Physical properties in MTEX, current status and future developments

Chemnitz MTEX Workshop 9-13 February 2015
Technische Universität Chemnitz, Germany

David Mainprice

(Géosciences Montpellier, Université de Montpellier, France)

CNRS - Université de Montpellier, 34095 Montpellier, France
Plan of this talk, is there a plan?

- A brief resumé of what I do …sometimes
- Single crystal introduction tensor basics – starting with 2\textsuperscript{nd} rank tensors
- Single crystal elasticity tensor basics – Young’s modulus to wave propagation
- Effective media: average properties for polycrystalline aggregates, Voigt, Reuss and Hill…
- Future developments 1; Self-consistent (SC) and Differential Effective Media (DEM), FFT methods
- Future developments 2; Importing single crystal tensors from a database, advantages and pitfalls
- Future developments 3; What are we going to do this afternoon?
A brief resumé of what I do …sometimes
What do I do?
Atomic Modelling & Experimentation at high P & T

- Atomic Modelling
- Experimentation
- Plasticity Modelling
- Crystal Preferred Orientation
- Elastic Tensors
- Seismology

- Slip Systems
- CRSS
- Multi-anvil 1400°C 16 GPa
- Paterson Press 0.3 GPa
- EBSD
- Geodynamics
- P<10^{-4} GPa

Sylvie Demouchy
Shear Wave Splitting

http://garnero.asu.edu
Mantle & Core: petrology & seismic anisotropy

Mainprice (2007)

Bottom up science: starting at the innercore
Innercore anisotropy
from the group of Arwen Deuss in Cambridge

Lythgoe et al. (2014)
Early of days innercore experiments and ab initio models

0° = c-axis
90° = basal plane for *ab initio* models
MTEX Reference papers on physical properties

http://mtex-toolbox.github.io/publications.html

Reference Publications

If you are using the library for your research, please cite this homepage with the following sample BibTeX entry.

2014


2011

Single crystal introduction tensor basics – starting with 2\textsuperscript{nd} rank tensors
Why are we interested in Single Crystals?

• To understand the anisotropic physical properties of polycrystalline rocks caused by crystal preferred orientation (CPO) it is important to know the about the simplest case, the single crystal.

• The single orientation (single crystal), has a perfectly defined ODF (orientation distribution function), PFs (pole figure) or IPFs (inverse pole figure).

• To understand the how crystal symmetry, sample symmetry, CPO and single crystal properties combined to produce anisotropic rock properties …
Physical properties of crystals

- Thermal conductivity and diffusivity (2<sup>th</sup> rank tensor) \( \rightarrow \) can be calculated from CPO
- Thermal expansion (2<sup>th</sup> rank tensor) \( \rightarrow \) can be calculated from CPO
- Electrical conductivity, electrical polarization and dielectric properties) \( \rightarrow \) can be calculated from CPO, BUT may not be relevant if conductivity controlled by high conductivity phases in the grain boundaries (e.g. water or carbon)
- Piezoelectricity (3<sup>rd</sup> rank tensor) \( \rightarrow \) can be calculated from CPO, if we can determine the CPO of the Left- and Right-handed crystals...

- Elasticity (4<sup>th</sup> rank tensor) \( \rightarrow \) seismic (elastic) properties, can be calculated from CPO
Anisotropic Properties

Calcite optical properties: 2nd Rank Tensor
Why are we interested in tensors of single Crystals?

• To understand the anisotropic physical properties of polycrystalline materials caused by crystal preferred orientation (CPO) or Texture it is important to know the about the simplest case, the single crystal.

• The single orientation (single crystal), has a perfectly defined ODF (orientation distribution function), PFs (pole figure) or IPFs (inverse pole figure).

• To understand the how crystal symmetry, sample symmetry, CPO or Texture and single crystal properties combined to produce anisotropic rock properties …
Thermodynamically reversible changes

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

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

where \( S_{ijkl} \) are the elastic compliance, \( d_{kij} \) piezo-electric, \( q_{lij} \) piezo-magnetic and \( \alpha_{ij} \) thermal expansion tensors.

A) Heckmann (1925) introduced a triangular diagram
B) 4 variables choses from triangular diagram at constant entropy (s) and temperature (T)
# Tensor rank of physical properties

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

- We shall only discuss tensors defined in *Cartesian orthogonal right-handed* reference frame.
- Cartesian (orthonormal or orthogonal) reference frame comprising of 3 unit vectors, with axes that we label X1, X2 and X3 e.g. Nye’s book 1957 or x,y,z in MTEX.
- The use of an *orthogonal reference frame* avoids the complications of the metric associated with the crystal unit cell axes a,b,c as a reference frame for tensors, in any case almost all measurements of single crystal properties use this convention.
- We will also restrict ourselves to linear physical properties that are properties than can be described by linear relation between cause and effect, such as *stress and strain for linear elasticity*, where derivatives of the property are restricted to first order of a Taylor expansion series.
- The definition of tensor requires that it obey the linear orthogonal transformation laws for Cartesian tensors describing physical properties of a crystal when it is rotated.
Typical choices for tensor reference frames

<table>
<thead>
<tr>
<th>Crystal Symmetry</th>
<th>x</th>
<th>y</th>
<th>z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orthorhombic, tetragonal, cubic</td>
<td>a</td>
<td>b</td>
<td>c</td>
</tr>
<tr>
<td>Trigonal, hexagonal</td>
<td>a</td>
<td>m</td>
<td>c</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>a*</td>
<td>b</td>
<td>c</td>
</tr>
<tr>
<td>Triclinic</td>
<td>a*</td>
<td>z x z</td>
<td>c*</td>
</tr>
</tbody>
</table>

For Monoclinic and Triclinic, the starred axes represent rotation axes.
Cartesian Tensors II

• Note it is a fundamental concept for tensors of physical properties *that the magnitude physical property does not change* (i.e. it is invariant) with the rotation of the co-ordinate frame, which is attached to the crystal.

• The crystal may rotate in the sample (external) reference frame, but the tensor reference frame is related to the crystal structure and rotates with the crystal, like a rigid body, in other words it is a co-ordinate transform.
Table 1. Linear orthogonal transformation laws for Cartesian tensors

<table>
<thead>
<tr>
<th>Name</th>
<th>Rank</th>
<th>New orientation in terms of old</th>
<th>Old orientation in terms of new</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scalar</td>
<td>0</td>
<td>( S' = S )</td>
<td>( S = S' )</td>
</tr>
<tr>
<td>Vector</td>
<td>1</td>
<td>( \mathbf{V}'<em>i = \mathbf{R}</em>{ij} \mathbf{V}_j )</td>
<td>( \mathbf{V}<em>i = \mathbf{R}</em>{ji} \mathbf{V}'_j )</td>
</tr>
<tr>
<td>2(^{nd}) rank Tensor</td>
<td>2</td>
<td>( \mathbf{T}'<em>{ij} = \mathbf{R}</em>{ik} \mathbf{R}<em>{j} \mathbf{T}</em>{kl} )</td>
<td>( \mathbf{T}<em>{ij} = \mathbf{R}</em>{kj} \mathbf{R}<em>{ij} \mathbf{T}'</em>{kl} )</td>
</tr>
<tr>
<td>3(^{rd}) rank Tensor</td>
<td>3</td>
<td>( \mathbf{T}'<em>{ijk} = \mathbf{R}</em>{il} \mathbf{R}<em>{jm} \mathbf{R}</em>{kn} \mathbf{T}_{lmn} )</td>
<td>( \mathbf{T}<em>{ijk} = \mathbf{R}</em>{il} \mathbf{R}<em>{mj} \mathbf{R}</em>{nk} \mathbf{T}'_{lmn} )</td>
</tr>
<tr>
<td>4(^{th}) rank Tensor</td>
<td>4</td>
<td>( \mathbf{T}'<em>{ijkl} = \mathbf{R}</em>{im} \mathbf{R}<em>{jn} \mathbf{R}</em>{ko} \mathbf{R}<em>{lp} \mathbf{T}</em>{mnop} )</td>
<td>( \mathbf{T}<em>{ijkl} = \mathbf{R}</em>{mj} \mathbf{R}<em>{nj} \mathbf{R}</em>{ok} \mathbf{R}<em>{pi} \mathbf{T}'</em>{mnop} )</td>
</tr>
</tbody>
</table>

\( S = \text{scalar}, \, \mathbf{V} = \text{vector}, \, \mathbf{T} = \text{tensor} \). \( \mathbf{T}'_{ij} \) is the new orientation of the tensor and \( \mathbf{T}_{ij} \) the old orientation.

