27-301
Microstructure-Properties
Tensors and Anisotropy, Part 3
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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 does it matter?

• Even an apparently simple device such as quartz oscillator is made from a single crystal (of quartz) whose elastic properties are crucial to the device performance.

• The microstructure of wood consists of bundles of elongated cells at the 1-100 µm scale. The cell walls themselves have a strongly aligned microstructure. This means that wood is inevitably a strongly anisotropic material. Engineering with such a material requires quantitative descriptions of its anisotropy.

• Any fiber reinforced composite is anisotropic because the fibers generally have higher modulus than their matrix. The symmetry that applies depends on the way in which the fibers are laid up, e.g. unidirectional versus random in-plane versus woven.

• The bottom line is that many engineering materials at all different length scales are anisotropic (and not just elastically), so the analysis that we do here is needed for quantitative descriptions.

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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 (4th rank) stiffness tensor and the stiffness matrix (6x6)? See the notes for details but, e.g., $\{11,22,33\}_{\text{tensor}}$ correspond to $\{1,2,3\}_{\text{matrix}}$. E.g., $C_{12}(\text{matrix}) = C_{1122}(\text{tensor})$. 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 (2nd 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.

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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\textsuperscript{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 $1/S_{11}$.

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**Notation**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>Stimulus (field)</td>
</tr>
<tr>
<td>R</td>
<td>Response</td>
</tr>
<tr>
<td>P</td>
<td>Property</td>
</tr>
<tr>
<td>j</td>
<td>electric current</td>
</tr>
<tr>
<td>E</td>
<td>electric field</td>
</tr>
<tr>
<td>D</td>
<td>electric polarization</td>
</tr>
<tr>
<td>ε</td>
<td>Strain</td>
</tr>
<tr>
<td>σ</td>
<td>Stress (or conductivity)</td>
</tr>
<tr>
<td>ρ</td>
<td>Resistivity</td>
</tr>
<tr>
<td>d</td>
<td>piezoelectric tensor</td>
</tr>
<tr>
<td>C</td>
<td>elastic stiffness (also k)</td>
</tr>
<tr>
<td>S</td>
<td>elastic compliance</td>
</tr>
<tr>
<td>a</td>
<td>rotation matrix</td>
</tr>
<tr>
<td>W</td>
<td>work done (energy)</td>
</tr>
<tr>
<td>I</td>
<td>identity matrix</td>
</tr>
<tr>
<td>O</td>
<td>symmetry operator (matrix)</td>
</tr>
<tr>
<td>Y</td>
<td>Young’s modulus</td>
</tr>
<tr>
<td>δ</td>
<td>Kronecker delta</td>
</tr>
<tr>
<td>e</td>
<td>axis (unit) vector</td>
</tr>
<tr>
<td>T</td>
<td>tensor</td>
</tr>
<tr>
<td>α</td>
<td>direction cosine</td>
</tr>
</tbody>
</table>

If the stress or strain symbol is written with one index then vector-matrix notation is being used; two indices indicate tensor notation. Similarly 2 indices on S or C denote vector-matrix and 4 denote tensor notation.

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Linear properties

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

\[ R = R_0 + PF \]

or if \( R_0 = 0 \),

\[ R = PF. \]

e.g. elasticity: \( \sigma = C \varepsilon \)

In tension, \( C \equiv Young’s \ modulus, \ Y \) or \( E \).

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Elasticity

- Elasticity: example of a property that requires 4\textsuperscript{th} rank tensors to describe it fully.
- Even in cubic metals, a crystal can be quite anisotropic. The [111] in many cubic metals is stiffer than the [100] direction, although there some where the opposite is true.
- Even in cubic materials, 3 different numbers/coefficients/moduli are required to describe elastic properties; isotropic materials only require 2.
- Familiarity with Miller indices is assumed.
Stress Tensor

Illustration of the action of each stress component on each face of an infinitesimal cubical volume element.

Note how the diagonal components act normal to each face, whereas the shear components exert transverse tractions.

