g., adjust C_{12} until the Zener ratio=1. Some care is required, however, because one might want to match some average Young's modulus, for example.

Rotated compliance (matrix)

- Given an orientation a_{ij}, we transform the compliance tensor, using cubic point group symmetry, and find that:

$$S'_{11} = S_{11}\left(a_{11}^4 + a_{12}^4 + a_{13}^4\right)$$

$$+\ 2S_{12}\left(a_{12}^2 a_{13}^2 + a_{11}^2 a_{12}^2 + a_{11}^2 a_{13}^2\right)$$

$$+\ S_{44}\left(a_{12}^2 a_{13}^2 + a_{11}^2 a_{12}^2 + a_{11}^2 a_{13}^2\right)$$

Rotated compliance (matrix)

- This can be further simplified with the aid of the standard relations between the direction cosines, $a_{ik}a_{jk}$ = 1 for $i=j$; $a_{ik}a_{jk}$ = 0 for $i \neq j$, ($a_{ik}a_{jk} = \delta_{ij}$) to read as follows.

$$s'_{11} = s_{11} - 2\left(s_{11} - s_{12} - \frac{s_{44}}{2}\right)\left\{\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2\right\}$$

- By definition, the Young's modulus in any direction is given by the reciprocal of the compliance, $E = 1/S'_{11}$.
- By definition, the Young's modulus along <100> is given by the reciprocal of the compliance for <100>:

$E_{100} = 1/S_{11} = \{(C_{11}\text{-}C_{12})(C_{11} + 2C_{12})\}/(C_{11} + C_{12})$.

Anisotropy in cubic materials

- Thus the second term on the RHS is zero for <100> directions and, for C_{44}/C'>1, a maximum in <111> directions (conversely a minimum for C_{44}/C'<1).
  The following table shows that most cubic metals have positive values of Zener's coefficient so that <100> is soft and <111> is hard, with the exceptions of V and NaCl.
- See the supplemental slides for how to go between C values and the *Lamé constants* used to describe isotropic materials.

Material	C_{44}/C'	E_{111}/E_{100}
Cu	3.21	2.87
Ni	2.45	2.18
Al	1.22	1.19
Fe	2.41	2.15
Ta	1.57	1.50
W (2000K)	1.23	1.35
W (R.T.)	1.01	1.01
V	0.78	0.72
Nb	0.55	0.57
β-CuZn	18.68	8.21
spinel	2.43	2.13
MgO	1.49	1.37
NaCl	0.69	0.74

Stiffness coefficients, cubics

Material class	Material	C_{11} (10^{10} N/m²)	C_{12} (10^{10} N/m²)	C_{44} (10^{10} N/m²)	Anisotropy ratio $(C_{11} - C_{12})/2C_{44}$
Metals	Ag	12.4	9.3	4.6	0.34
	Al	10.8	6.1	2.9	0.81
	Au	18.6	15.7	4.2	0.35
	Cu	16.8	12.1	7.5	0.31
	α-Fe	23.7	14.1	11.6	0.41
	Mo	46.0	17.6	11.0	1.29
	Na	0.73	0.63	0.42	0.12
	Ni	24.7	14.7	12.5	0.40
	Pb	5.0	4.2	1.5	0.27
	W	50.1	19.8	15.1	1.00
Covalent solids	Si	16.6	6.4	8.0	0.64
	Diamond	107.6	12.5	57.6	0.83
	TiC	51.2	11.0	17.7	1.14
Ionic solids	LiF	11.2	4.6	6.3	0.52
	MgO	29.1	9.0	15.5	0.65
	NaCl	4.9	1.3	1.3	1.38

Table 2.2
Stiffness coefficients for selected cubic materials

[Courtney]

Anisotropy in terms of moduli

- Another way to write the above equation is to insert the values for the Young's modulus in the soft and hard directions, assuming that the <100> are the most compliant direction(s). (Courtney uses α, β, and γ in place of my α_1, α_2, and α_3.) The advantage of this formula is that moduli in specific directions can be used directly.

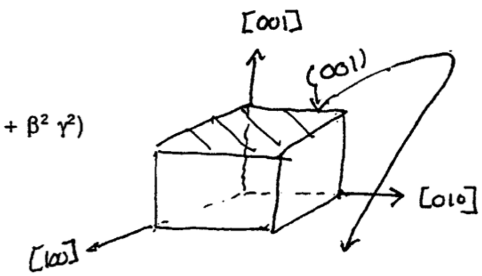
$$\frac{1}{E_{uvw}} = \frac{1}{E_{100}} - 3\left\{\frac{1}{E_{100}} - \frac{1}{E_{111}}\right\}\left(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2\right)$$

Example Problem

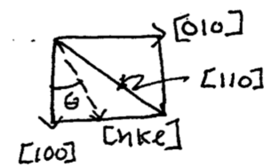
2.11 a Sketch a (001) plane in a face-centered cubic material and an arbitrary vector within it making an angle θ with the [100] direction. Plot the Young's modulus for copper as a function of θ for directions between [110] and [100].
b Sketch a (110) plane in Cu and a vector in the plane making an angle α with the [110] direction. Plot E vs. α for directions between [110] and [001].

Solution: (a) The plane is illustrated to the right.
Use Eq. (3.22).

$$1/E_{[hkl]} = 1/E_{<100>} - 3\{1/E_{<100>} - 1/E_{<111>}\}(\alpha^2\beta^2 + \alpha^2\gamma^2 + \beta^2\gamma^2)$$



where α is the cosine of the angle between the direction [100] and [hkl], β is the cosine of the angle between [010] and [hkl], and γ is the like cosine between [001] and [hkl]. From the sketches provided we see that α = cosθ, β = cos(90°-θ) = sin θ and γ =0. Employing moduli in units of 10^{10} N/m², with $E_{<100>}$ = 6.7, $E_{<111>}$ =11.2 the above equation becomes

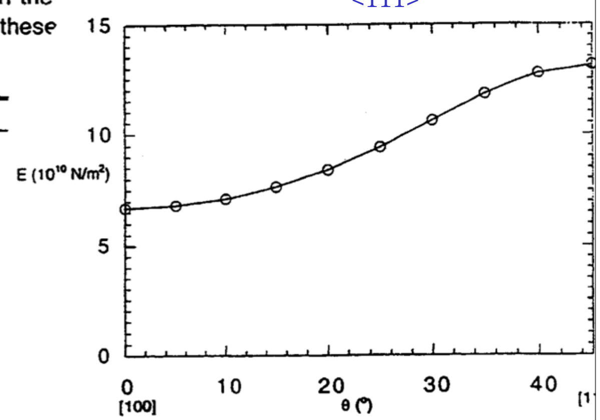


$$1/E_{[hkl]} = 0.149 - 0.2915\cos^2\theta\sin^2\theta$$

Should be $E_{<111>}$= 18.89

The table below presents results obtained with the above formula; the figure to the right graphs these results.

θ (°)	$\cos^2\theta\sin^2\theta$	E (10^{10}N/m²)
0	0	6.7
5	0.0075	6.81
10	0.0292	7.12
15	0.0625	7.65
20	0.1033	8.41
25	0.1467	9.41
30	0.1875	10.6
35	0.2207	11.82
40	0.2425	12.77
45 (=[110])	0.25	13.14



[Courtney]

Alternate Vectorization

$$\mathbf{b}^{(1)}=\frac{1}{\sqrt{6}}\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&2\end{pmatrix};\ \mathbf{b}^{(2)}=\frac{1}{\sqrt{2}}\begin{pmatrix}-1&0&0\\0&1&0\\0&0&0\end{pmatrix};\ \mathbf{b}^{(3)}=\frac{1}{\sqrt{2}}\begin{pmatrix}0&0&0\\0&0&1\\0&1&0\end{pmatrix}$$

$$\mathbf{b}^{(4)}=\frac{1}{\sqrt{2}}\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix};\quad \mathbf{b}^{(5)}=\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&0\\0&0&0\end{pmatrix};\ \mathbf{b}^{(6)}=\frac{1}{\sqrt{3}}\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$$

An alternate vectorization, discussed by Tomé on p287 of the Kocks et al. textbook, is to use the above set of eigentensors. For both stress and strain, one can matrix multiply each eigentensor into the stress/strain tensor in turn and obtain the coefficient of the corresponding stress/strain vector. Work conjugacy is still satisfied. The first two eigentensors represent shears in the {110} planes; the next three are simple shears on {110}<110> systems, and the last (6^{th}) is the hydrostatic component. The same vectorization can be used for plastic anisotropy, except in this case, the sixth, hydrostatic component is (generally) ignored.

