Physical properties in MTEX, current status and future developments

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

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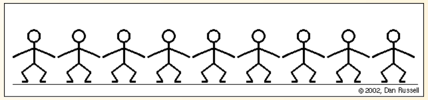

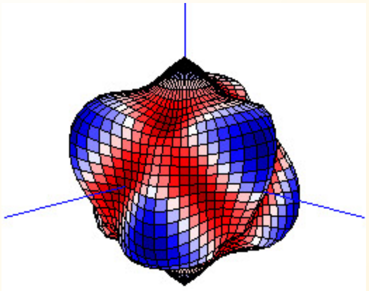

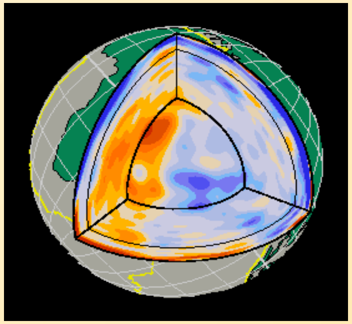

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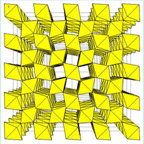
Plan of this talk, is there a plan ?

- A brief resumé of what I do …sometimes
- Single crystal introduction tensor basics – starting with 2nd 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 ?

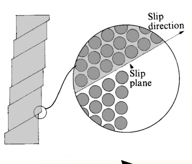
A brief resumé of what I do …sometimes

What do I do ?
Atomic Modelling & Experimentation at high P & T