The rotation or transformation matrix \( \mathbf{R}_{ij} \) used to calculate the tensor in new orientation is replaced by its transpose \( \mathbf{R}_{ji} \) to calculate the old orientation.

Cartesian tensors have orthogonal reference axes (labelled \( x, y \) and \( z \) in MTEX)
Representing single crystal properties

```matlab
%%
% Plot thermal conductivity tensor (W/m/K units)
%******************************************************************************
plot(k,'complete');
colorbar
% annotate with tensor orthogonal axes X1,X2 and X3
hold on
plot([xvector,yvector,zvector],'data',{X1,'X2','X3'},'backgroundcolor','w');
hold off
% save plot as *.png file
savefigure('Plot_Orthoclase_Single_Crystal_TC_Quadric.png');
```
% Plot rotated thermal conductivity tensor (W/m/K units)
% define rotation
G = orientation('Euler', 10*degree, 20*degree, 30*degree, cs_tensor);
% rotate tensor
k_rot = rotate(k, G);
% plot
plot(k_rot, 'complete');
colorbar

% annotate with tensor orthogonal axes X1, X2 and X3
hold on
plot([xvector, yvector, zvector], 'data', {'X1', 'X2', 'X3'}, 'backgroundcolor', 'w');
hold off
% save plot as *.png file
savefigure('Plot_Orthoclase_Single_Crystal_TC_Quadric_rot.png');
2\textsuperscript{nd} Rank Tensors - important for geophysics

- Typically relates 2 vectors – for example thermal conductivity: applied vector (negative) temperature gradient and resulting vector heat flow density, exception thermal expansion relates temperature (0) and strain (2).

- The generic 2\textsuperscript{nd} rank tensor $T$ is the relation between an applied vector $p$ and resultant vector $q$. We can write relation between $p$ and $q$ as a tensor equation

$$p = T q \quad \text{or} \quad p_i = T_{ij} q_j \quad (i=1,2,3 ; j=1,2,3)$$

- In general the vectors $p$ and $q$ are not parallel.
Difference between a transformation matrix \( R_{ij} \) and a 2\(^{nd}\) rank tensor \( T_{ij} \)

\( R_{ij} \) is an 3 by 3 matrix relating two (right-handed) reference frames [orthogonal matrix \( R^t R = R R^t = I \), \( R^t = R^{-1} \) and \( \text{Det}(R) = +1 \) where the rows and columns are orthogonal (orthonormal) unit vectors.] (e.g. rotation or orientation matrix) N.B. when \( R_{ij} \) is relating right-handed to left-handed reference frames \( \text{Det}(R) = -1 \).

\( T_{ij} \) is a physical quantity (e.g. 2\(^{nd}\) rank tensor) that for a given set of reference axes is represented by 9 numbers (a 3 by 3 table).
The representation **quadric** for 2\(^{nd}\) Rank Tensors

Geometrical representation of symmetrical second-rank tensors as a second-degree surface (called a **quadric**). The quadric may be an ellipsoid or a hyperboloid. Most common second-rank tensors are symmetric (\(T_{ij} = T_{ji}\)) and when the 3 principal coefficients are all positive then the property is represented by an ellipsoid with axes \(1/\sqrt{T_1}\), \(1/\sqrt{T_2}\) and \(1/\sqrt{T_3}\), which is the case for electric polarization, electrical and thermal conductivity and optical properties.
The representation **hyperboloid** for 2\(^{nd}\) Rank Tensors

If **one** of the principal coefficients is **negative** then surface is a hyperboloid of one sheet (e.g. thermal expansion of plagioclase feldspar). If **two** of the principal coefficients are **negative** then surface is a hyperboloid of two sheets or caps, this the case for the thermal expansion of calcite with contraction the basal plane. If all three of the principal coefficients are negative then surface is an imaginary ellipsoid, this is the case for many susceptibilities of paramagnetic and diamagnetic minerals, such as quartz, calcite and aragonite.
Radius-normal property of the representation quadric

\[ \frac{1}{\sqrt{r_{33}}} \]
\[ \frac{1}{\sqrt{r_{11}}} \]

\( q \) = heat flux  \( \Delta T \) = thermal gradient

Thermal Resistivity \((r)\)
\[ \Delta T_i = - r_{ij} q_j \]

Thermal Conductivity \((k)\)
\[ q_i = - k_{ij} \Delta T_i \]

where \( r_{11} = 1/k_{11} \) etc
The stimulus vector and response vectors for 2\textsuperscript{nd} rank tensors

In general in anisotropic crystals the stimulus vector (e.g. \( \Delta T \)) is not parallel to the response vector (e.g. \( q \))

\[
\theta \\
r = \Delta T \cos \theta / q
\]

In certain directions (e.g. principal axes) the stimulus vectors and the response vectors may be parallel in anisotropic crystals. It is always the case for isotropic crystals (e.g. 2nd rank tensors of cubic crystals)
Fundamental concept for tensors

1. Physical properties are anisotropic when the applied tensor is not aligned with resultant tensor.

2. Physical properties are isotropic when the applied tensor is aligned with resultant tensor for all directions.

3. In specific directions in an anisotropic crystal, the applied and resultant tensor may be aligned giving rise to local isotropic or pseudo-isotropic behaviour.
Effect of symmetry on Physical Properties: Neumann’s Principle

F.E. Neumann’s principle (1885) states that “symmetry elements of any physical property of a crystal must include ALL the symmetry elements of the point group of the crystal”. This implies that a given physical property may possess a higher symmetry than that possessed by the crystal and it cannot be of a lower symmetry than that of the crystal. Some physical properties are inherently centrosymmetric (all symmetric second order tensors and elasticity) which will add a center of symmetry in many minerals (e.g. quartz) and result in a higher symmetry than the possessed by the crystal.
### Symmetric 2nd rank tensors for all crystal symmetries