Summary

- We have covered the following topics:
  - Linear properties
  - Non-linear properties
  - Examples of properties
  - Tensors, vectors, scalars, tensor transformation law.
  - Elasticity, as example as of higher order property, also as example as how to apply (crystal) symmetry.

Supplemental Slides

- The following slides contain some useful material for those who are not familiar with all the detailed mathematical methods of matrices, transformation of axes, tensors etc.

Einstein Convention

- The Einstein Convention, or summation rule for suffixes looks like this:

$$A_i = B_{ij}\, C_j$$

where "i" and "j" both are integer indexes whose range is {1,2,3}. So, to find each "ith" component of A on the LHS, we sum up over the repeated index, "j", on the RHS:

$$A_1 = B_{11}C_1 + B_{12}C_2 + B_{13}C_3$$
$$A_2 = B_{21}C_1 + B_{22}C_2 + B_{23}C_3$$
$$A_3 = B_{31}C_1 + B_{32}C_2 + B_{33}C_3$$

Matrix Multiplication

- Take each row of the LH matrix in turn and multiply it into each column of the RH matrix.
- In suffix notation, $a_{ij} = b_{ik}c_{kj}$

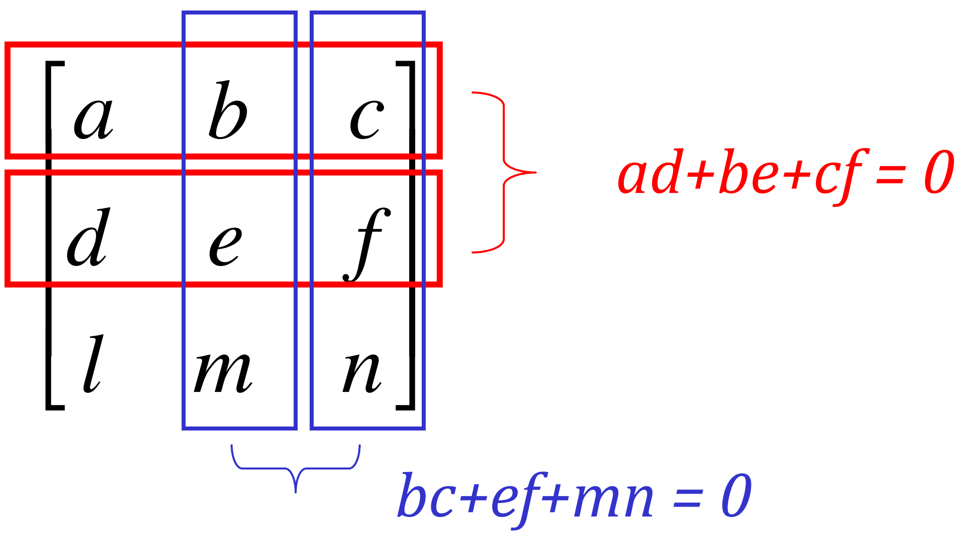
$$\begin{bmatrix} a\alpha + b\delta + c\gamma & a\beta + b\varepsilon + c\mu & a\gamma + b\phi + c\nu \\ d\alpha + e\delta + f\gamma & d\beta + e\varepsilon + f\mu & d\gamma + e\phi + f\nu \\ l\alpha + m\delta + n\gamma & l\beta + m\varepsilon + n\mu & l\gamma + m\phi + n\nu \end{bmatrix}$$

$$= \begin{bmatrix} a & b & c \\ d & e & f \\ l & m & n \end{bmatrix} \times \begin{bmatrix} \alpha & \beta & \gamma \\ \delta & \varepsilon & \phi \\ \lambda & \mu & \nu \end{bmatrix}$$

Properties of Rotation Matrix

- The rotation matrix is an *orthogonal matrix*, meaning that any row is orthogonal to any other row (the dot products are zero). In physical terms, each row represents a unit vector that is the position of the corresponding (new) old axis in terms of the (old) new axes.
- The same applies to columns: in suffix notation -

$$a_{ij}a_{kj} = \delta_{ik},\ a_{ji}a_{jk} = \delta_{ik}$$



Direction Cosines, contd.

- That the set of direction cosines are not independent is evident from the following construction:

$$\hat{e}'_i \cdot \hat{e}'_j = a_{ik} a_{jl} \hat{e}_k \cdot \hat{e}_l = a_{ik} a_{jl} \delta_{kl} = a_{ik} a_{jk} = \delta_{ij}$$

  Thus, there are *six* relationships (*i* takes values from 1 to 3, and *j* takes values from 1 to 3) between the *nine* direction cosines, and therefore, as stated above, only *three* are independent, exactly as expected for a rotation.

- Another way to look at a rotation: combine an axis (described by a unit vector with two parameters) and a rotation angle (one more parameter, for a total of 3).

Orthogonal Matrices

- Note that the direction cosines can be arranged into a *3x3 matrix*, Λ, and therefore the relation above is equivalent to the expression

$$\Lambda\Lambda^T = \mathrm{I}$$

where Λ^T denotes the transpose of Λ. This relationship identifies Λ as an orthogonal matrix, which has the properties

$$\Lambda^{-1} = \Lambda^T \qquad \det \Lambda = \pm 1$$

Relationships

- When both coordinate systems are right-handed, *det*(Λ)=+1 and Λ is a *proper orthogonal matrix*. The orthogonality of Λ also insures that, in addition to the relation above, the following holds:

$$\hat{e}_j = a_{ij}\hat{e}'_i$$

Combining these relations leads to the following inter-relationships between components of vectors in the two coordinate systems:

$$v_i = a_{ji}v'_j \;,\; v'_j = a_{ji}v_i$$

Transformation Law

- These relations are called the *laws of transformation* for the components of vectors. They are a consequence of, and equivalent to, the parallelogram law for addition of vectors. That such is the case is evident when one considers the scalar product expressed in two coordinate systems:

$$\vec{u} \cdot \vec{v} = u_i v_i = a_{ji} u'_j a_{ki} v'_k =$$

$$\delta_{jk} u'_j v'_k = u'_j v'_j = u'_i v'_i$$

Invariants

Thus, the transformation law as expressed preserves the lengths and the angles between vectors. Any function of the components of vectors which remains unchanged upon changing the coordinate system is called an *invariant* of the vectors from which the components are obtained. The derivations illustrate the fact that the scalar product $\vec{u} \cdot \vec{v}$ is an *invariant* of $\vec{u}$ and $\vec{v}$. Other examples of *invariants* include the vector product of two vectors and the triple scalar product of three vectors. The reader should note that the transformation law for vectors also applies to the components of points when they are referred to a common origin.

Orthogonality

- A rotation matrix, Λ, is an *orthogonal matrix*, however, because each row is mutually orthogonal to the other two.

$$a_{ki}a_{kj} = \delta_{ij}, \quad a_{ik}a_{jk} = \delta_{ij}$$

- Equally, each column is orthogonal to the other two, which is apparent from the fact that each row/column contains the direction cosines of the new/old axes in terms of the old/new axes and we are working with [mutually perpendicular] Cartesian axes.

Anisotropy

- *Anisotropy* as a word simply means that something varies with direction.
- Anisotropy is from the Greek: *aniso* = different, varying; *tropos* = direction.
- Almost all crystalline materials are anisotropic; many materials are engineered to take advantage of their anisotropy (beer cans, turbine blades, microchips…)
- Older texts use trigonometric functions to describe anisotropy but tensors offer a general description with which it is much easier to perform calculations.
- For materials, what we know is that some properties are anisotropic. This means that several numbers, or *coefficients*, are needed to describe the property - one number is not sufficient.
- Elasticity is an important example of a property that, when examined in single crystals, is often highly anisotropic. In fact, the lower the crystal symmetry, the greater the anisotropy is likely to be.
- *Nomenclature:* in general, we need to use *tensors* to describe fields and properties. The simplest case of a tensor is a *scalar* which is all we need for isotropic properties. The next "level" of tensor is a *vector*, e.g. electric current.