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Elastic Anisotropy: 1

• First we restate the linear elastic relations for the properties Compliance, written $S$, and Stiffness, written $C$ (!), which connect stress, $\sigma$, and strain, $\varepsilon$. 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):

\[
\sigma = C : \varepsilon \\
\varepsilon = S : \sigma
\]

• In component form (with suffixes),

\[
\sigma_{ij} = C_{ijkl} \varepsilon_{kl} \\
\varepsilon_{ij} = S_{ijkl} \sigma_{kl}
\]

• In vector-matrix form (with suffixes, to be explained),

\[
\sigma_i = C_{ij} \varepsilon_j \\
\varepsilon_i = S_{ij} \sigma_j
\]

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**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,

\[ S_{ijkl} = S_{jikl} \]

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

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**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 \( (4^{\text{th}} \) rank) tensor from crystal coordinates to sample coordinates using the orientation (matrix), \( a \) (see parts 1 & 2):

\[
c'_{ijkl} = a_{im} a_{jn} a_{ko} a_{lp} c_{mnop}
\]

- Note how the transformation matrix appears four times because we are transforming a 4th rank tensor!
- The axis transformation matrix, \( a \), is also written as \( \lambda \) in some texts.

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Young’s modulus from compliance

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

\[ E = \frac{1}{s'_{1111}}. \]

• 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,

\[ s'_{ijkl} = a_{im} a_{jn} a_{ko} a_{lp} s_{mnop} \]

which, substituting “1” for i, j, k & l, becomes

\[ s'_{1111} = a_{1m} a_{1n} a_{1o} a_{1p} s_{mnop} \]

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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.

\[
\begin{pmatrix}
\sigma_{11} & \sigma_{12} & \sigma_{13} \\
\sigma_{21} & \sigma_{22} & \sigma_{23} \\
\sigma_{31} & \sigma_{32} & \sigma_{33}
\end{pmatrix}
\quad
\begin{pmatrix}
\sigma_1 \\
\sigma_2 \\
\sigma_3 \\
\sigma_4 \\
\sigma_5 \\
\sigma_6
\end{pmatrix}
\]

\[
\begin{pmatrix}
\sigma_{11} & \sigma_{12} & \sigma_{13} \\
\sigma_{21} & \sigma_{22} & \sigma_{23} \\
\sigma_{31} & \sigma_{32} & \sigma_{33}
\end{pmatrix}
\begin{pmatrix}
\sigma_6 \\
\sigma_2 \\
\sigma_4 \\
\sigma_3 \\
\sigma_5 \\
\sigma_1
\end{pmatrix}
\]

Newnham, Ch. 10

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Voigt or “matrix” notation, contd.

• Similarly for strain:

\[
\begin{pmatrix}
\varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\
\varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\
\varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33}
\end{pmatrix}
\leftrightarrow
\begin{pmatrix}
\frac{1}{2}\varepsilon_{6} & \varepsilon_{2} & \frac{1}{2}\varepsilon_{5} \\
\frac{1}{2}\varepsilon_{5} & \frac{1}{2}\varepsilon_{4} & \varepsilon_{3}
\end{pmatrix}
\leftrightarrow
(\varepsilon_{1}, \varepsilon_{2}, \varepsilon_{3}, \varepsilon_{4}, \varepsilon_{5}, \varepsilon_{6})
\]

The particular definition of shear strain used in the reduced notation happens to correspond to that used in mechanical engineering such that \(\varepsilon_{4}\) 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. Stress and strain are linked (conjugated) because it is their product that gives the energy associated with elastic loading.

\[ dW = \sigma : d\varepsilon = \sigma_{ij} : d\varepsilon_{ij} = \sigma_k \cdot d\varepsilon_k \]

This means that the 6x6 matrix of stiffness coefficients is symmetric, i.e. \( C_{ij} = C_{ji} \). Likewise, \( S_{ij} = S_{ji} \).

• Also we can combine the expressions \( \sigma = C\varepsilon \) and \( \varepsilon = S\sigma \) to give:

\[ \sigma = CS\sigma, \text{ which shows that:} \]
\[ I = CS, \text{ or, } C = S^{-1} \]

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Tensor conversions: stiffness

• Lastly we need a system for converting the tensor coefficients of stiffness and compliance (4 indices) to the matrix coefficients (2 indices). For stiffness, it is very simple because one substitutes values according to the following table, such that \( \text{matrix} C_{11} = \text{tensor} C_{1111} \) for example.

<table>
<thead>
<tr>
<th>Tensor</th>
<th>11</th>
<th>22</th>
<th>33</th>
<th>23</th>
<th>32</th>
<th>13</th>
<th>31</th>
<th>12</th>
<th>21</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>4</td>
<td>5</td>
<td>5</td>
<td>6</td>
<td>6</td>
</tr>
</tbody>
</table>

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(General) 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)

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Tensor conversions: compliance

- For compliance some factors of two are required (by work conjugacy) and so the rule becomes:

\[ pS_{ijkl} = S_{mn} \]

\[ p = 1 \quad m \text{ AND } n \in [1,2,3] \]
\[ p = 2 \quad m \text{ XOR } n \in [1,2,3] \]
\[ p = 4 \quad m \text{ AND } n \in [4,5,6] \]