<table>
<thead>
<tr>
<th>Crystal Symmetry (Independent constants)</th>
<th>Symmetry and tensor axes</th>
<th>Tensor</th>
</tr>
</thead>
</table>
| Cubic (1)                               | Isotropic                | \[
\begin{bmatrix}
T_{11} & 0 & 0 \\
0 & T_{11} & 0 \\
0 & 0 & T_{11}
\end{bmatrix}
\] |
| Hexagonal (2)                           | 6-fold // z              | \[
\begin{bmatrix}
T_{11} & 0 & 0 \\
0 & T_{11} & 0 \\
0 & 0 & T_{33}
\end{bmatrix}
\] |
| Trigonal on hexagonal axes (2)          | 3-fold // z              |        |
| Tetragonal (2)                          | 4-fold // z              |        |
| Orthorhombic (3)                        | 2-fold // x              | \[
\begin{bmatrix}
T_{11} & 0 & 0 \\
0 & T_{22} & 0 \\
0 & 0 & T_{33}
\end{bmatrix}
\] |
|                                        | 2-fold // y              |        |
|                                        | 2-fold // z              |        |
| Mononclinic (4)                         | 2-fold // y              | \[
\begin{bmatrix}
T_{11} & 0 & T_{13} \\
0 & T_{22} & 0 \\
T_{13} & 0 & T_{33}
\end{bmatrix}
\] |
| Triclinic (6)                           | x, y & z in arbitrary orientations | \[
\begin{bmatrix}
T_{11} & T_{12} & T_{13} \\
T_{12} & T_{22} & T_{23} \\
T_{13} & T_{23} & T_{33}
\end{bmatrix}
\] |
Thermal expansion of calcite

3D plot
%***************************************************************************
% Step 1 : Define the tensor reference frame for Calcite
%***************************************************************************
cs_tensor = crystalSymmetry('3m1', 4.9896, 4.9896, 17.0610,...
[90, 90, 120]*degree,'mineral','calcite','x||a','z||c');
%***************************************************************************
% Step 2 : Import 2nd rank tensor as 3 by 3 matrix M
%***************************************************************************
% Thermal expansion Tensor for Calcite given by Fei (1995) AGU Bookshelf
% Series Mineral Physics vol.2 Chapter 6 Thermal expansion
% in x 10^-6 1/K units
% a11=-3.20 a12=0.00 a13=0.00
% a21=0.00 a22=-3.20 a23=0.00
% a33=0.00 a32=0.00 a33=13.3
%
% Enter tensor as matrix,M, line by line.
% M = [ [-3.20 0.00 0.00 ]; ...
%       [ 0.00 -3.20 0.00 ]; ...
%       [ 0.00 0.00 13.30 ]];
% Define tensor object with MTEX command tensor
% for the alpha(ij) thermal expansion with units x10^-6 1/K
% alpha_calcite = tensor(M,'name','thermal expansion','unit','x10^-6
% 1/K',cs_tensor)
%***************************************************************************
% Step 3 : Plot thermal expansion tensor of calcite
%***************************************************************************
% Create list of crystallographic directions
List = [Miller(2,-1,-1,0,cs_tensor,'UVTW'),...
        Miller(0,1,-1,0,cs_tensor,'UVTW'),...
        Miller(0,0,0,1,cs_tensor,'UVTW')]
% plot 2nd rank tensor
plot(alpha_calcite,'complete')
colorbar
% annotate with crystal directions
hold on
plot(List,'labeled')
hold off
% save plot as *.pdf file
saveFigure('Plot_Calcite_Single_Crystal_alpha_tensor.pdf')
Single crystal thermal expansion – effect of symmetry

\( \alpha \)-Quartz (trigonal -3m)

Diopside (monoclinic 12/m1)

Bytownite An76 (triclinic -1)

Forsterite (orthogonal mmm)
Optical properties - olivine

**Figure 4.2.3-8:** Left: (A) Variation of interference colour in differently oriented forsterite grains; (B) to (D) Decreasing interference colours at wedging-out edges of sections of forsterite grains that have different orientation in thin section. Right: Determination of birefringence using crystal thickness and interference colour; example of forsterite grain (D).

M.M. Raith, P. Raase, J. Reinhardt (2011)
Guide To Thin Section Microscopy.
e-book ISBN 978-3-00-033606-5 (PDF) – it is free!
Olivine – refractive index and retardation in MTEX

Refactive index

Retardation (nm): Michel Levy colours
Single crystal elasticity tensor basics – Young’s modulus to wave propagation
4th Rank Tensors - important for geophysics

- In any crystalline material there is balance between **Coulomb attractive** forces between oppositely charge ions and **Born repulsive** forces due to the overlap of electron shells. At any given thermodynamic state the crystal will tend toward an equilibrium structure.

- For a change in hydrostatic or non-hydrostatic stress, the crystal structure will adjust at the atomic level to the new **thermodynamic state**.

- The fundamental nature of atomic forces in the determination of elastic properties has been illustrated by the emergence of **first principles atomic modeling** to predict single crystal elastic tensors of geophysical importance at **very high PT conditions** of interior of planets.
Elastic (small linear) Strains

Typical stress-strain relation for a solid material.
Hooke’s Law

\[ \sigma = c \varepsilon \quad \text{and} \quad \varepsilon = s \sigma \]

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

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

or

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

i,j,k,l can have the values 1,2 or 3
so \( 3 \times 3 \times 3 \times 3 = 3^4 = 81 \) coefficients.

But due to the symmetry of the deformation and stress tensors the 81 coefficients are not independent. In addition thermodynamic considerations of the crystal energy also reduce the number of independent coefficients. In Voigt notation we can write the \( C_{ijkl} \) tensor as 6 by 6 symmetric tensor \( C_{ij} \) with 21 independent values for a triclinic crystal.
81 elastic constants 9 x 9

- If stress and strain were NOT symmetric
- 9 values of stress and strain

\[
\begin{bmatrix}
\sigma_{11} & \sigma_{22} & \sigma_{33} & \sigma_{12} & \sigma_{31} & \sigma_{13} & \sigma_{21}
\end{bmatrix}
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} & c_{14} & c_{15} & c_{16}
c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} & c_{24} & c_{25} & c_{26}
c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} & c_{34} & c_{35} & c_{36}
c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} & c_{44} & c_{45} & c_{46}
c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} & c_{55} & c_{56} & c_{56}
c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} & c_{56} & c_{66} & c_{66}
c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} & c_{44} & c_{45} & c_{46}
c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} & c_{55} & c_{56} & c_{56}
c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} & c_{56} & c_{66} & c_{66}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
\varepsilon_{31} \\
\varepsilon_{12} \\
\varepsilon_{32} \\
\varepsilon_{13} \\
\varepsilon_{21}
\end{bmatrix}
\]
Stress and Strain Tensors

• Both symmetric for small linear elastic strains

• 6 Independent values \( ij = ji \) (not 9 because \( ij \neq ji \))
\[ \sigma_{ij} = C_{ijkl} \varepsilon_{kl} \]

- \( C_{ijkl} = (\partial \sigma_{ij} / \partial \varepsilon_{kl}) \) and \( S_{ijkl} = (\partial \varepsilon_{ij} / \partial \sigma_{kl}) \)
- Stress tensor \( \sigma_{ij} = \sigma_{ji} \) hence \( C_{ijkl} = C_{jikl} \)
- Strain tensor \( \varepsilon_{kl} = \varepsilon_{lk} \) hence \( C_{ijkl} = C_{ijlk} \)
- The elastic constants can be expressed as a function of the crystal energy per unit volume of crystal (\( U \)) as
  \[ C_{ijkl} = (\partial^2 U / \partial \varepsilon_{ij} \partial \varepsilon_{kl}) \]
  where the strains \( \partial \varepsilon_{ij} \) and \( \partial \varepsilon_{kl} \) can be inter-changed, hence \( C_{ijkl} = C_{klij} \)

Life was not meant to be easy in elasticity!
21 independent elastic constants
6 x 6 symmetric tensor

- Stress and strain tensor are symmetric
- 6 values of stress and strain
- The strains $\partial \varepsilon_{ij}$ and $\partial \varepsilon_{kl}$ are inter-changable
Uniaxial tensile (or compressive) stress. Poisson’s ratio, \( v \), is the ratio of transverse to axial strain. Dashed lines represent initial stress-free shape: a cube of edge length \( l_0 \).