Scalars, Vectors, Tensors

- *Scalar*:= quantity that requires only one number, e.g. density, mass, specific heat. Equivalent to a zero-rank tensor.
- *Vector*:= quantity that has direction as well as magnitude, e.g. velocity, current, magnetization; requires 3 numbers or *coefficients* (in 3D). Equivalent to a first-rank tensor.
- *Tensor*:= quantity that requires higher order descriptions but is the same, no matter what coordinate system is used to describe it, e.g. stress, strain, elastic modulus; requires 9 (or more, depending on rank) numbers or *coefficients*.

Vector field, response

- If we have a vector response, R, that we can write in component form, a vector field, F, that we can also write in component form, and a property, P, that we can write in matrix form (with nine coefficients) then the linearity of the property means that we can write the following ($R_0 = 0$):

$$R_i = P_{\mathrm{ij}} F_j$$

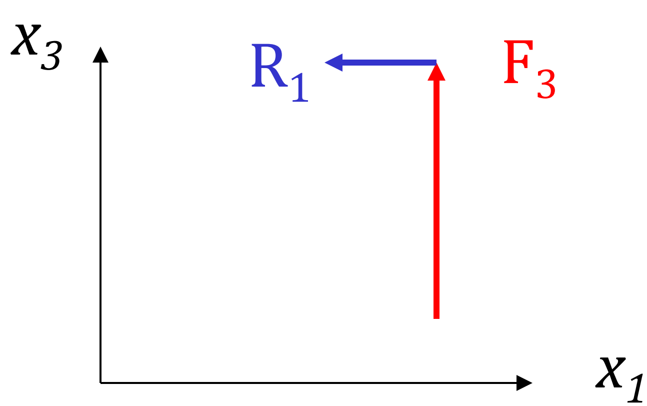
- A *scalar* (e.g. pressure) can be called a *zero-rank tensor*.
- A *vector* (e.g. electric current) is also known as a *first-rank tensor*.

Linear anisotropic property

- This means that each component of the response is *linearly* related to each component of the field and that the proportionality constant is the appropriate coefficient in the matrix. Example:

$$R_1 = P_{13}F_3,$$

which says that the first component of the response is linearly related to the third field component through the property coefficient P_{13}.



Example: electrical conductivity

- An example of such a linear anisotropic (second order tensor, discussed in later slides) property is the electrical conductivity of a material:

  - Field: Electric Field, E
  - Response: Current Density, J
  - Property: Conductivity, σ
  - $J_i = \sigma_{ij} E_j$

Anisotropic electrical conductivity

- We can illustrate anisotropy with Nye's example of electrical conductivity, σ:

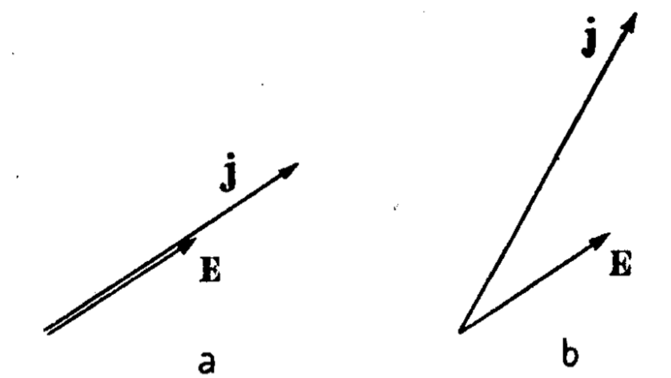


FIG. 1.1. The relation between the electric current density **j** and the electric field **E** in (*a*) an isotropic conductor and (*b*) an anisotropic conductor.

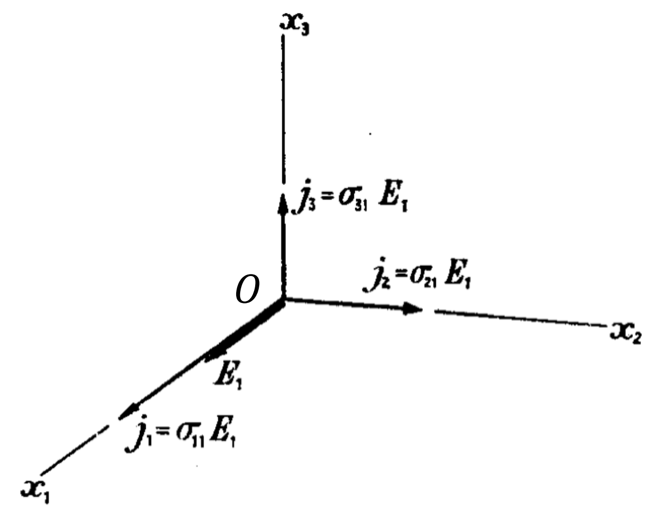


FIG. 1.2. The components of current density when a field is applied along Ox_1.

Stimulus/ Field: $E_1 \neq 0, E_2=E_3=0$

Response: $j_1=\sigma_{11}E_1, j_2=\sigma_{21}E_1, j_3=\sigma_{31}E_1,$

Changing the Coordinate System

- Many different choices are possible for the orthonormal base vectors and origin of the Cartesian coordinate system. A vector is an example of an entity which is independent of the choice of coordinate system. Its direction and magnitude must not change (and are, in fact, invariants), although its components will change with this choice.
- Why would we want to do something like this? For example, although the *properties* are conveniently expressed in a crystal reference frame, experiments often place the crystals in a non-symmetric position with respect to an experimental frame. Therefore we need some way of converting the coefficients of the property into the experimental frame.
- Changing the coordinate system is also known as *axis transformation*.

Motivation for Axis Transformation

- One motivation for axis transformations is the need to solve problems where the specimen shape (and the stimulus direction) does not align with the crystal axes. Consider what happens when you apply a force parallel to the sides of this specimen …

The direction parallel to the long edge does not line up with any simple, low index crystal direction. Therefore we have to find a way to *transform* the properties that we know for the material into the frame of the problem (or vice versa).

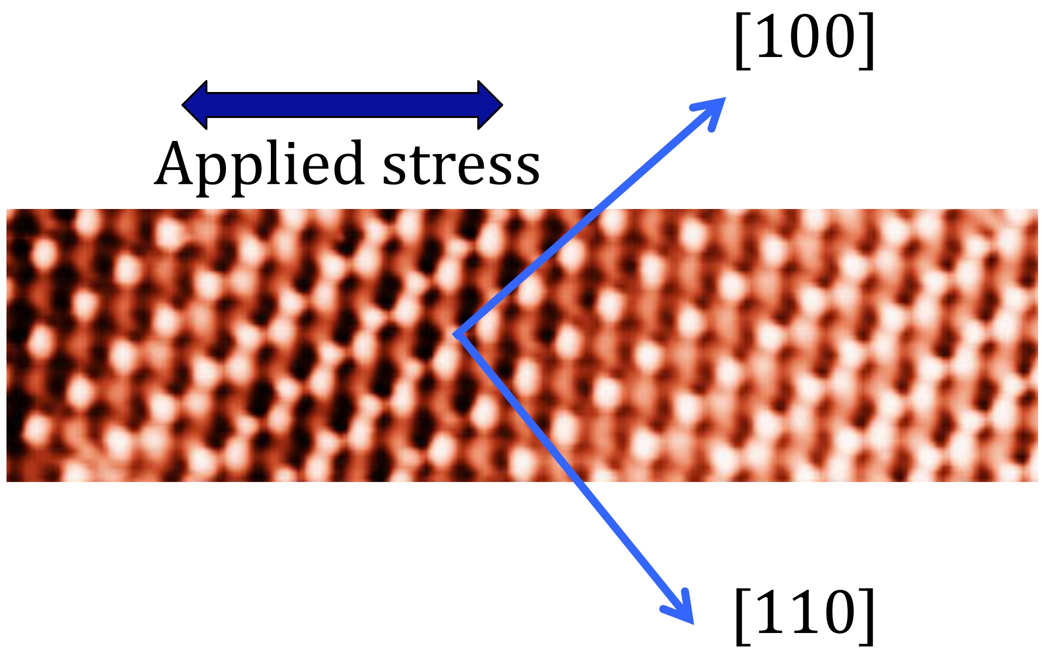


Image of Pt surface from www.cup.uni-muenchen.de/pc/wintterlin/IMGs/pt10p3.jpg

New Axes

- Consider a *new* orthonormal system consisting of right-handed base vectors: $\hat{e}'_1, \hat{e}'_2 \text{ and } \hat{e}'_3$
  These all have the same origin, o, associated with $\hat{e}'_1, \hat{e}'_2 \text{ and } \hat{e}'_3$