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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

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Relationships between coefficients: 
\( C \) in terms of \( S \)

- Recall that we stated that the compliance and stiffness tensors are the inverse of each other, or, \( C = S^{-1} \).
- Determining the relationship can be done, but not required here.
- Useful relationships between coefficients for cubic materials are as follows. Symmetrical relationships exist for compliance coefficients in terms of stiffness values (next slide).

\[
C_{11} = \frac{(S_{11}+S_{12})}{(S_{11}-S_{12})(S_{11}+2S_{12})}
\]

\[
C_{12} = \frac{-S_{12}}{(S_{11}-S_{12})(S_{11}+2S_{12})}
\]

\[
C_{44} = \frac{1}{S_{44}}
\]
**S in terms of C**

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

\[
S_{11} = \frac{(C_{11}+C_{12})}{(C_{11}-C_{12})(C_{11}+2C_{12})}
\]

\[
S_{12} = \frac{-C_{12}}{(C_{11}-C_{12})(C_{11}+2C_{12})}
\]

\[
S_{44} = \frac{1}{C_{44}}
\]

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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.
Effect of symmetry on stiffness matrix

- Following Reid, p.66 et seq.:
  Apply a -90° rotation about the crystal-z axis (axis 3)*,

\[
C'_{ijkl} = O_{im} O_{jn} O_{ko} O_{lp} C_{mnop}:
\]

\[
C' = C
\]

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

\[
O^z_4 = \begin{pmatrix}
0 & 1 & 0 \\
-1 & 0 & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

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

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Effect of symmetry, 2

- Using \( P' = P \), we can equate all the coefficients in the 6x6 matrix and find that:
  \[
  C_{11} = C_{22}, \ C_{13} = C_{23}, \ C_{44} = C_{35}, \ C_{16} = -C_{26}, \\
  C_{14} = C_{15} = C_{24} = C_{25} = C_{34} = C_{35} = C_{36} = C_{45} = C_{46} = C_{56} = 0.
  \]

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

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Stiffness matrix, cubic symmetry

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. In fact, one need only apply two successive 90° rotations about two orthogonal axes (e.g., 100 and 010) to demonstrate this result. The number of coefficients decreases to two in the case of isotropic elasticity.

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

Symmetrized 6x6 matrices for other point groups given on next slide.