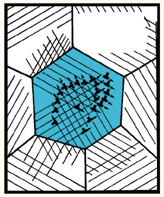
Atomic
Modelling *



Slip Systems
CRSS



Plasticity
Modelling



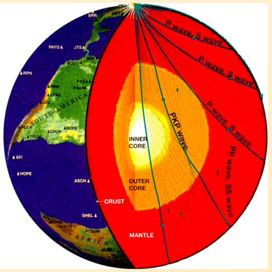
Crystal
Preferred
Orientation

Elastic
Tensors

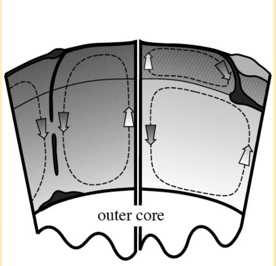
Orthorhombic
222, *mm*2, *mmm*

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

Seismology

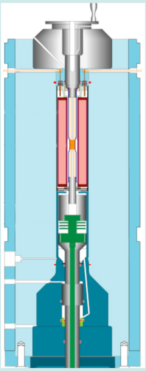


Geodynamics



Experimentation

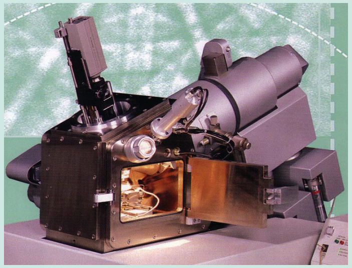
Multi-anvil 1400°C 16 GPa



Paterson
Press *
0.3 GPa

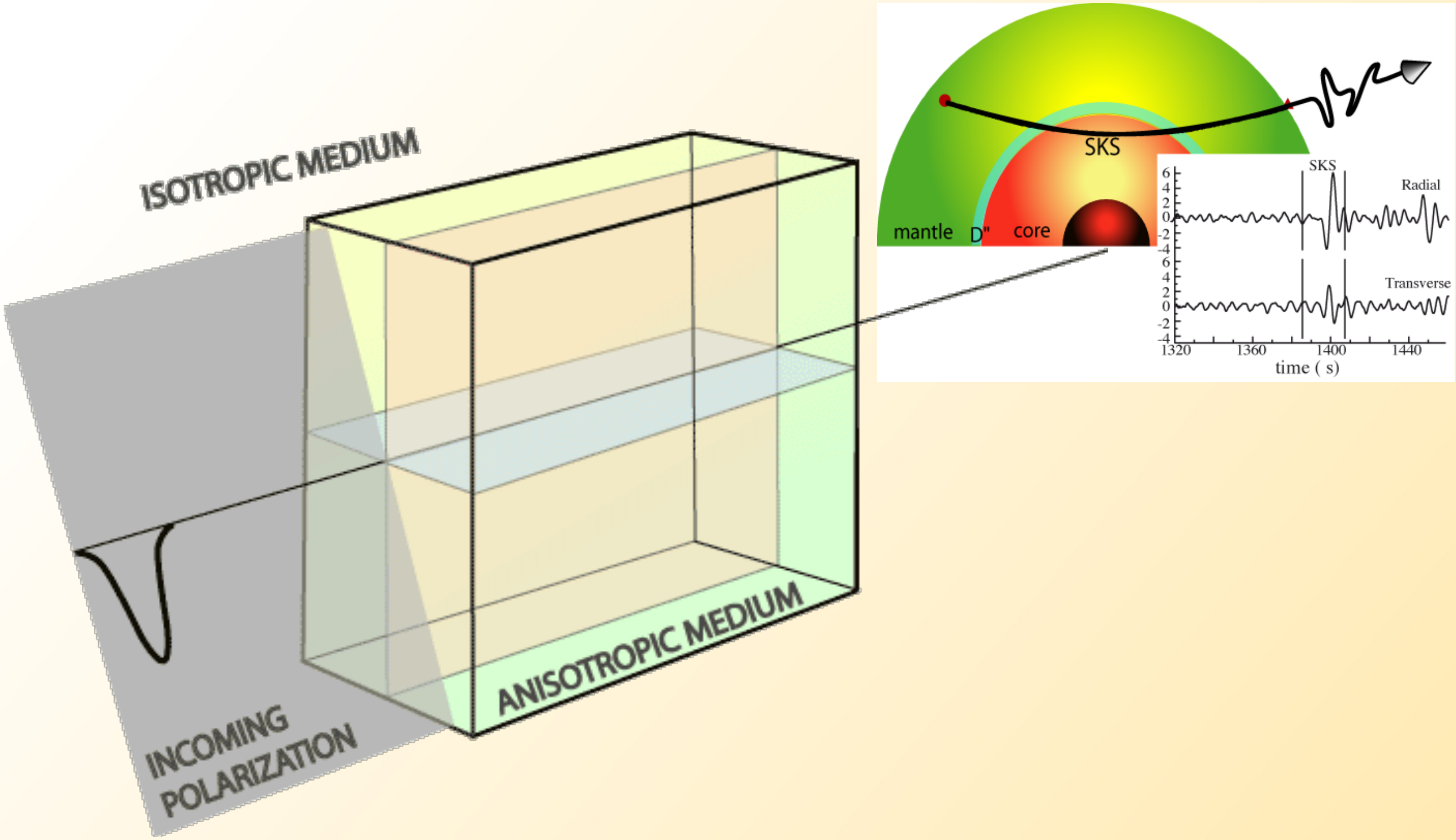
Sylvie Demouchy

EBSD *



P<10^{-4} GPa

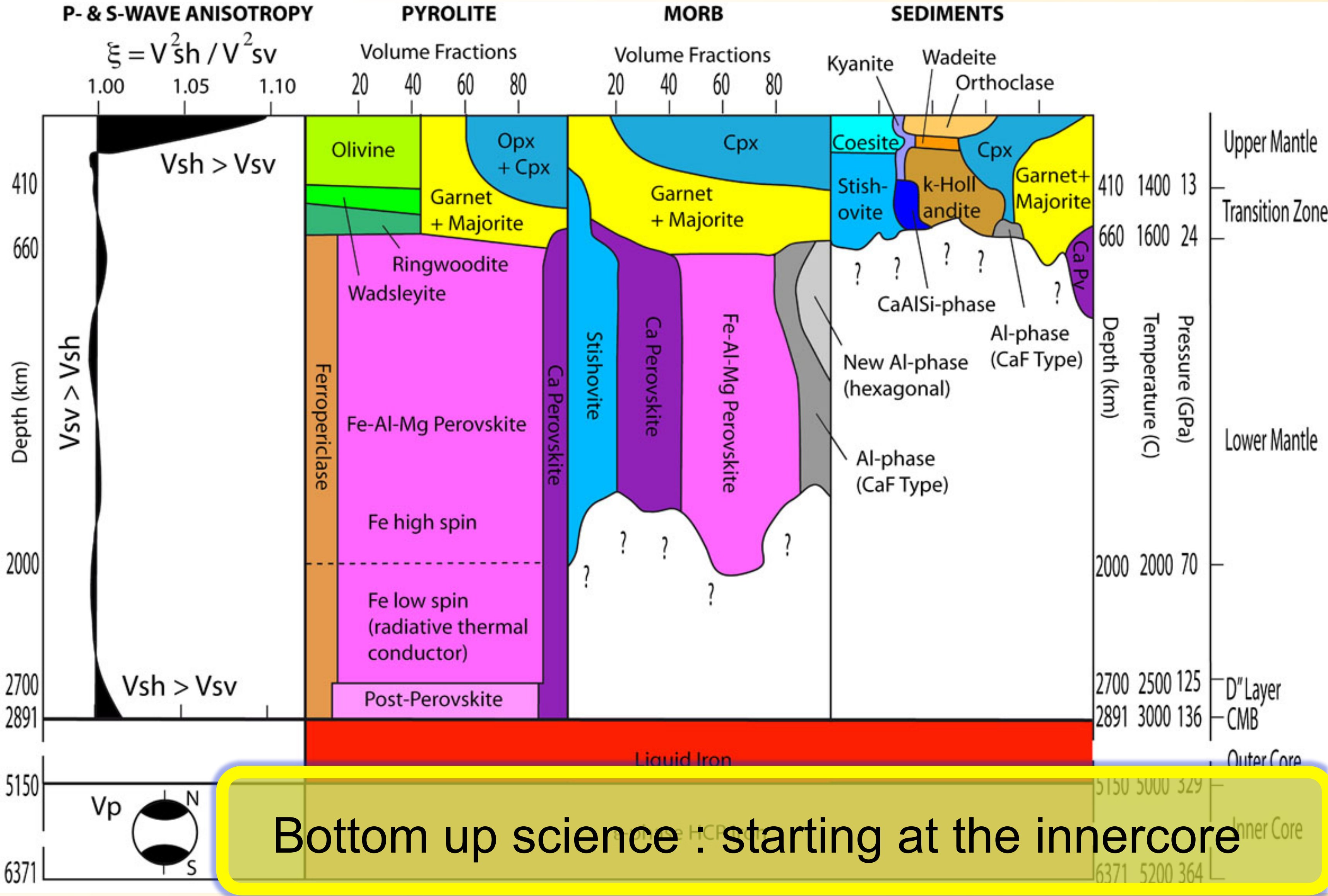
Shear Wave Splitting



http://garnero.asu.edu

Mantle & Core : petrology & seismic anisotropy

Mainprice (2007)