- The vector *v* is clearly expressed equally well in either coordinate system:

$$\vec{v} = v_i \hat{e}_i = v'_i \hat{e}'_i$$

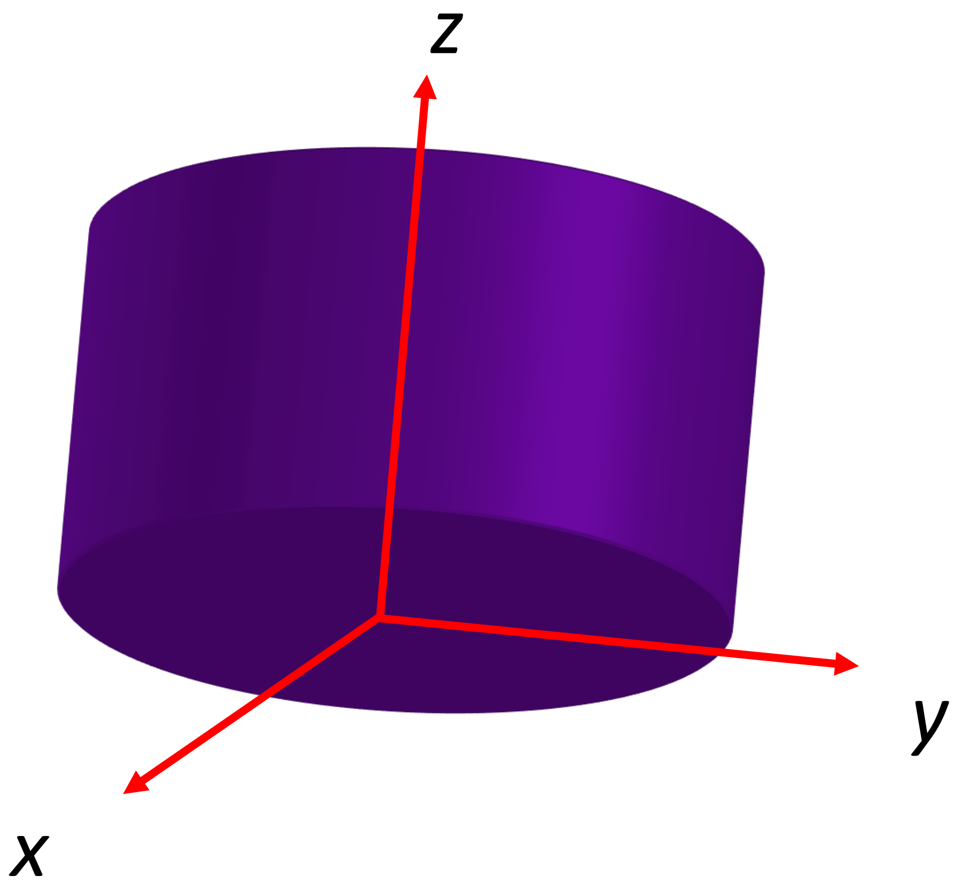
  Note - same physical vector but different values of the components.

- We need to find a relationship between the two sets of components for the vector.

Anisotropy in Composites

- The same methods developed here for describing the anisotropy of single crystals can be applied to composites.
- Anisotropy is important in composites, *not* because of the intrinsic properties of the components but because of the *arrangement* of the components.
- As an example, consider (a) a uniaxial composite (e.g. tennis racket handle) and (b) a flat panel cross-ply composite (e.g. wing surface).

Fiber Symmetry



Fiber Symmetry

- We will use the same *matrix notation* for stress, strain, stiffness and compliance as for single crystals.
- The compliance matrix, **s**, has 5 independent coefficients.

$$\begin{bmatrix} s_{11} & s_{12} & s_{13} & 0 & 0 & 0 \\ s_{12} & s_{11} & s_{13} & 0 & 0 & 0 \\ s_{13} & s_{13} & s_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\left(s_{11} - s_{12}\right) \end{bmatrix}$$

Relationships

- For a uniaxial stress along the z (3) direction,

$$E_3 = \frac{\sigma_3}{\varepsilon_3} = \frac{1}{s_{33}} \left(= \frac{\sigma_{zz}}{\varepsilon_{zz}} \right)$$

- This stress causes strain in the transverse plane: $e_{11} = e_{22} = s_{12}\sigma_{33}$. Therefore we can calculate Poisson's ratio as:

$$\nu_{13} = \frac{e_1}{e_3} = \frac{s_{13}}{s_{33}} \left(= \frac{e_{xx}}{e_{zz}} \right)$$

- Similarly, stresses applied perpendicular to z give rise to different moduli and Poisson's ratios.

$$E_1 = \frac{\sigma_1}{\varepsilon_1} = \frac{1}{s_{11}}, \quad \nu_{21} = \frac{-s_{12}}{s_{11}}, \quad \nu_{31} = \frac{-s_{13}}{s_{11}}$$

Relationships, contd.

- Similarly the torsional modulus is related to shears involving the z axis, i.e. *yz* or *xz* shears:

$$s_{44} = s_{55} = 1/G$$

- Shear in the x-y plane (1-2 plane) is related to the other compliance coefficients:

$$s_{66} = 2(s_{11}-s_{12}) = 1/G_{xy}$$

Plates: Orthotropic Symmetry

- Again, we use the same *matrix notation* for stress, strain, stiffness and compliance as for single crystals.
- The compliance matrix, **s**, has *9 independent coefficients*.
- This corresponds to *othorhombic sample symmetry:* see the following slide with Table from Nye's book.

$$\begin{bmatrix} s_{11} & s_{12} & s_{13} & 0 & 0 & 0 \\ s_{12} & s_{22} & s_{23} & 0 & 0 & 0 \\ s_{13} & s_{23} & s_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{66} \end{bmatrix}$$

Plates: 0° and 90° plies

- If the composite is a laminate composite with fibers laid in at 0° and 90° in equal thicknesses then the symmetry is higher because the x and y directions are equivalent.
- The compliance matrix, **s**, has *6 independent coefficients*.
- This corresponds to (tetragonal) *4mm sample symmetry:* see the following slide with Table from Nye's book.

$$\begin{bmatrix} s_{11} & s_{12} & s_{13} & 0 & 0 & 0 \\ s_{12} & s_{11} & s_{13} & 0 & 0 & 0 \\ s_{13} & s_{13} & s_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{66} \end{bmatrix}$$

Effect of Symmetry on the Elasticity Tensors, S, C

TABLE 9

Form of the (s_{ij}) ***and*** (c_{ij}) ***matrices***

KEY TO NOTATION

- zero component
- non-zero component
- equal components
- components numerically equal, but opposite in sign