**Poisson’s ratio**, \( v \), another elastic constant, is the ratio of transverse to axial strain

\[
v = \frac{-\varepsilon_y}{\varepsilon_z}
\]
Auxetic behaviour – negative Poisson’s ratio

At low strain the Poisson’s ratio is 0.2, nearly zero – ideal to pushing into the bottle, or even better drawing it out! At high strains, beware the Poisson’s ratio can become negative -0.01 and the cork is impossible to pull out without braking it!

The Voigt Notation

Voigt

\( p, q = 1 \text{ to } 6 \)

Tensors

\( i, j, k, l = 1 \text{ to } 3 \)

Matrix \((p,q)\)

\[
\begin{array}{cccccc}
1 & 2 & 3 & 4 & 5 & 6 \\
\end{array}
\]

Tensor \((ij \text{ or } kl)\)

\[
\begin{array}{cccccc}
11 & 22 & 33 & 23 \text{ or } 32 & 31 \text{ or } 13 & 12 \text{ or } 21 \\
\end{array}
\]

\[
\sigma_{ij} = \begin{bmatrix}
\sigma_{11} & \sigma_{12} & \sigma_{13} \\
\sigma_{12} & \sigma_{22} & \sigma_{23} \\
\sigma_{13} & \sigma_{23} & \sigma_{33}
\end{bmatrix} \Rightarrow \sigma_i = \begin{bmatrix}
\sigma_1 & \sigma_6 & \sigma_5 \\
\sigma_6 & \sigma_2 & \sigma_4 \\
\sigma_5 & \sigma_4 & \sigma_3
\end{bmatrix}
\]

\[
\varepsilon_{ij} = \begin{bmatrix}
\varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\
\varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\
\varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33}
\end{bmatrix} \Rightarrow \varepsilon_i = \begin{bmatrix}
\varepsilon_1 & \varepsilon_{6/2} & \varepsilon_{5/2} \\
\varepsilon_{6/2} & \varepsilon_2 & \varepsilon_{4/2} \\
\varepsilon_{5/2} & \varepsilon_{4/2} & \varepsilon_3
\end{bmatrix}
\]

Life was not meant to be easy in elasticity!
The Voigt Notation 2

In addition we need to introduce factors of 2 and 4 into the equations relating compliance in tensor and matrix notations due the factor of 2 due to shear strain tensor $\varepsilon \rightarrow$ shear strain matrix $\varepsilon/2$.

$S_{ijkl} = S_{pq} \quad \text{for } p=1,2,3 \text{ and } q = 1,2,3$

$2S_{ijkl} = S_{pq} \quad \text{for either } p= \text{ or } q = 4,5,6$

$4S_{ijkl} = S_{pq} \quad \text{for either } p= \text{ and } q = 4,5,6$

However

$C_{ijkl} = C_{pq}$

for all $i,j,k,l$ and all $p$ and $q$ (for $i,j,k,l = 1,2,3$ and $p,q = 1$ to $6$)

**Transformation law**

$p = \delta ij.i + (1-\delta ij)(9-i-j)$

$q = \delta kl.k + (1-\delta kl)(9-k-l)$

with the Kronecker delta , $\delta ij = 0$ when $i \neq j$ and $\delta ij = 1$ when $i=j$

Life was not meant to be easy in elasticity!
Crystal symmetry classes and their Elastic tensors

<table>
<thead>
<tr>
<th>Cubic (3) 23, m3, 432, 43m, m3m</th>
<th>Hexagonal (5) 6, 6̅, 6/m, 622, 6mm, 6̅2m, 6/mmm</th>
<th>Orthorhombic (9) 222, mm2, mmm</th>
<th>Monoclinic (13) 2, m, 2/m</th>
</tr>
</thead>
</table>
| \[
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\
c_{12} & c_{13} & c_{13} & 0 & 0 & 0 \\
c_{13} & c_{13} & c_{13} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & c_{44}
\end{bmatrix}
\] | \[
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\
c_{12} & c_{12} & c_{13} & 0 & 0 & 0 \\
c_{13} & c_{13} & c_{13} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{2}(c_{11}-c_{12})
\end{bmatrix}
\] | \[
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\
c_{12} & c_{22} & c_{23} & 0 & 0 & 0 \\
c_{13} & c_{23} & c_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{55} & 0 \\
0 & 0 & 0 & 0 & 0 & c_{66}
\end{bmatrix}
\] | \[
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\
c_{12} & c_{22} & c_{23} & 0 & 0 & 0 \\
c_{13} & c_{23} & c_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{46} & 0 \\
0 & 0 & 0 & 0 & 0 & c_{66}
\end{bmatrix}
\] |

<table>
<thead>
<tr>
<th>Trigonal (6) 32, 3m, 3̅m</th>
<th>Triclinic (21) 1, (\overline{1})</th>
</tr>
</thead>
</table>
| \[
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\
c_{12} & c_{11} & c_{13} & -c_{14} & 0 & 0 \\
c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\
c_{14} & -c_{14} & 0 & c_{44} & c_{44} & c_{14} \\
0 & 0 & 0 & 0 & c_{44} & \frac{1}{2}(c_{11}-c_{12})
\end{bmatrix}
\] | \[
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\
c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\
c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\
c_{14} & c_{24} & c_{24} & c_{44} & c_{45} & c_{46} \\
c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\
c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66}
\end{bmatrix}
\] |

<table>
<thead>
<tr>
<th>Trigonal (7) 3, 3̅</th>
<th>Tetragonal (6) 422, 4mm, 42m, 4/mmm</th>
</tr>
</thead>
</table>
| \[
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & c_{14} & -c_{25} & 0 \\
c_{12} & c_{11} & c_{13} & -c_{14} & c_{25} & 0 \\
c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\
c_{14} & -c_{14} & 0 & c_{44} & 0 & c_{29} \\
-c_{25} & c_{25} & 0 & 0 & c_{44} & c_{14} \\
0 & 0 & 0 & c_{25} & c_{14} & \frac{1}{2}(c_{11}-c_{12})
\end{bmatrix}
\] | \[
\begin{bmatrix}
c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\
c_{12} & c_{11} & c_{13} & 0 & -c_{16} & 0 \\
c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{44} & 0 \\
-c_{16} & -c_{16} & 0 & 0 & 0 & c_{66}
\end{bmatrix}
\] |

| Tetragonal (7), 4, 4̅, 4/m | |
|-----------------------------| |
## Elastic Stiffness Cij