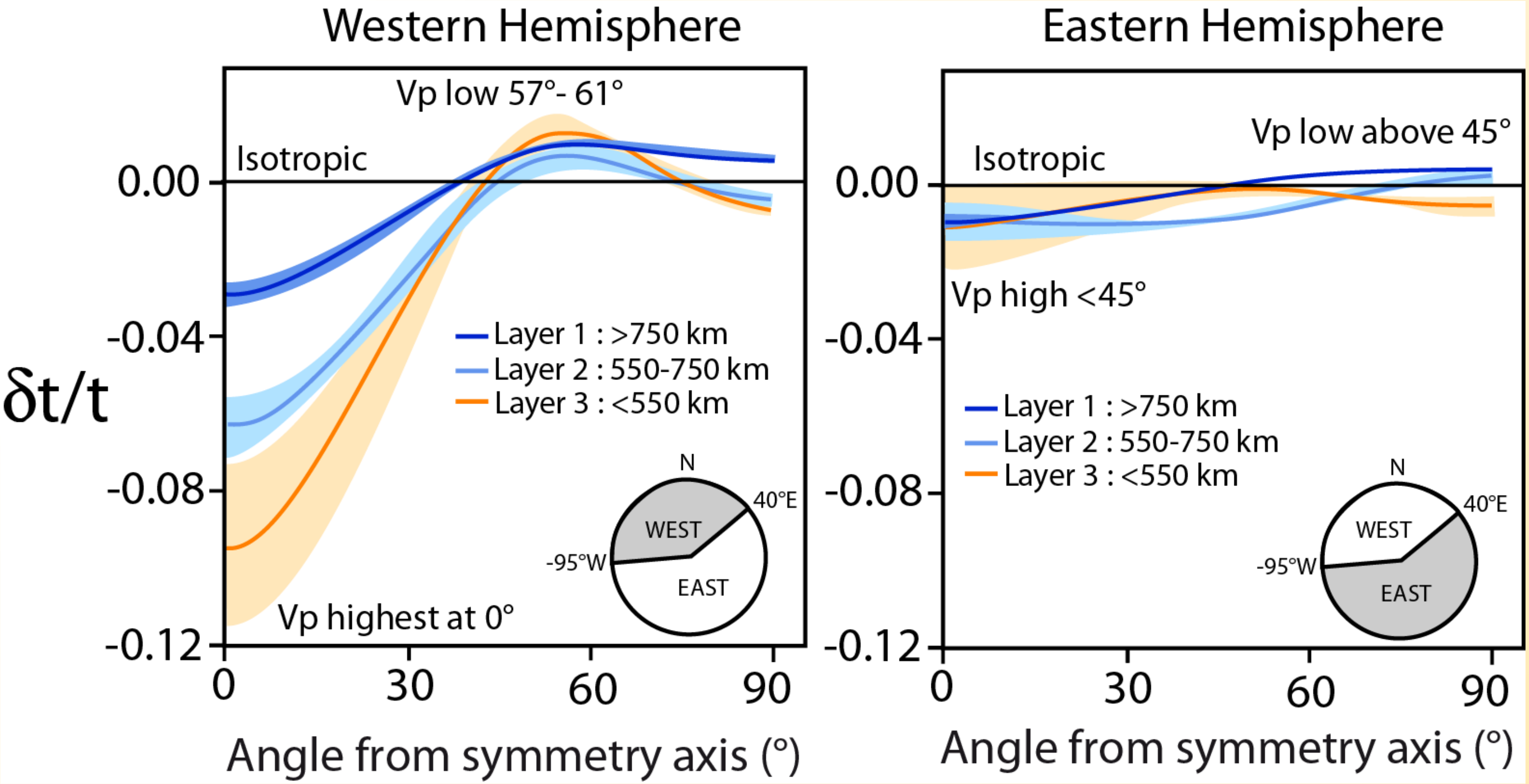


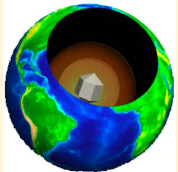
Bottom up science : starting at the innercore

Panning & Romanowicz 06 Ono & Oganov 05 Perrillat et al. 06 Irifune et al. 94 modif. by Poli & Schmidt 02