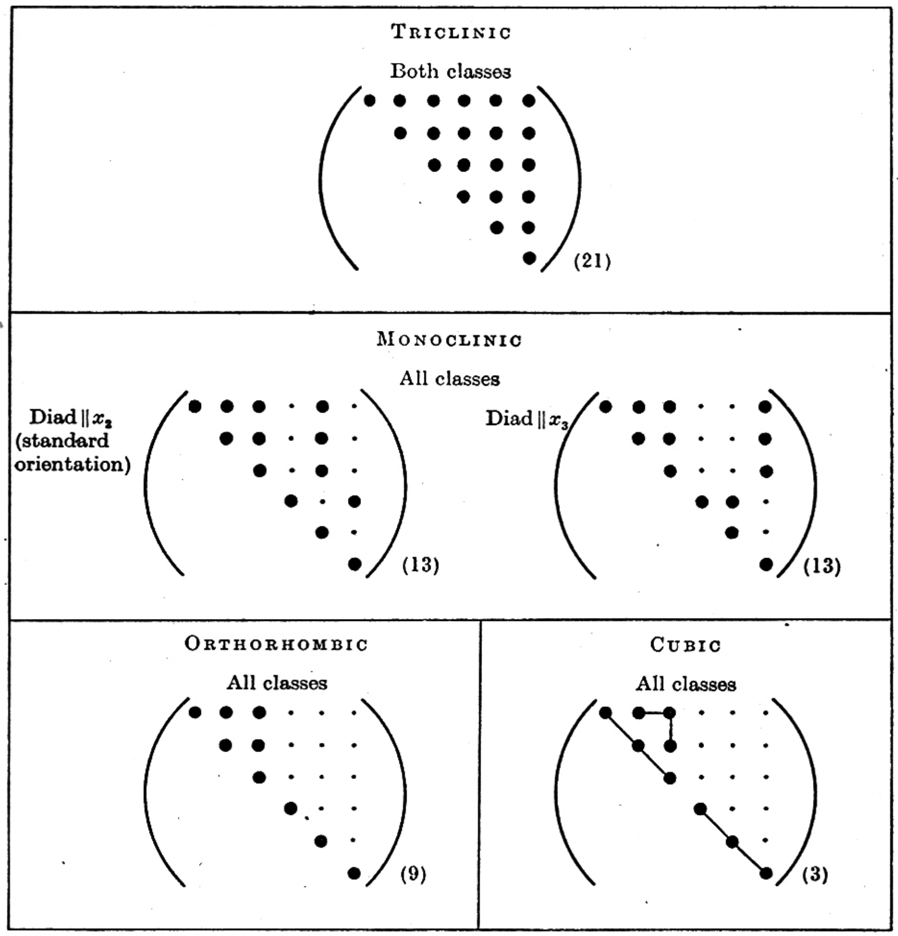
For s — twice the numerical equal of the heavy dot component to which it is joined

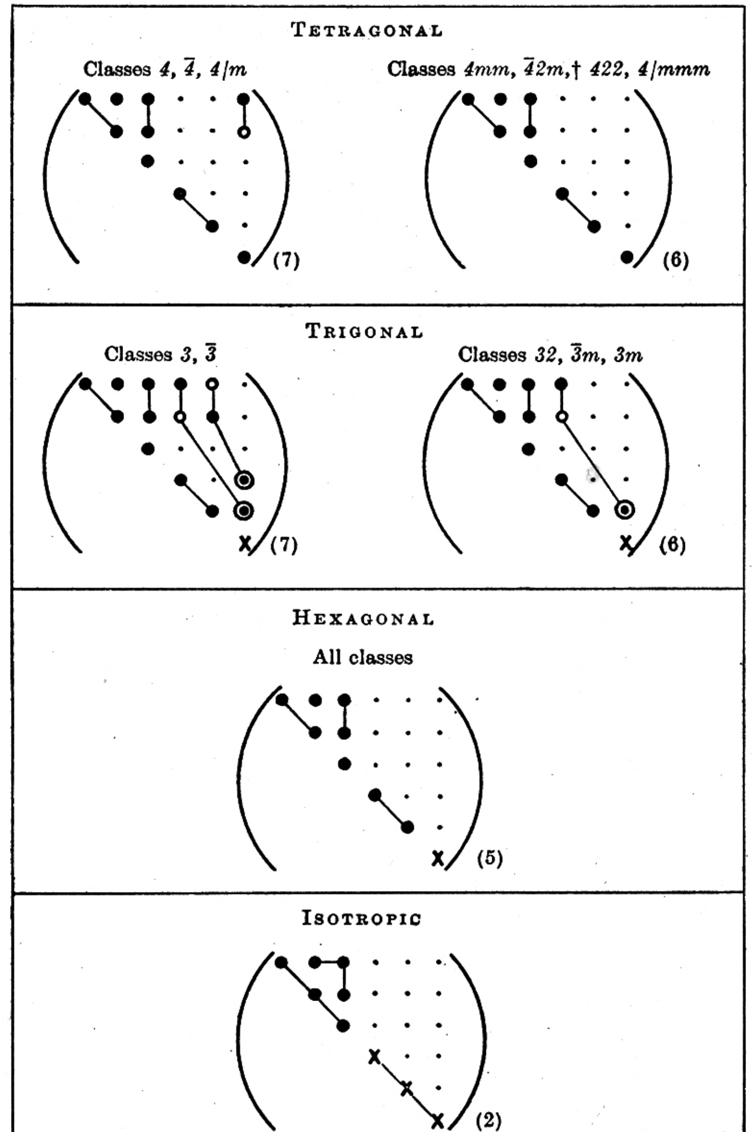
For c — the numerical equal of the heavy dot component to which it is joined

For s — $2(s_{11}-s_{12})$

For c — $\frac{1}{2}(c_{11}-c_{12})$

All the matrices are symmetrical about the leading diagonal.





Lamé constants (isotropic elasticity)

For an elastically isotropic body, there are only 2 elastic moduli, known as the Lamé constants.

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix} = \begin{pmatrix} \lambda + 2G & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda + 2G & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & \lambda + 2G & 0 & 0 & 0 \\ 0 & 0 & 0 & G & 0 & 0 \\ 0 & 0 & 0 & 0 & G & 0 \\ 0 & 0 & 0 & 0 & 0 & G \end{pmatrix} \begin{pmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ 2\epsilon_{23} \\ 2\epsilon_{13} \\ 2\epsilon_{12} \end{pmatrix}$$

This means that, if you know the Lamé constants, then you can obtain the stiffness values thus:

$$C_{11} = \lambda + 2G$$
$$C_{12} = \lambda$$
$$C_{44} = G$$

Stiffnesses in terms of E and ν

$$C_{11} = \frac{E}{(1+\nu)}\left(1+\frac{\nu}{1-2\nu}\right)$$

$$C_{12} = \frac{E}{(1+\nu)}\frac{\nu}{(1-2\nu)}$$

$$C_{44} = \frac{E}{2(1+\nu)}$$

$S_{11} = (C_{11}+C_{12})/\{(C_{11}-C_{12})(C_{11}+2C_{12})\}$
$S_{11} = (\lambda+2G+\lambda) / \{(\lambda+2G-\lambda)(\lambda+2G+2\lambda)\}$
$S_{11} = (\lambda+G) / \{G(2G+3\lambda)\}$

$S_{12} = -C_{12}/\{(C_{11}-C_{12})(C_{11}+2C_{12})\}$
$S_{12} = -\lambda / \{2G(2G+3\lambda)\}$

$S_{44} = 1 / G$

Young's, Bulk moduli, Poisson's ratio

1. Young's modulus : the ratio of longitudinal stress to longitudinal strain under uniaxial normal loading in the longitudinal direction.

$$E = 2G + \frac{G\lambda}{G+\lambda} \qquad E = 2G(1+\nu) => G = \frac{E}{2(1+\nu)}$$

2. Poisson's ratio : minus the ratio of lateral strain to longitudinal strain.

$$2\nu = \frac{\lambda}{\lambda + G} \qquad \nu = \frac{\lambda}{2(\lambda+G)} \qquad \lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}$$

3. Bulk modulus : minus the ratio of pressure to dilatation.

$$K = -\frac{1}{3}\frac{\sigma_{xx}+\sigma_{yy}+\sigma_{zz}}{\epsilon_{xx}+\epsilon_{yy}+\epsilon_{zz}} = \frac{E}{3(1-2\nu)}$$

$\nu = \lambda/2(G+\lambda) => 1-\nu = \{2(G+\lambda) - \lambda\}/2(G+\lambda)$
$1-\nu = \{2G+\lambda)\}/2(G+\lambda)$
$1-2\nu = \{2(G+\lambda) - 2\lambda\}/2(G+\lambda) = G/(G+\lambda)$
$1-(1-2\nu)/(1-2\nu) = \lambda/G$
$2\nu/(1-2\nu) = \lambda/G$
$G\,2\nu/(1-2\nu) = \lambda$
$\lambda = G\,2\nu/(1-2\nu)$
$\lambda = E/\,2\{1+\nu\} * 2\nu/(1-2\nu)$
$\lambda = \nu E/\,\{(1+\nu)\,(1-2\nu)\}$
$\lambda = E/(1+\nu)\,\{\nu/(1-2\nu)\}$

$E = 2\{2G(G+\lambda) + G\lambda\}/2(G+\lambda)$
$E = 2\{2G^2 + 3G\lambda\}/2(G+\lambda)$
$E/\,1-2\nu = 2G\{2G+3\lambda\}\,/\,2G = 2G+3\lambda$
$E/\,1-2\nu = 2G\{2G+3\lambda\}\,/\,2G = 2G+3G\{2\nu/(1-2\nu)\}$
$E/\,1-2\nu = 2G\{1+\nu\}/(1-2\nu)$
$E = 2G\{1+\nu\} => G = E/\,2\{1+\nu\}$

$C_{11} = E/\,\{1+\nu\} + \nu E/\,\{(1+\nu)\,(1-2\nu)\}$
$C_{11} = E\,[1 + (\nu/\,(1-2\nu))]\,/\,\{1+\nu\}$

General Anisotropic Properties

- Many different properties of crystals can be described as tensors.
- The rank of each tensor property depends, naturally, on the nature of the quantities related by the property.