### Orthorhombic Crystals

<table>
<thead>
<tr>
<th>Material</th>
<th>$\rho$ (Mg/m³)</th>
<th>11</th>
<th>22</th>
<th>33</th>
<th>44</th>
<th>55</th>
<th>66</th>
<th>12</th>
<th>13</th>
<th>23</th>
<th>G (GPa)</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>MgSiO₃</td>
<td>4.108</td>
<td>515</td>
<td>525</td>
<td>435</td>
<td>179</td>
<td>202</td>
<td>175</td>
<td>117</td>
<td>117</td>
<td>139</td>
<td>246.4</td>
<td>184.2</td>
</tr>
<tr>
<td>NaMgF₃</td>
<td>3.058</td>
<td>125.7</td>
<td>147.3</td>
<td>142.5</td>
<td>46.7</td>
<td>44.8</td>
<td>50.4</td>
<td>49.5</td>
<td>45.1</td>
<td>43.1</td>
<td>75.7</td>
<td>46.7</td>
</tr>
<tr>
<td>Enstatite (En₁₀₀₀), MgSiO₃</td>
<td>3.198</td>
<td>224.7</td>
<td>177.9</td>
<td>213.6</td>
<td>77.6</td>
<td>75.9</td>
<td>81.6</td>
<td>72.4</td>
<td>54.1</td>
<td>52.7</td>
<td>107.8</td>
<td>75.7</td>
</tr>
<tr>
<td>Ferrosilite (Fs₁₀₀₀), FeSiO₃</td>
<td>4.002</td>
<td>198</td>
<td>136</td>
<td>175</td>
<td>59</td>
<td>58</td>
<td>49</td>
<td>84</td>
<td>72</td>
<td>55</td>
<td>101</td>
<td>52</td>
</tr>
<tr>
<td>En₄₄ Fs₆</td>
<td>3.272</td>
<td>229.3</td>
<td>167.0</td>
<td>193.9</td>
<td>79.7</td>
<td>76.1</td>
<td>77.1</td>
<td>73.6</td>
<td>49.8</td>
<td>46.6</td>
<td>102.3</td>
<td>73.9</td>
</tr>
<tr>
<td>En₄₂ Fs₁₅.₂</td>
<td>3.335</td>
<td>229.9</td>
<td>165.4</td>
<td>205.7</td>
<td>83.1</td>
<td>76.4</td>
<td>78.5</td>
<td>70.1</td>
<td>57.3</td>
<td>49.6</td>
<td>105.0</td>
<td>75.5</td>
</tr>
<tr>
<td>En₆₀ Fs₂₀</td>
<td>3.354</td>
<td>228.6</td>
<td>160.5</td>
<td>210.4</td>
<td>81.8</td>
<td>75.5</td>
<td>77.7</td>
<td>71.0</td>
<td>54.8</td>
<td>46.0</td>
<td>103.5</td>
<td>74.9</td>
</tr>
<tr>
<td>Protoenstatite, MgSiO₃</td>
<td>3.052</td>
<td>213</td>
<td>152</td>
<td>246</td>
<td>81</td>
<td>44</td>
<td>67</td>
<td>76</td>
<td>59</td>
<td>70</td>
<td>112</td>
<td>63</td>
</tr>
<tr>
<td>Forsterite (Fo₁₀₀₀), Mg₂SiO₄</td>
<td>3.221</td>
<td>328</td>
<td>200</td>
<td>235</td>
<td>66.7</td>
<td>81.3</td>
<td>80.9</td>
<td>69</td>
<td>69</td>
<td>73</td>
<td>29.5</td>
<td>81.1</td>
</tr>
<tr>
<td>Fayalite (Fo₁₂₈), Mg₂SiO₄</td>
<td>3.18</td>
<td>266</td>
<td>168</td>
<td>232</td>
<td>32.3</td>
<td>46.5</td>
<td>57</td>
<td>94</td>
<td>92</td>
<td>92</td>
<td>34</td>
<td>50.7</td>
</tr>
<tr>
<td>Fo₉₃ Fa₇</td>
<td>3.311</td>
<td>320.2</td>
<td>195.9</td>
<td>233.8</td>
<td>63.5</td>
<td>76.9</td>
<td>78.1</td>
<td>67.9</td>
<td>70.5</td>
<td>78.5</td>
<td>29.5</td>
<td>77.6</td>
</tr>
<tr>
<td>Fo₉₃ Fa₇</td>
<td>3.311</td>
<td>320.2</td>
<td>195.9</td>
<td>233.8</td>
<td>63.5</td>
<td>76.9</td>
<td>78.1</td>
<td>67.9</td>
<td>70.5</td>
<td>78.5</td>
<td>29.5</td>
<td>77.6</td>
</tr>
<tr>
<td>Fo₉₁₃ Fa₈₁</td>
<td>3.316</td>
<td>324</td>
<td>196</td>
<td>232</td>
<td>63.9</td>
<td>77.9</td>
<td>78.8</td>
<td>71.5</td>
<td>71.5</td>
<td>68.8</td>
<td>28.1</td>
<td>78.7</td>
</tr>
<tr>
<td>Fo₉₂ Fa₈</td>
<td>3.299</td>
<td>319</td>
<td>192</td>
<td>238</td>
<td>63.8</td>
<td>78.3</td>
<td>79.7</td>
<td>59</td>
<td>76</td>
<td>72</td>
<td>26.7</td>
<td>79.0</td>
</tr>
<tr>
<td>Mn₂SiO₄</td>
<td>4.129</td>
<td>258.4</td>
<td>165.6</td>
<td>206.8</td>
<td>45.3</td>
<td>55.6</td>
<td>57.8</td>
<td>87</td>
<td>95</td>
<td>92</td>
<td>28</td>
<td>54</td>
</tr>
<tr>
<td>Monticellite, CaMgSiO₄</td>
<td>3.116</td>
<td>216</td>
<td>150</td>
<td>184</td>
<td>50.6</td>
<td>56.5</td>
<td>59.2</td>
<td>59</td>
<td>71</td>
<td>77</td>
<td>30.6</td>
<td>55.2</td>
</tr>
<tr>
<td>Ni₂SiO₄</td>
<td>4.933</td>
<td>340</td>
<td>238</td>
<td>253</td>
<td>71</td>
<td>87</td>
<td>78</td>
<td>109</td>
<td>110</td>
<td>113</td>
<td>65</td>
<td>80</td>
</tr>
<tr>
<td>Co₂SiO₄</td>
<td>4.706</td>
<td>307.8</td>
<td>194.7</td>
<td>234.2</td>
<td>46.7</td>
<td>63.9</td>
<td>64.8</td>
<td>102</td>
<td>105</td>
<td>103</td>
<td>48</td>
<td>62</td>
</tr>
<tr>
<td>Mg₂GeO₄</td>
<td>4.029</td>
<td>312</td>
<td>187</td>
<td>217</td>
<td>57.2</td>
<td>66.1</td>
<td>71</td>
<td>60</td>
<td>65</td>
<td>66</td>
<td>20</td>
<td>72</td>
</tr>
</tbody>
</table>

AGU Bookshelf Reference Books (free !)
http://www.agu.org/reference/minphys.html
Defining a single crystal elastic tensor in MTEX

1. cs_Tensor with frame ‘x||a’ & ‘z||c’
2. Tensor in Voigt matrix form M
3. C = tensor(M,cs_tensor…)

Editor Window

```
%**********************************************
% Define elastic stiffness tensor (GPa)
%**********************************************

% Reference Elastic constants

% Reference Crystal Structure
San Carlos OLIVINE Fo93 room pressure d=3.311 g/cm3

% Define density (g/cm3)
rho = 3.311;

% Define Cartesian tensor crystal symmetry tensor frame X and Z
cs_Tensor = symmetry('mmm',[ 4.7646 10.2296 5.9942],...
[ 90.0000 90.0000 90.0000]*degree,'X||a','Z||c',...
'mineral','Olivine Fo93');

% Elastic Cij stiffness tensor (GPa) as matrix M
M = ...
[ 323.70 66.40 71.60 0.00 0.00 0.00];...
[ 66.40 197.60 75.60 0.00 0.00 0.00];...
[ 71.60 75.60 235.10 0.00 0.00 0.00];...
[ 0.00 0.00 0.00 64.60 0.00 0.00];...
[ 0.00 0.00 0.00 0.00 78.10 0.00];...
[ 0.00 0.00 0.00 0.00 0.00 79.00];

M as stiffness tensor C with MTEX tensor command
C = tensor(M,cs_Tensor,'rank',4,'propertyname',...
'Olivine Fo93 Stiffness tensor 1969','unit','GPa')
```