Innercore anisotropy

from the group of Arwen Deuss in Cambridge

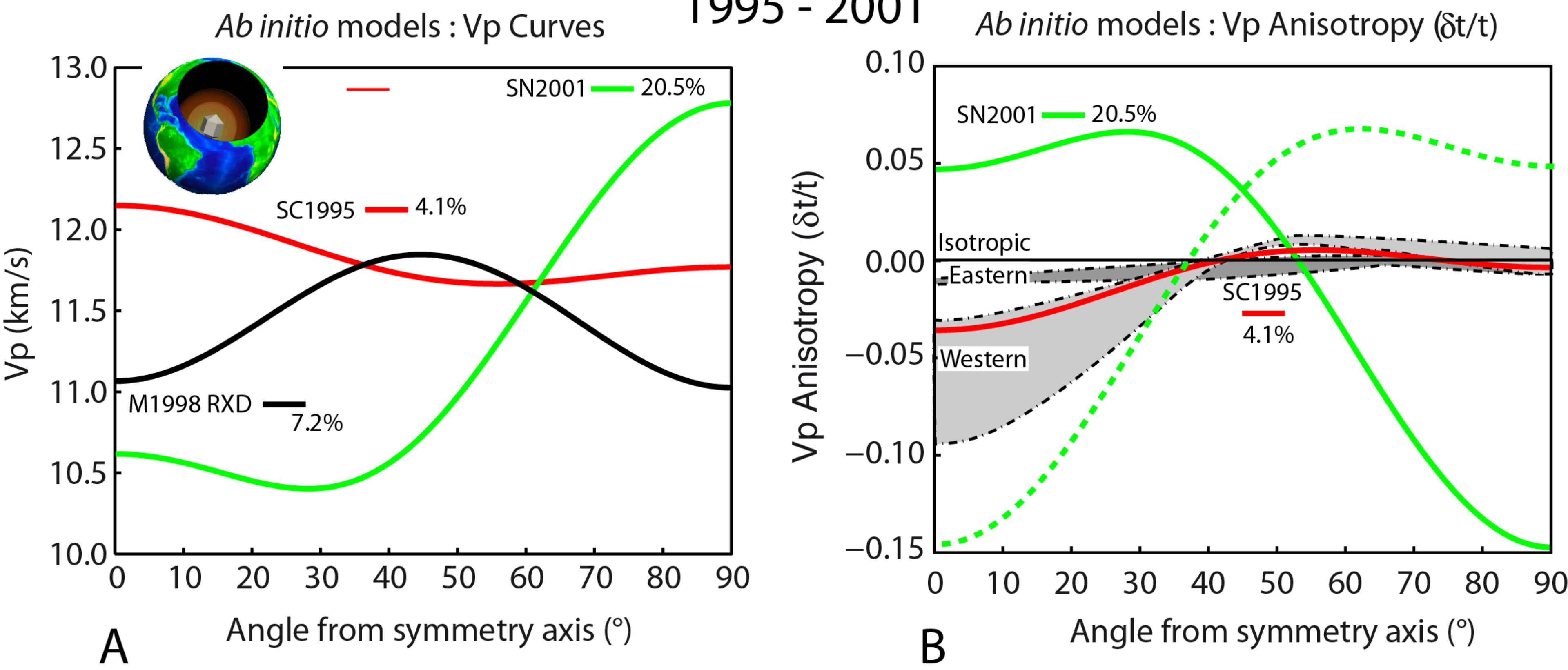




Lythgoe et al. (2014)