Examples of Materials Properties as Tensors

- Table 1 shows a series of tensors that are of importance for material science. The tensors are grouped by rank, and are also labeled (in the last column) by *E* (equilibrium property) or *T* (transport property). The number following this letter indicates the maximum number of independent, nonzero elements in the tensor, taking into account symmetries imposed by thermodynamics.
- The Field and Response columns contain the following symbols: ΔT = *temperature difference*, ΔS = *entropy change*, E_i = electric field components, H_i = magnetic field components, ε_{ij} = mechanical strain, D_i = electric displacement, B_i = magnetic induction, σ_{ij} = mechanical stress, $\Delta\beta_{ij}$ = change of the impermeability tensor, j_i = electrical current density, $\nabla_j T$ = temperature gradient, h_i = heat flux, $\nabla_j c$ = concentration gradient, m_i = mass flux, $\rho^a{}_i$ = anti-symmetric part of resistivity tensor, $\rho^s{}_i$ = symmetric part of resistivity tensor, $\Delta\rho_{ij}$ = change in the component *ij* of the resistivity tensor, l_i = direction cosines of wave direction in crystal, *G* = gyration constant,

Property	Symbol	Field	Response	Type#
Tensors of Rank 0 (Scalars)				
Specific Heat	C	ΔT	$T\Delta S$	E1
Tensors of Rank 1 (Vectors)				
Electrocaloric	p_i	E_i	ΔS	E3
Magnetocaloric	q_i	H_i	ΔS	E3
Pyroelectric	p'_i	ΔT	D_i	E3
Pyromagnetic	q'_i	ΔT	B_i	E3
Tensors of Rank 2				
Thermal expansion	α_{ij}	ΔT	ϵ_{ij}	E6
Piezocaloric effect	α'_{ij}	σ_{ij}	ΔS	E6
Dielectric permittivity	κ_{ij}	E_j	D_i	E6
Magnetic permeability	μ_{ij}	H_j	B_i	E6
Optical activity	g_{ij}	$l_i l_j$	G	E6
Magnetoelectric polarization	λ_{ij}	H_j	D_i	E9
Converse magnetoelectric polarization	λ'_{ij}	E_j	B_i	E9
Electrical conductivity (resistivity)	$\sigma_{ij}\ (\rho_{ij})$	$E_j\ (j_j)$	$j_i\ (E_i)$	T6
Thermal conductivity	K_{ij}	$\nabla_j T$	h_i	T6
Diffusivity	D_{ij}	$\nabla_j c$	m_i	T6
Thermoelectric power	Σ_{ij}	$\nabla_j T$	E_i	T9
Hall effect	R_{ij}	B_j	ρ_i^a	T9

Tensors of Rank 3				
Piezoelectricity	d_{ijk}	σ_{jk}	D_i	E18
Converse piezoelectricity	d'_{ijk}	E_k	ϵ_{ij}	E18
Piezomagnetism	Q_{ijk}	σ_{jk}	B_i	E18
Converse piezomagnetism	Q'_{ijk}	H_k	ϵ_{ij}	E18
Electro-optic effect	r_{ijk}	E_k	$\Delta\beta_{ij}$	E18
Nernst tensor	Σ_{ijk}	$\nabla_j T B_k$	E_i	T27
Tensors of Rank 4				
Elasticity	s_{ijkl} (c_{ijkl})	σ_{kl} (ϵ_{kl})	ϵ_{ij} (σ_{ij})	E21
Electrostriction	γ_{ijkl}	$E_k E_l$	ϵ_{ij}	E36
Photoelasticity	q_{ijkl}	σ_{kl}	$\Delta\beta_{ij}$	E36
Kerr effect	p_{ijkl}	$E_k E_l$	$\Delta\beta_{ij}$	E36
Magnetoresistance	ξ_{ijkl}	$B_k B_l$	ρ^s_{ij}	T36
Piezoresistance	Π_{ijkl}	σ_{kl}	$\Delta\rho_{ij}$	T36
Magnetothermoelectric power	Σ_{ijkl}	$\nabla_j T B_k B_l$	E_i	T54
Second order Hall effect	ρ_{ijkl}	$B_j B_k B_l$	ρ^2_i	T30
Tensors of Rank 6				
Third order elasticity	c_{ijklmn}	$\epsilon_{kl}\epsilon_{mn}$	σ_{ij}	E56

Courtesy of Prof. M. De Graef

$$
\begin{pmatrix} \Delta S \\ D_x \\ D_y \\ D_z \\ B_x \\ B_y \\ B_z \\ \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{yz} \\ \epsilon_{xz} \\ \epsilon_{xy} \end{pmatrix}
=
\left(\begin{array}{c|ccc|ccc|cccccc}
\frac{C}{T} & p_x & p_y & p_z & q_x & q_y & q_z & \alpha'_{xx} & \alpha'_{yy} & \alpha'_{zz} & \alpha'_{yz} & \alpha'_{xz} & \alpha'_{xy} \\
\hline
p'_x & \kappa_{xx} & \kappa_{xy} & \kappa_{xz} & \lambda_{xx} & \lambda_{xy} & \lambda_{xz} & d_{xxx} & d_{xyy} & d_{xzz} & d_{xyz} & d_{xxz} & d_{xxy} \\
p'_y & \kappa_{yx} & \kappa_{yy} & \kappa_{yz} & \lambda_{yx} & \lambda_{yy} & \lambda_{yz} & d_{yxx} & d_{yyy} & d_{yzz} & d_{yyz} & d_{yxz} & d_{yxy} \\
p'_z & \kappa_{zx} & \kappa_{zy} & \kappa_{zz} & \lambda_{zx} & \lambda_{zy} & \lambda_{zz} & d_{zxx} & d_{zyy} & d_{zzz} & d_{zyz} & d_{zxz} & d_{zxy} \\
\hline
q'_x & \lambda'_{xx} & \lambda'_{xy} & \lambda'_{xz} & \mu_{xx} & \mu_{xy} & \mu_{xz} & Q_{xxx} & Q_{xyy} & Q_{xzz} & Q_{xyz} & Q_{xxz} & Q_{xxy} \\
q'_y & \lambda'_{yx} & \lambda'_{yy} & \lambda'_{yz} & \mu_{yx} & \mu_{yy} & \mu_{yz} & Q_{yxx} & Q_{yyy} & Q_{yzz} & Q_{yyz} & Q_{yxz} & Q_{yxy} \\
q'_z & \lambda'_{zx} & \lambda'_{zy} & \lambda'_{zz} & \mu_{zx} & \mu_{zy} & \mu_{zz} & Q_{zxx} & Q_{zyy} & Q_{zzz} & Q_{zyz} & Q_{zxz} & Q_{zxy} \\
\hline
\alpha_{xx} & d'_{xxx} & d'_{xxy} & d'_{xxz} & Q'_{xxx} & Q'_{xxy} & Q'_{xxz} & s_{xxxx} & s_{xxyy} & s_{xxzz} & s_{xxyz} & s_{xxxz} & s_{xxxy} \\
\alpha_{yy} & d'_{yyx} & d'_{yyy} & d'_{yyz} & Q'_{yyx} & Q'_{yyy} & Q'_{yyz} & s_{yyxx} & s_{yyyy} & s_{yyzz} & s_{yyyz} & s_{yyxz} & s_{yyxy} \\
\alpha_{zz} & d'_{zzx} & d'_{zzy} & d'_{zzz} & Q'_{zzx} & Q'_{zzy} & Q'_{zzz} & s_{zzxx} & s_{zzyy} & s_{zzzz} & s_{zzyz} & s_{zzxz} & s_{zzxy} \\
\alpha_{yz} & d'_{yzx} & d'_{yzy} & d'_{yzz} & Q'_{yzx} & Q'_{yzy} & Q'_{yzz} & s_{yzxx} & s_{yzyy} & s_{yzzz} & s_{yzyz} & s_{yzxz} & s_{yzxy} \\
\alpha_{xz} & d'_{xzx} & d'_{xzy} & d'_{xzz} & Q'_{xzx} & Q'_{xzy} & Q'_{xzz} & s_{xzxx} & s_{xzyy} & s_{xzzz} & s_{xzyz} & s_{xzxz} & s_{xzxy} \\
\alpha_{xy} & d'_{xyx} & d'_{xyy} & d'_{xyz} & Q'_{xyx} & Q'_{xyy} & Q'_{xyz} & s_{xyxx} & s_{xyyy} & s_{xyzz} & s_{xyyz} & s_{xyxz} & s_{xyxy}
\end{array}\right)
\begin{pmatrix} \Delta T \\ E_x \\ E_y \\ E_z \\ H_x \\ H_y \\ H_z \\ \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{pmatrix}
$$