Command Window

```
C = tensor (show methods, plot)
propertyname: Olivine Fo93 Stiffness tensor 1969
unit : GPa
rank : 4 (3 x 3 x 3 x 3)
mineral : Olivine Fo93 (mm)
tensor in Voigt matrix representation:
323.7 66.4 71.6 0 0 0
66.4 197.6 75.6 0 0 0
71.6 75.6 235.1 0 0 0
0 0 0 64.6 0 0
0 0 0 0 78.1 0
0 0 0 0 0 79
```
Single crystal velocity calculation

Solve Christoffel symmetric tensor (3 by 3) at each grid point $n$

$$T_{ik}(n) = C_{ijkl} n_j n_l$$

$$V_p = \sqrt{\frac{\lambda_1}{\rho}}, \quad V_{s1} = \sqrt{\frac{\lambda_2}{\rho}}, \quad V_{s2} = \sqrt{\frac{\lambda_3}{\rho}}$$

Single Crystal $C_{ij}$ for Olivine (orthorhombic)

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

crystal coordinates

pcrystal coordinates

plot(C_Crystal,'density',rho_Crystal,'PlotType',velocity,'vp',complete,'contourf')
Plot and rotate a tensor of any rank

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

Plot(C,'density',rho,'PlotType','velocity','vp','complete','contourf')
annotate([xvector,yvector,zvector],'label',
{'[100] ','[010] ','[001] '
,...
,'BackgroundColor','w'});
colorbar
savefigure('/MatLab_Programs/Plot_Olivine_Single_Crystal_Vp_Label.pdf')

% rotate and plot
r = rotation('Euler',45*degree,30*degree,60*degree)
% rotate elastic tensor
C_rotated = rotate(C,r)
% rotate specimen frame vectors
x_rotated = rotate(xvector,r)
y_rotated = rotate(yvector,r)
z_rotated = rotate(zvector,r)
% plot tensor
plot(C_rotated,'density',rho,'PlotType','velocity','vp',... 
   'complete','contourf')
annotate([x_rotated,y_rotated,z_rotated],'label',... 
   {'[100] ','[010] ','[001] '},'BackgroundColor','w');
colorbar
savefigure(...
'/MatLab_Programs/Plot_Olivine_Single_Crystal_Vp_rotated.pdf');
In MTEX the reference frames are defined

The command to define the crystal reference of the Euler frame is

\[
\text{CS} = \text{crystalSymmetry}('\text{triclinic}',[5.2957,9.1810,9.4228]..., [90.372,98.880,90.110]*\text{degree},'x\text{lla}','z\text{llc}','\text{mineral}','\text{Talc}')
\]

The command to define the crystal reference of the Tensor frame is

\[
\text{CS\_tensor} = \text{crystalSymmetry}('\text{triclinic}',[5.2957,9.1810,9.4228]..., [90.372,98.880,90.110]*\text{degree},'x\text{lla}','z\text{llc}*','\text{mineral}','\text{Talc}')
\]

N.B. in Euler frame 'x\text{lla}','z\text{llc}' and in the Tensor frame 'x\text{lla}','z\text{llc}''

MTEX knows the orientation of each reference frame and automatically applies all corrections for the orientation difference between Euler and Tensor frames.
What can we do with elastic constants?

- Volume compressibility
- Linear compressibility
- Young’s modulus
- Shear modulus
- Poission’s ratio
- Christoffel Tensor
- Etc

Life was not meant to be easy in elasticity! But there is MTEX!
Define Elastic tensor in MTEX

Editor window m-file

```matlab
%%
% Specify Crystal Symmetry (cs)
% crystal symmetry - Orthorhombic mmm
% Olivine structure:
% (4.7646, 10.2296, 5.9942, 90.00, 90.00, 90.00) - Orthorhombic
cs_tensor = symmetry('mmm',[4.7646,10.2296,5.9942],...
[90.00,90.00,90.00]*degree,'xIIa','zIIc','mineral','Olivine');
%
% Import 4th rank tensor as 6 by 6 matrix
% Olivine elastic stiffness (Cij) Tensor in GPa
% The elastic constants of San Carlos olivine to 17 GPa.
%
320.5 68.15 71.6 0 0 0
68.15 196.5 76.8 0 0 0
71.6 76.8 233.5 0 0 0
0 0 0 64 0 0
0 0 0 0 77 0
0 0 0 0 0 78.7
%
Enter tensor as 6 by 6 matrix, M line by line.
M = [[320.5 68.15 71.6 0 0 0];...
[68.15 196.5 76.8 0 0 0];...
[71.6 76.8 233.5 0 0 0];...
[0 0 0 64 0 0];...
[0 0 0 0 77 0];...
[0 0 0 0 0 78.7]];
%
% Define tensor object in MTEX
% Cij -> Cijkl - elastic stiffness tensor
%
C = tensor(M,cs_tensor);
% Define density (g/cm3)
% rho=3.355;
%
```

Command window

```matlab
cs_tensor = crystal symmetry (show methods, plot)
mineral : Olivine
symmetry: mmm (mmm)
a, b, c : 4.8, 10, 6

C = tensor (show methods, plot)
rank : 4 (3 x 3 x 3 x 3)
mineral: Olivine (mmm)

tensor in Voigt matrix representation:
320.5 68.2 71.6 0 0 0
68.2 196.5 76.8 0 0 0
71.6 76.8 233.5 0 0 0
0 0 0 64 0 0
0 0 0 0 77 0
0 0 0 0 0 78.7

rho = 3.3550
```
MTEX: calculate Young's modulus in a specific crystallographic direction

```
% Calculate Young's Modulus in directions [100],[010],[001],[111] and (111)
% Define crystallographic directions in reference frame of "cs_tensor"
uvw_100 = Miller(1,0,0,cs_tensor,'uvw');
uvw_010 = Miller(0,1,0,cs_tensor,'uvw');
uvw_001 = Miller(0,0,1,cs_tensor,'uvw');
uvw_111 = Miller(1,1,1,cs_tensor,'uvw');
hkl_111 = Miller(1,1,1,cs_tensor,'hkl');
% Calculate Young's modulus (GPa)
E_100 = YoungsModulus(C,uvw_100);
E_010 = YoungsModulus(C,uvw_010);
E_001 = YoungsModulus(C,uvw_001);
E_111_uvw = YoungsModulus(C,uvw_111);
E_111_hkl = YoungsModulus(C,hkl_111);
% Calculate angle between [111] and (111) in degrees
theta = angle(uvw_111,hkl_111)/degree;
```
MTEX: calculate Young’s modulus in a specific crystallographic direction