Early of days innercore experiments and ab initio models

1995 - 2001



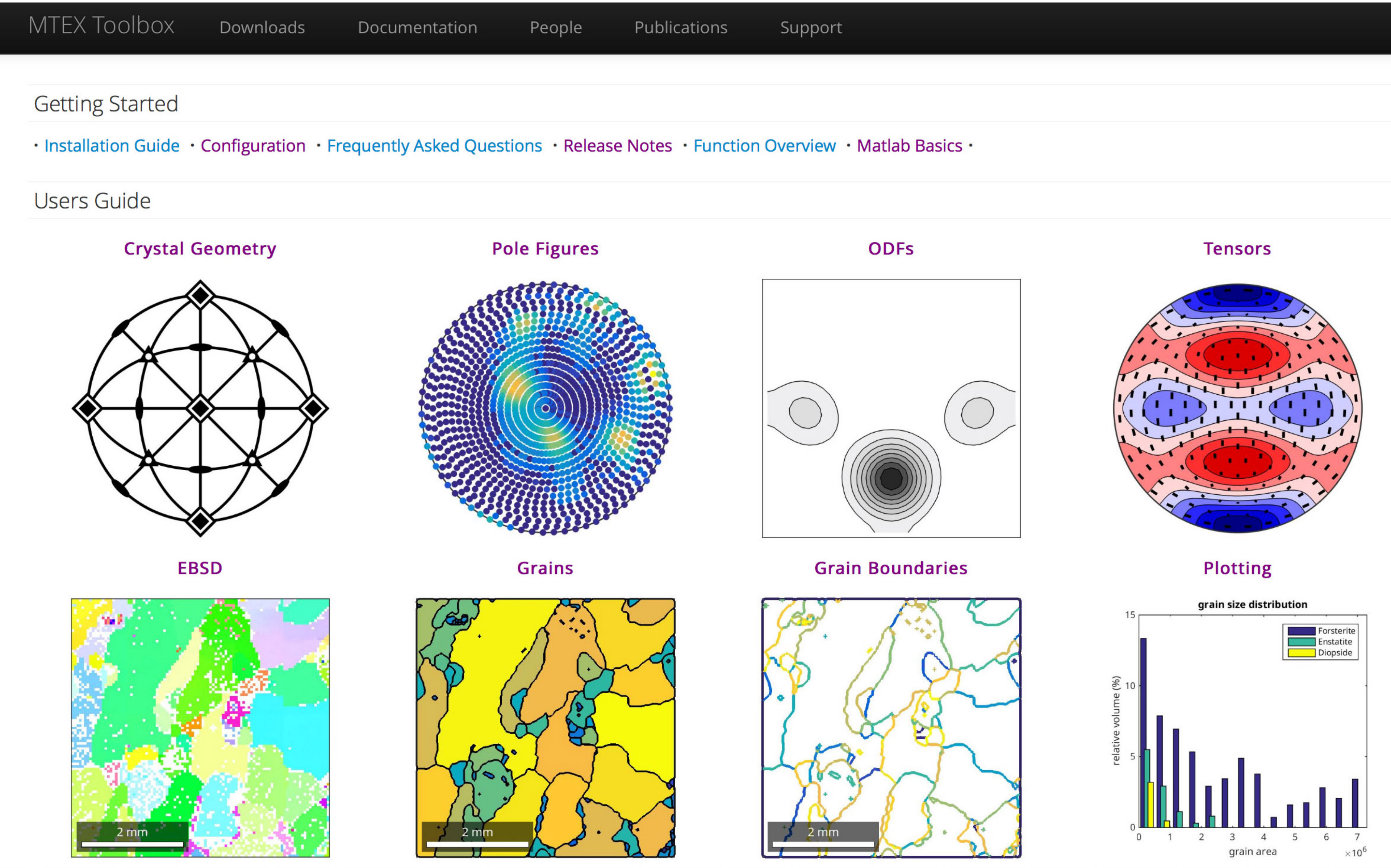
Ab initio models : Vp Curves

Ab initio models : Vp Anisotropy (δt/t)

0° = c-axis

90°=basal plane for *ab initio* models

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



MTEX Toolbox Downloads Documentation People Publications Support

Getting Started

· Installation Guide · Configuration · Frequently Asked Questions · Release Notes · Function Overview · Matlab Basics ·