- Principal Effects
- Electrocaloric = pyroelectric
- Magnetocaloric = pyromagnetic
- Thermal expansion = piezocaloric
- Magnetoelectric and converse magnetoelectric
- Piezoelectric and converse piezoelectric
- Piezomagnetic and converse piezomagnetic

Courtesy of Prof. M. De Graef

$$\Delta S = \frac{C}{T}\Delta T + p_i E_i + q_i H_i + \alpha'_{ij}\sigma_{ij};$$

$$D_i = p'_i \Delta T + \kappa_{ij} E_j + \lambda_{ij} H_j + d_{ijk}\sigma_{jk};$$

$$B_i = q'_i \Delta T + \lambda'_{ij} E_j + \mu_{ij} H_j + Q_{ijk}\sigma_{jk};$$

$$\epsilon_{ij} = \alpha_{ij}\Delta T + d'_{ijk} E_k + Q'_{ijk} H_k + s_{ijkl}\sigma_{kl}.$$

Principal Effects

Courtesy of Prof. M. De Graef

1st rank cross effects

2nd rank cross effects

3rd rank cross effects

$$
\begin{pmatrix} \Delta S \\ D_x \\ D_y \\ D_z \\ B_x \\ B_y \\ B_z \\ \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{yz} \\ \epsilon_{xz} \\ \epsilon_{xy} \end{pmatrix}
=
\begin{pmatrix}
\frac{C}{T} & p_x & p_y & p_z & q_x & q_y & q_z & \alpha'_{xx} & \alpha'_{yy} & \alpha'_{zz} & \alpha'_{yz} & \alpha'_{xz} & \alpha'_{xy} \\
p'_x & \kappa_{xx} & \kappa_{xy} & \kappa_{xz} & \lambda_{xx} & \lambda_{xy} & \lambda_{xz} & d_{xxx} & d_{xyy} & d_{xzz} & d_{xyz} & d_{xxz} & d_{xxy} \\
p'_y & \kappa_{yx} & \kappa_{yy} & \kappa_{yz} & \lambda_{yx} & \lambda_{yy} & \lambda_{yz} & d_{yxx} & d_{yyy} & d_{yzz} & d_{yyz} & d_{yxz} & d_{yxy} \\
p'_z & \kappa_{zx} & \kappa_{zy} & \kappa_{zz} & \lambda_{zx} & \lambda_{zy} & \lambda_{zz} & d_{zxx} & d_{zyy} & d_{zzz} & d_{zyz} & d_{zxz} & d_{zxy} \\
q'_x & \lambda'_{xx} & \lambda'_{xy} & \lambda'_{xz} & \mu_{xx} & \mu_{xy} & \mu_{xz} & Q_{xxx} & Q_{xyy} & Q_{xzz} & Q_{xyz} & Q_{xxz} & Q_{xxy} \\
q'_y & \lambda'_{yx} & \lambda'_{yy} & \lambda'_{yz} & \mu_{yx} & \mu_{yy} & \mu_{yz} & Q_{yxx} & Q_{yyy} & Q_{yzz} & Q_{yyz} & Q_{yxz} & Q_{yxy} \\
q'_z & \lambda'_{zx} & \lambda'_{zy} & \lambda'_{zz} & \mu_{zx} & \mu_{zy} & \mu_{zz} & Q_{zxx} & Q_{zyy} & Q_{zzz} & Q_{zyz} & Q_{zxz} & Q_{zxy} \\
\alpha_{xx} & d'_{xxx} & d'_{xxy} & d'_{xxz} & Q'_{xxx} & Q'_{xxy} & Q'_{xxz} & s_{xxxx} & s_{xxyy} & s_{xxzz} & s_{xxyz} & s_{xxxz} & s_{xxxy} \\
\alpha_{yy} & d'_{yyx} & d'_{yyy} & d'_{yyz} & Q'_{yyx} & Q'_{yyy} & Q'_{yyz} & s_{yyxx} & s_{yyyy} & s_{yyzz} & s_{yyyz} & s_{yyxz} & s_{yyxy} \\
\alpha_{zz} & d'_{zzx} & d'_{zzy} & d'_{zzz} & Q'_{zzx} & Q'_{zzy} & Q'_{zzz} & s_{zzxx} & s_{zzyy} & s_{zzzz} & s_{zzyz} & s_{zzxz} & s_{zzxy} \\
\alpha_{yz} & d'_{yzx} & d'_{yzy} & d'_{yzz} & Q'_{yzx} & Q'_{yzy} & Q'_{yzz} & s_{yzxx} & s_{yzyy} & s_{yzzz} & s_{yzyz} & s_{yzxz} & s_{yzxy} \\
\alpha_{xz} & d'_{xzx} & d'_{xzy} & d'_{xzz} & Q'_{xzx} & Q'_{xzy} & Q'_{xzz} & s_{xzxx} & s_{xzyy} & s_{xzzz} & s_{xzyz} & s_{xzxz} & s_{xzxy} \\
\alpha_{xy} & d'_{xyx} & d'_{xyy} & d'_{xyz} & Q'_{xyx} & Q'_{xyy} & Q'_{xyz} & s_{xyxx} & s_{xyyy} & s_{xyzz} & s_{xyyz} & s_{xyxz} & s_{xyxy}
\end{pmatrix}
\begin{pmatrix} \Delta T \\ E_x \\ E_y \\ E_z \\ H_x \\ H_y \\ H_z \\ \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{pmatrix}
$$

General crystal symmetry shown above.