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<table>
<thead>
<tr>
<th>Crystal Class</th>
<th>Point groups</th>
<th>Elastic moduli tensor</th>
</tr>
</thead>
</table>
| Triclinic          | 1, $\bar{1}$ | \[
\begin{pmatrix}
 k_{11} & k_{12} & k_{13} & k_{14} & k_{15} & k_{16} \\
 k_{12} & k_{22} & k_{23} & k_{24} & k_{25} & k_{26} \\
 k_{13} & k_{23} & k_{33} & k_{34} & k_{35} & k_{36} \\
 k_{14} & k_{24} & k_{34} & k_{44} & k_{45} & k_{46} \\
 k_{15} & k_{25} & k_{35} & k_{45} & k_{55} & k_{56} \\
 k_{16} & k_{26} & k_{36} & k_{46} & k_{56} & k_{66}
\end{pmatrix}
\] |
| Monoclinic         | 2, m, $2/m$  | \[
\begin{pmatrix}
 k_{11} & k_{12} & k_{13} & 0 & 0 & k_{16} \\
 k_{12} & k_{22} & k_{23} & 0 & 0 & k_{26} \\
 k_{13} & k_{23} & k_{33} & 0 & 0 & k_{36} \\
 0 & 0 & 0 & k_{44} & k_{45} & 0 \\
 0 & 0 & 0 & k_{45} & k_{55} & 0 \\
 k_{16} & k_{26} & k_{36} & 0 & 0 & k_{66}
\end{pmatrix}
\] |
| Orthorhombic       | 222, mm2, mmm | \[
\begin{pmatrix}
 k_{11} & k_{12} & k_{13} & 0 & 0 & 0 \\
 k_{12} & k_{12} & k_{12} & 0 & 0 & 0 \\
 k_{13} & k_{13} & k_{13} & 0 & 0 & 0 \\
 0 & 0 & 0 & k_{44} & 0 & 0 \\
 0 & 0 & 0 & 0 & k_{55} & 0 \\
 0 & 0 & 0 & 0 & 0 & k_{66}
\end{pmatrix}
\] |
| Lower Tetragonal   | 4, $\bar{4}$, $4/m$ | \[
\begin{pmatrix}
 k_{11} & k_{12} & k_{13} & 0 & 0 & k_{16} \\
 k_{12} & k_{12} & k_{13} & 0 & 0 & 0 \\
 k_{13} & k_{13} & k_{13} & 0 & 0 & 0 \\
 0 & 0 & 0 & k_{44} & 0 & 0 \\
 0 & 0 & 0 & 0 & k_{44} & 0 \\
 k_{16} & 0 & 0 & 0 & 0 & k_{66}
\end{pmatrix}
\] |
| Upper Tetragonal   | 422, 4mm, 42m, 4/mmm | \[
\begin{pmatrix}
 k_{11} & k_{12} & k_{13} & 0 & 0 & 0 \\
 k_{12} & k_{12} & k_{13} & 0 & 0 & 0 \\
 k_{13} & k_{13} & k_{13} & 0 & 0 & 0 \\
 0 & 0 & 0 & k_{44} & 0 & 0 \\
 0 & 0 & 0 & 0 & k_{44} & 0 \\
 0 & 0 & 0 & 0 & 0 & k_{66}
\end{pmatrix}
\] |
<table>
<thead>
<tr>
<th>Crystal Class</th>
<th>Point groups</th>
<th>Elastic moduli tensor</th>
</tr>
</thead>
</table>
| Lower Trigonal  | $3, \bar{3}$ | \[
\begin{pmatrix}
  k_{11} & k_{12} & k_{13} & k_{14} & k_{15} & 0 \\
  k_{12} & k_{11} & k_{13} & -k_{14} & -k_{15} & 0 \\
  k_{13} & k_{13} & k_{33} & 0 & 0 & 0 \\
  k_{14} & -k_{14} & 0 & k_{44} & 0 & -\sqrt{2}k_{15} \\
  k_{15} & -k_{15} & 0 & 0 & k_{44} & \sqrt{2}k_{14} \\
  0 & 0 & 0 & -\sqrt{2}k_{15} & \sqrt{2}k_{14} & k_{11} - k_{12} \\
\end{pmatrix}
\] |
| Upper Trigonal  | $32, 3m, 3m$ | \[
\begin{pmatrix}
  k_{11} & k_{12} & k_{13} & k_{14} & 0 & 0 \\
  k_{12} & k_{11} & k_{13} & k_{14} & 0 & 0 \\
  k_{13} & k_{13} & k_{33} & 0 & 0 & 0 \\
  k_{14} & -k_{14} & 0 & k_{44} & 0 & 0 \\
  0 & -\sqrt{2}k_{14} & \sqrt{2}k_{14} & k_{11} - k_{12} \\
\end{pmatrix}
\] |
| Lower Hexagonal | $6, \bar{6}, 6/m$ | \[
\begin{pmatrix}
  k_{11} & k_{12} & k_{13} & 0 & 0 & 0 \\
  k_{12} & k_{11} & k_{13} & 0 & 0 & 0 \\
  k_{13} & k_{13} & k_{33} & 0 & 0 & 0 \\
  0 & 0 & 0 & k_{44} & 0 & 0 \\
  0 & 0 & 0 & 0 & k_{44} & 0 \\
  0 & 0 & 0 & 0 & 0 & k_{11} - k_{12} \\
\end{pmatrix}
\] |
| Upper Hexagonal | $622, 6mm, \bar{6}m2, 6/mmm$ | \[
\begin{pmatrix}
  k_{11} & k_{12} & k_{13} & 0 & 0 & 0 \\
  k_{12} & k_{11} & k_{13} & 0 & 0 & 0 \\
  k_{13} & k_{13} & k_{33} & 0 & 0 & 0 \\
  0 & 0 & 0 & k_{44} & 0 & 0 \\
  0 & 0 & 0 & 0 & k_{44} & 0 \\
  0 & 0 & 0 & 0 & 0 & k_{11} - k_{12} \\
\end{pmatrix}
\] |
| Lower Cubic     | $23, m3$     | \[
\begin{pmatrix}
  k_{11} & k_{12} & k_{12} & 0 & 0 & 0 \\
  k_{12} & k_{11} & k_{12} & 0 & 0 & 0 \\
  k_{12} & k_{12} & k_{11} & 0 & 0 & 0 \\
  0 & 0 & 0 & k_{44} & 0 & 0 \\
  0 & 0 & 0 & 0 & k_{44} & 0 \\
  0 & 0 & 0 & 0 & 0 & k_{44} \\
\end{pmatrix}
\] |
| Upper Cubic     | $432, \bar{4}3m, m\bar{3}m$ | \[
\begin{pmatrix}
  k_{11} & k_{12} & k_{12} & 0 & 0 & 0 \\
  k_{12} & k_{11} & k_{12} & 0 & 0 & 0 \\
  k_{12} & k_{12} & k_{11} & 0 & 0 & 0 \\
  0 & 0 & 0 & k_{44} & 0 & 0 \\
  0 & 0 & 0 & 0 & k_{44} & 0 \\
  0 & 0 & 0 & 0 & 0 & k_{44} \\
\end{pmatrix}
\] |