\[
\begin{align*}
\text{uvw} \_100 &= \text{Miller (show methods, plot)} \\
\text{size: } 1 \times 1 \\
\text{options: } uvw \\
\text{mineral: } \text{Olivine (mmm)} \\
u &= 1 \\
v &= 0 \\
w &= 0 \\
\text{uvw} \_010 &= \text{Miller (show methods, plot)} \\
\text{size: } 1 \times 1 \\
\text{options: } uvw \\
\text{mineral: } \text{Olivine (mmm)} \\
u &= 0 \\
v &= 1 \\
w &= 0 \\
\text{uvw} \_001 &= \text{Miller (show methods, plot)} \\
\text{size: } 1 \times 1 \\
\text{options: } uvw \\
\text{mineral: } \text{Olivine (mmm)} \\
u &= 0 \\
v &= 0 \\
w &= 1 \\
\text{uvw} \_111 &= \text{Miller (show methods, plot)} \\
\text{size: } 1 \times 1 \\
\text{options: } uvw \\
\text{mineral: } \text{Olivine (mmm)} \\
u &= 1 \\
v &= 1 \\
w &= 1 \\
\text{hkl} \_111 &= \text{Miller (show methods, plot)} \\
\text{size: } 1 \times 1 \\
\text{mineral: } \text{Olivine (mmm)} \\
h &= 1 \\
k &= 1 \\
l &= 1 \\
E\_100 &= 286.9284 \\
E\_010 &= 164.5770 \\
E\_001 &= 196.6730 \\
E\_111\_uvw &= 170.9797 \\
E\_111\_hkl &= 200.2764 \\
\theta &= 34.6431
\end{align*}
\]
MTEX : Plotting Young's modulus

```matlab
%%
%***************************************************************************%
% Plotting section                                                      %
%***************************************************************************%
%
% plotting convention
% set the default plot direction of the X-axis
% plotx2north;
%
% plot YoungsModulus
% setpref('mtex','defaultColorMap',WhiteJetColorMap);
plot(C,'PlotType','YoungsModulus','complete')
colorbar
hold on
plot([xvector,yvector,zvector],'data',{[100 ],[010 ],[001 ]},'backgroundcolor','w');
hold off
% save plot as *.png file
savefigure('/MatLab_Programs/Plot_Olivine_Single_Crystal_Young_colour.png');
% plot YoungsModulus
setpref('mtex','defaultColorMap',grayColorMap);
plot(C,'PlotType','YoungsModulus','complete')
colorbar
hold on
plot([xvector,yvector,zvector],'data',{[100 ],[010 ],[001 ]},'backgroundcolor','w');
hold off
% save plot as *.png file
savefigure('/MatLab_Programs/Plot_Olivine_Single_Crystal_Young_gray.png');
```
MTEX : Plotting Young’s modulus

setMTEXpref('defaultColorMap', WhiteJetColorMap)

setMTEXpref('defaultColorMap', white2blackColorMap)
MTEX – calculate velocities (plot x2north)

%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Compute elastic wave velocities and polarizations in direction x = 1 0 0
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%
% compute Vp,Vs1,Vs2, particale motion for P,S1,S2 for direction
% xvector = 1,0,0 unit vector in coordinates of X1,X2, and X3 tensor frame
[vp,vsl,vss,pp,ps1,ps2] = velocity(C,xvector,rho);
%

Velocities in km/s

vp =
  9.7739

vs1 =
  4.8433

vs2 =
  4.7907

pp = vector3d (show methods, plot)
size: 1 x 1
xyz
1 0 0

ps1 = vector3d (show methods, plot)
size: 1 x 1
xyz
0 1 0

ps2 = vector3d (show methods, plot)
size: 1 x 1
xyz
0 0 1
Sample co-ordinates for plotting in MTEX

Default
plotx2north

Defined in upper hemisphere

N.B. only rotates
Plots, does not affect numerical results
MTEX – plot velocities

```matlab
%%
% Plotting section
%**************************************************************************
%
% plotting convention
% set the default plot direction of the X-axis
% plotx2north;
%
% set colour map to seismicColorMap
setattr('mtex','defaultColorMap',seismicColorMap);
%**************************************************************************
% Plot P-wave velocity (km/s)
%**************************************************************************
%
% *** need density rho in plot command for velocity ***
%
% Plot P-wave velocity (km/s)
% plot(C,'density',rho,'PlotType','velocity','vp','complete','contourf')
colorbar;
%
% Add to the plot the P-wave polarization directions
%
hold on
plot(C,'density',rho,'PlotType','velocity','pp','complete');
% add tensor orthogonal axes X1,X2 and X3
hold on
plot([xvector,yvector,zvector],'data',{[100]','[010]','[001]'},'backgroundcolor','w');
hold off
%
% save plot as *.png file
savefigure('/MatLab_Programs/Plot_Olivine_Single_Crystal_Vp_PP.png');
```
MTEX : Plot seismic velocities

setMTEXpref('defaultColorMap',blue2redColorMap)
References – Tensors and Crystal Physics

• Curie, P., Oeuvres , pp. 118, Paris, Société Français de Physique (1908)
• D.McKie and C.McKie Crystalline Solids Nelson, 1974 (Chapter 11)
Effective media: average properties for polycrystalline aggregates, Voigt, Reuss and Hill...

2 Germans & 1 Englishman
Microscopic and Macroscopic

Microscopic

\[ c_i = \sigma_i \ e_i^{-1} \]

Macroscopic

\[ c^* = <\sigma> \ <e>^{-1} \]

\[ c^* = \text{effective medium elastic constants} \]

\[ <\sigma> = \text{volume averaged stress} = \sum v_i \sigma_i = \sum v_i (c_i e_i) \]

\[ <e> = \text{volume averaged strain} = \sum v_i e_i \]
Simple volume averages

**Voigt Average**

- Constant strain

\[ e_i = \text{constant}: \quad C^* \langle \sigma \rangle = \sum V_i (C_i \ e_i) \]

\[ C^{* \approx \text{Voigt}} = \sum V_i C_i \]

**Reuss Average**

- Constant stress

\[ \sigma_i = \text{constant}: \quad C^* \langle e \rangle^{-1} = \left( \sum V_i e_i \right)^{-1} \left( \sum V_i (s_i \sigma_i) \right)^{-1} \]

\[ C^{* \approx \text{Reuss}} = \left( \sum V_i s_i \right)^{-1} \]

- easy to calculate
- widely separated bounds for strongly anisotropic minerals
- cannot introduce microstructure e.g. shape
- very poor bounds for mixtures with very different stiffnesses e.g. solids, liquids and voids
Voigt & Reuss micro-structural models

Voigt-Reuss-Hill (VRH) or Hill = \( \frac{V + R}{2} \)

No microstructural or theoretical basis, but in practice it is close to the experimentally measured values.

(a) Grain structure of a polycrystal for which Voigt’s assumption is valid. (b) Grain structure of a polycrystal for which Reuss’s assumption is valid.
Macromodel composite laminates

Aligned metal rods (black) in polyurethane matrix grey where lighter greys - larger shear strains
Oklahoma Gabbro
Stereo & Vp YZ profile

Confining pressure = 800 MPa

Physical Properties & Microstructure - Composite materials approach

Crystal Orientation

P Wave Profile: Z to XY plane

Voigt
Reuss

Microstructure

Crystal Orientation "signal" = 5 x Microstructure "signal"
Interaction between inclusions

A photoelastic image (Puck 1967), showing isochromatic (equal birefringence) fringes for a macromodel composite loaded in transverse tension (vertical direction).
Ellipsoidal inclusion - special properties

Uniform stress and strain field within the inclusion
Ellipsoid and Cylinder

homogeneous stress & strain fields

heterogeneous stress & strain fields
Self Consistent (SC) Method

\[ e_i = \frac{\sigma_i}{\epsilon_i}, \sigma_i \neq \text{constant} \quad \Rightarrow \quad C^* = \langle \sigma \rangle \langle \epsilon \rangle^{-1} \]
\[ C^* = \langle \sigma \rangle \langle \epsilon \rangle^{-1} \]
\[ <\sigma> = \sum V_i (C_{ij} e_j) \quad <\epsilon> = \sum V_i \epsilon_i \]
\[ C^* \approx c^{SC} = \langle \sigma \rangle \cdot <\epsilon>^{-1} = \left[ \sum V_i (C_{ij} e_j) \right] \cdot \left[ \sum V_i \epsilon_i \right]^{-1} \]

The value of \( e_i \) is found using a generalization of Eshelby's inclusion theory to anisotropic inclusions in anisotropic background media.

\[ e_i = \left[ I + G ( C_i - C^* ) \right]^{-1} \]

Where \( I \) is the 4th rank identity tensor and \( G \) is a Green's tensor involving elliptical integrals over the inclusion shape.