Courtesy of Prof. M. De Graef

$$
\begin{pmatrix} \Delta S \\ D_x \\ D_y \\ D_z \\ B_x \\ B_y \\ B_z \\ \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{yz} \\ \epsilon_{xz} \\ \epsilon_{xy} \end{pmatrix} = \begin{pmatrix}
\frac{C}{T} & p_x & p_x & p_z & q_x & q_x & q_z & \alpha_{xx} & \alpha_{xx} & \alpha_{zz} & 0 & 0 & 0 \\
p_x & \kappa_{xx} & 0 & 0 & \lambda_{xx} & \lambda_{xy} & 0 & 0 & 0 & 0 & d_{xyz} & d_{xxz} & 0 \\
p_x & 0 & \kappa_{xx} & 0 & -\lambda_{xy} & \lambda_{xx} & 0 & 0 & 0 & 0 & -d_{xxz} & d_{xyz} & 0 \\
p_z & 0 & 0 & \kappa_{zz} & 0 & 0 & \lambda_{zz} & d_{zxx} & d_{zxx} & d_{zzz} & 0 & 0 & 0 \\
q_x & \lambda_{xx} & -\lambda_{xy} & 0 & \mu_{xx} & 0 & 0 & 0 & 0 & 0 & Q_{xyz} & Q_{xxz} & 0 \\
q_x & \lambda_{xy} & \lambda_{xx} & 0 & 0 & \mu_{xx} & 0 & 0 & 0 & 0 & -Q_{xxz} & Q_{xyz} & 0 \\
q_z & 0 & 0 & \lambda_{zz} & 0 & 0 & \mu_{zz} & Q_{zxx} & Q_{zxx} & Q_{zzz} & 0 & 0 & 0 \\
\alpha_{xx} & 0 & 0 & d_{zxx} & 0 & 0 & Q_{zxx} & s_{xxxx} & s_{xxyy} & s_{xxzz} & 0 & 0 & s_{xxxy} \\
\alpha_{xx} & 0 & 0 & d_{zxx} & 0 & 0 & Q_{zyy} & s_{xxyy} & s_{xxxx} & s_{xxzz} & 0 & 0 & -s_{xxxy} \\
\alpha_{zz} & 0 & 0 & d_{zzz} & 0 & 0 & Q_{zzz} & s_{xxzz} & s_{xxzz} & s_{zzzz} & 0 & 0 & 0 \\
0 & d_{xyz} & -d_{xxz} & 0 & Q_{xyz} & -Q_{xxz} & 0 & 0 & 0 & 0 & s_{xzxz} & -s_{xzyz} & 0 \\
0 & d_{xxz} & d_{xyz} & 0 & Q_{xxz} & Q_{xyz} & 0 & 0 & 0 & 0 & s_{xzyz} & s_{xzxz} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & s_{xxxy} & -s_{xxxy} & 0 & 0 & 0 & s_{xyxy}
\end{pmatrix} \begin{pmatrix} \Delta T \\ E_x \\ E_y \\ E_z \\ H_x \\ H_y \\ H_z \\ \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{pmatrix}
$$

Point group 4

Courtesy of Prof. M. De Graef

$$
\begin{pmatrix} \Delta S \\ D_x \\ D_y \\ D_z \\ B_x \\ B_y \\ B_z \\ \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{yz} \\ \epsilon_{xz} \\ \epsilon_{xy} \end{pmatrix} = \begin{pmatrix}
\frac{C}{T} & 0 & 0 & 0 & 0 & 0 & 0 & \alpha & \alpha & \alpha & 0 & 0 & 0 \\
0 & \kappa & 0 & 0 & \lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \kappa & 0 & 0 & \lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \kappa & 0 & 0 & \lambda & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \lambda & 0 & 0 & \mu & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \lambda & 0 & 0 & \mu & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \lambda & 0 & 0 & \mu & 0 & 0 & 0 & 0 & 0 & 0 \\
\alpha & 0 & 0 & 0 & 0 & 0 & 0 & s_{xxxx} & s_{xxyy} & s_{xxyy} & 0 & 0 & 0 \\
\alpha & 0 & 0 & 0 & 0 & 0 & 0 & s_{xxyy} & s_{xxxx} & s_{xxyy} & 0 & 0 & 0 \\
\alpha & 0 & 0 & 0 & 0 & 0 & 0 & s_{xxyy} & s_{xxyy} & s_{xxxx} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s_{yzyz} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s_{yzyz} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s_{yzyz}
\end{pmatrix} \begin{pmatrix} \Delta T \\ E_x \\ E_y \\ E_z \\ H_x \\ H_y \\ H_z \\ \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{pmatrix}
$$

Point group m$\bar{3}$m

Note how many fewer independent coefficients there are!
Note how the center of symmetry eliminates many of the properties, such as pyroelectricity

Courtesy of Prof. M. De Graef

Homogeneity

- Stimuli and responses of interest are, in general, not scalar quantities but tensors. Furthermore, some of the properties of interest, such as the plastic properties of a material, are far from linear at the scale of a polycrystal. Nonetheless, they can be treated as linear at a suitably local scale and then an averaging technique can be used to obtain the response of the polycrystal. The local or microscopic response is generally well understood but the validity of the averaging techniques is still controversial in many cases. Also, we will only discuss cases where a homogeneous response can be reasonably expected.
- There are many problems in which a non-homogeneous response to a homogeneous stimulus is of critical importance. Stress-corrosion cracking, for example, is a wildly non-linear, non-homogeneous response to an approximately uniform stimulus which depends on the mechanical and electro-chemical properties of the material.

Use of MuPAD inside Matlab

- Note that the 6x6 transformation matrix can be programmed inside Matlab just as a 3x3 can.
- In order to apply a transformation (e.g. a symmetry operator) to a 6x6 stiffness or compliance matrix, the formula is the same as before, i.e.:

$$C' = O\, C\, O^T$$

Matrix representation of the *rotation point groups*

What is a *group*? A group is a set of objects that form a closed set: if you combine any two of them together, the result is simply a different member of that same group of objects. Rotations in a given point group form closed sets - try it for yourself!

Note: the 3rd matrix in the 1st column (x-diad) is missing a "-" on the 33 element; this is corrected in this slide. Also, in the 2nd from the bottom, last column: the 33 element should be +1, not -1. In some versions of the book, in the last matrix (bottom right corner) the 33 element is incorrectly given as -1; here the +1 is correct.

Kocks, Tomé & Wenk: Ch. 1 Table II

Table II. Symmetry operators of rotation groups

tetragonal branch

			group
1	0	0	
0	1	0	
0	0	1	1
-1	0	0	
0	1	0	
0	0	-1	2
1	0	0	
0	-1	0	
0	0	-1	
-1	0	0	
0	-1	0	
0	0	1	222
0	1	0	
-1	0	0	
0	0	1	
0	-1	0	
1	0	0	
0	0	1	
0	1	0	
1	0	0	
0	0	-1	
0	-1	0	
-1	0	0	
0	0	-1	42

hexagonal branch

			group
1	0	0	
0	1	0	
0	0	1	
-.5	a	0	
-a	-.5	0	
0	0	1	
-.5	-a	0	
a	-.5	0	
0	0	1	3
.5	a	0	
-a	.5	0	
0	0	1	
-1	0	0	
0	-1	0	
0	0	1	
.5	-a	0	
a	.5	0	
0	0	1	6
-.5	-a	0	
-a	.5	0	
0	0	-1	
1	0	0	
0	-1	0	
0	0	-1	
-.5	a	0	
a	.5	0	
0	0	-1	
.5	a	0	
a	-.5	0	
0	0	-1	
-1	0	0	
0	1	0	
0	0	-1	
.5	-a	0	
-a	-.5	0	
0	0	-1	622

a = √3/2

cubic branch

						group
1	0	0	0	0	-1	
0	1	0	0	-1	0	
0	0	1	-1	0	0	
0	0	1	0	0	1	
1	0	0	0	-1	0	
0	1	0	1	0	0	
0	1	0	0	0	1	
0	0	1	0	1	0	
1	0	0	-1	0	0	
0	-1	0	0	0	-1	
0	0	1	0	1	0	
-1	0	0	1	0	0	
0	-1	0	-1	0	0	
0	0	-1	0	0	-1	
1	0	0	0	-1	0	
0	1	0	1	0	0	
0	0	-1	0	0	-1	
-1	0	0	0	1	0	
0	0	-1	1	0	0	
1	0	0	0	0	1	
0	-1	0	0	-1	0	
0	0	-1	-1	0	0	
-1	0	0	0	0	1	
0	1	0	0	1	0	
0	0	1	0	-1	0	
-1	0	0	0	0	-1	
0	-1	0	-1	0	0	
-1	0	0	0	1	0	
0	1	0	-1	0	0	
0	0	-1	0	0	1	
-1	0	0	0	1	0	
0	-1	0	1	0	0	
0	0	1	0	0	-1	
1	0	0	0	-1	0	
0	-1	0	1	0	0	
0	0	-1	0	0	1	23 / 432

The dashed boxes in this column make up group 4.

The dashed boxes in this column make up group 32.

The dashed box in this column comprises the 3-fold axes only.

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