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Summary

- We have covered the following topics:
  - Linear elasticity
  - Stiffness (C) and Compliance (S) tensors
  - Tensor versus vector-matrix notation for stress, strain and elastic tensors, with conversion factors.
  - Effect of symmetry in stress, strain tensors.
  - Elasticity, reduction in number of independent coefficients as example as how to apply (crystal) symmetry.
  - Isotropic elasticity: moduli, Lamé constants

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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 etc.

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Bibliography

- De Graef, M., lecture notes for 27-201.

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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.

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Non-Linear properties, example

- Another important example of non-linear 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, \( n \sim 50 \). The stress is scaled by the \( crss \), and be expressed as either shear stress-shear strain rate [graph], or tensile stress-tensile strain [equation].

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

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**Einstein Convention**

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

  \[ A_i = B_{ij} C_j \]

  \[ A_i = \sum_j B_{ij} C_j \]

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

  \[ A_1 = B_{11} C_1 + B_{12} C_2 + B_{13} C_3 \]

  \[ A_2 = B_{21} C_1 + B_{22} C_2 + B_{23} C_3 \]

  \[ A_3 = B_{31} C_1 + B_{32} C_2 + B_{33} C_3 \]

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Matrix Multiplication

- Take each row of the LH matrix in turn and multiply it into each column of the RH matrix.

- In suffix notation, $a_{ij} = b_{ik}c_{kj}$

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

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

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Properties of Rotation Matrix

- The rotation matrix is an \textit{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 determinant = +1.
- The same applies to columns: in suffix notation -
  \[
  a_{ij}a_{kj} = \delta_{ik}, \quad a_{ji}a_{jk} = \delta_{ik}
  \]

\[
\begin{bmatrix}
  a & b & c \\
  d & e & f \\
  l & m & n
\end{bmatrix}
\]

\[
\begin{align*}
  ad+be+cf &= 0 \\
  bc+ef+mn &= 0
\end{align*}
\]

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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.

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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 an extremely non-linear, non-homogeneous response to an approximately uniform stimulus which depends on the mechanical and electro-chemical properties of the material.
The “RVE”

• In order to describe the properties of a material, it is useful to define a *representative volume element* (RVE) that is large enough to be statistically representative of that region (but small enough that one can subdivide a body).

• For example, consider a polycrystal: how many grains must be included in order for the element to be representative of that point in the material?
Transformations of Stress & Strain Vectors

- It is useful to be able to transform the axes of stress tensors when written in vector form (equation on the left). The table (right) is taken from Newnham’s book. In vector-matrix form, the transformations are:

\[
\begin{align*}
\sigma_i' &= \alpha_{ij} \sigma_j \\
\sigma_i &= \alpha_{ij}^{-1} \sigma'_j \\
\epsilon_i' &= \alpha_{ij} \epsilon_j \\
\epsilon_i &= \alpha_{ij}^T \epsilon'_j
\end{align*}
\]

| Table 10.1 Transformation matrices for stresses and strains written in matrix form |
|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|---------------------------------|
| \((a)\)                         | \((a)\)                         | \((a)\)                         | \((a)\)                         | \((a)\)                         | \((a)\)                         |
| \([\sigma_1']\)                 | \([\sigma_1]\)                 | \([\sigma_2]\)                 | \([\sigma_2]\)                 | \([\sigma_3]\)                 | \([\sigma_3]\)                 |
| \([\sigma_2']\)                 | \([\sigma_3]\)                 | \([\sigma_3']\)                | \([\sigma_4]\)                 | \([\sigma_4']\)                | \([\sigma_5]\)                 |
| \([\sigma_3']\)                 | \([\sigma_4]\)                 | \([\sigma_4']\)                | \([\sigma_5]\)                 | \([\sigma_5']\)                | \([\sigma_6]\)                 |
| \([\sigma_4']\)                 | \([\sigma_5]\)                 | \([\sigma_5']\)                | \([\sigma_6]\)                 | \([\sigma_6']\)                |                                |

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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.:

\[ C' = O C O^T \]