- much more complex to calculate
- "best" bounds for strongly anisotropic minerals
- can introduce microstructure e.g. shape via Green's tensor as ellipsoidal inclusion
- "best" bounds for mixtures with very different stiffnesses e.g. solids, liquids and voids
- treats every object (grain, void, fracture) in an identical manner
- further information about neighbour interaction could be introduced via two-point correlation functions
DEM Method

Developed for two phase aggregates type AB (McLaughlin, 1977) where $V_b = 1 - V_a$. The phase B is the included phase and phase A is the host phase. Requires some initial value of $C^*$ at a composition $V_b$ - this may be a pure end member. The incremental nature of the differential approach preserves the percolating (connectivity) properties of the initial estimate. For example if starting from pure A, A will always be connected. If starting from 50:50 A:B then both phases will be connected.

- now phases A and B are microstructurally different (A=Host, B=Inclusion)
- preserves connectivity of initial estimate
Velocity Cube – with melt inclusions
VpX and VpZ Gabbro - Basalt : Effect of Aspect Ratio

CPO dominated anisotropy

Basalt dominated anisotropy

Inversion at 4% melt for aspect ratio 1:4

Aspect Ratio

Ellipsoid Shape X=Y:Z given as X:Z

% Basalt

Elastic Properties

max

Single crystal values

Voigt - volume fractions

Hashin-Shtrikman (HS\(^+\))

min

0

1

2

3

\(C_{sc}\) moduli

\(S_{sc}\) compliance

self-consistent

n-point correlation function

\[ C_{sc}^{-1} = S_{sc} \]
Cluster method

EBSD maps in MTEX microstructure at the pixel level

- Orientations – variations with position, gradients …
- Grains, sub-grains and twins and their boundaries
- Phases
- Properties: indexing quality
- Properties: diffraction contrast (band contrast)
- Properties: 2\textsuperscript{nd} rank tensors e.g. chemical diffusivity
- Properties: 3\textsuperscript{rd} rank tensors e.g. piezoelectricity
- Properties: 4\textsuperscript{th} rank tensors e.g. Young’s modulus
- Schmid factors for slip systems
- Superposed maps with transparency
- Select individual grains and line profiles interactively
- Select complex sub-regions interactively
- Chose from an extensive range of color options or make your own color scales
- And any thing else you care to add!
Ca-diffusion in olivine
Figure 4: 3D plot of the piezoelectric tensor $d$ for right-handed $\alpha$-quartz 32 using plot($d$,'3D'). Note the 3-fold $c$-axis repeating the red (positive) and blue (negative) lobes, 2-fold $a$-axes, $+a$-axes have negative values, and the zero value along the $c$-axis.
Figure 5: 3D plot of the piezoelectric tensor $d$ Sphalerite 43m using plot(d,'3D'). Note the 3-fold [111] cube axes repeating the red (positive) and blue (negative) lobes and 2-fold axes along $a$, $b$ and $c$. 
MTEX – 3D plots of longitudinal surface ($d_{111}$)
Lithium Niobate

a-axis (red)    m-axis (green)    c-axis (blue)
Future developments 1; Self-consistent (SC) and Differential Effective Media (DEM), FFT methods

- SC and DEM already developed in FORTRAN – algorithms require Green’s tenor integration for Eshelby inclusion. **Allows grain interaction and grain shape.** New 2014 optimised Gauss-Legendre Quadrature functions available for MATLAB. But could it more efficient in Fourier space.

- FFT method introduced in 1994 by Moulinec H. and Suquet P. **Allows variation of stress/strain fields within the grains.** Free complied application available “CraFT” some test using EBSD data can be done with “CraFT”, need to develop an export file from MTEX of map structure.
Polycrystal models: full-field vs. mean-field (statistical) approaches
Lebensohn, Tome & Ponte Castaneda, Phil Mag 87, 4287 (2007)

**Full-field solution**

**Mean-field statistical solution**

Solving equilibrium + compatibility:

- Grain structure
- Stress field

Local behavior inside grains with a particular orientation and a particular neighborhood

Average behavior of grains with same orientation and different neighborhoods

Validation of mean-field formulations with full-field models requires ensemble averages of the latter
Future developments 2;
Importing single crystal tensors from a database, advantages and pitfalls

- Over a hundred files for the elasticity in MTEX format for copy and pasting into MTEX M-files.
- It was envisaged to use the Materials Open Database “MPOD” initiated by Daniel Chateigner (http://materialproperties.org). However no provision for the tensor frame in this database that is supervised by International Union of Crystallography (IUC).
- Need to agree on the MTEX file format that includes the tensor frame.
- **Problems with minerals** using a different **unit cell parameters** in tensor file and imported EBSD Euler frame can lead error messages from MTEX
- Some times need to substitute a tensor from mineral of different composition and **unit cell parameters**.
- **Need to substitute** the cell parameters used by EBSD into cs_tensor
Future developments 3; What are we going to do this afternoon?

- Exercise – from the thermal expansion measurements ($\alpha$) in 4 directions determine the $\alpha_{11}$, $\alpha_{22}$, $\alpha_{33}$ and $\alpha_{13}$ for a monoclinic mineral with $b$ as the two-fold axis.
- Run scripts of 2nd and 4th rank single crystal tensors
- Run a full analysis of a multi-phase aggregate
- Run a general EBSD script
ESF-MicroDice conference and training workshop
'Microstructural evolution during HT deformation: advances in the characterization techniques and consequences to physical properties'

**Day 1: Microstructure, Texture and Evolution**
Evolution of microstructures and textures during deformation and recrystallization.
**Martyn Drury** (Univ. Utrecht, Nederlands)
In-situ micro-macro tracking of the deformation field. **Michel Bornert** (Univ. Paris-Est, France)
Modelling evolving microstructures. **Albert Griera** (Univ. Autonoma de Barcelona, Spain)

**Day 2: High resolution study of microstructures**
High Resolution EBSD. **Claire Maurice** (Ecole de Mines de St. Etienne, France)
Characterization of the dislocation content of EBSD maps. **John Wheeler** (Univ. Liverpool, UK)

**Day 3: Rheology: consequences of microstructure and texture evolution to large-scale flow**
Non-stationary rheology and changing microstructure. **Brian Evans** (MIT, USA)
Impact of texture-induced anisotropy on glaciers flow. **Fabien Gillet-Chaulet** (Grenoble, France)

- Montpellier, France
- 30 March 1 April 2015  3-day Conference
- 2-3 April 2015  2-day MTEX open source & free texture analysis training workshop
- Conference web site: [http://lgge.osug.fr/article920.html](http://lgge.osug.fr/article920.html)

- Registration for the conference (30th March-1st April) must be done online (https://www.azur-colloque.fr/DR13/AzurInscription)
- Deadline for registration and submission of abstracts: **15 February, 2015**
- Registration Fees: Senior researchers **100 €** PhD & Post-docs **50 €**
Thank you

• I thank Ralf for inviting me to this workshop.
• I thank you all for listening.
• Most things I talked about (programs, pdf of publications, MTEX examples and link to the MTEX site) can accessed via my webpage http://www.gm.univ-montp2.fr/PERSO/mainprice/
• Also look at MTEX website http://mtex-toolbox.github.io