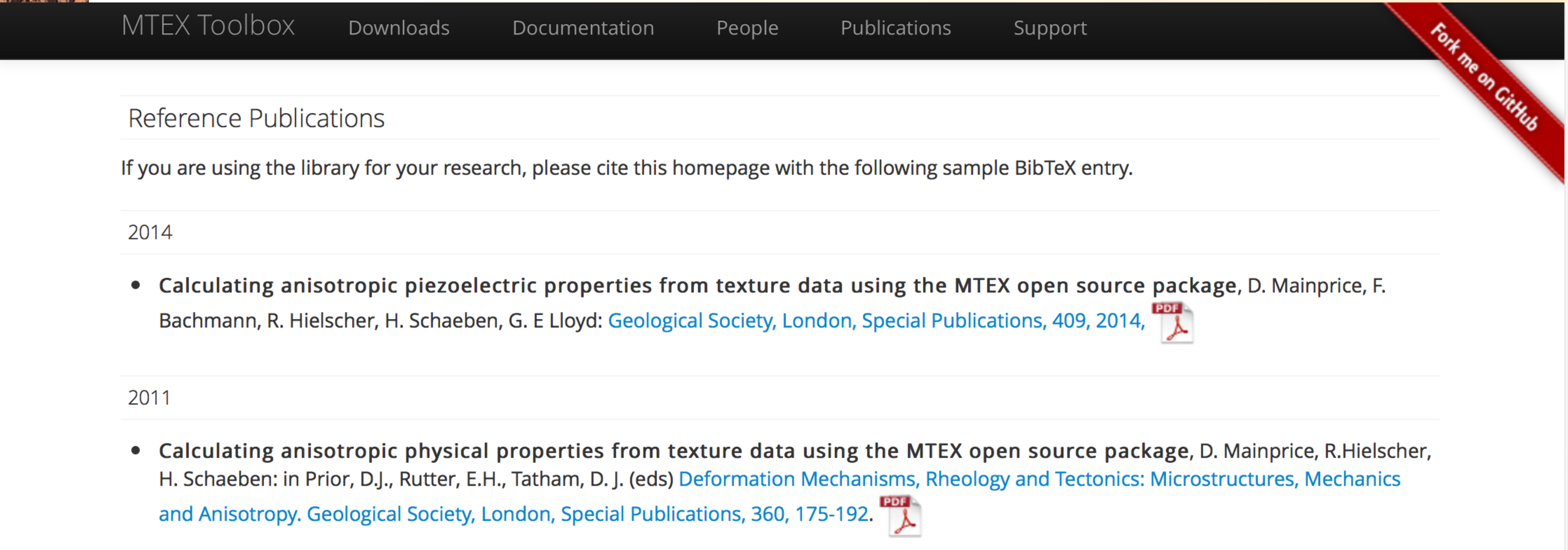
Users Guide

Crystal Geometry **Pole Figures** **ODFs** **Tensors**

EBSD **Grains** **Grain Boundaries** **Plotting**

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

- **Calculating anisotropic piezoelectric properties from texture data using the MTEX open source package**, D. Mainprice, F. Bachmann, R. Hielscher, H. Schaeben, G. E Lloyd: Geological Society, London, Special Publications, 409, 2014,

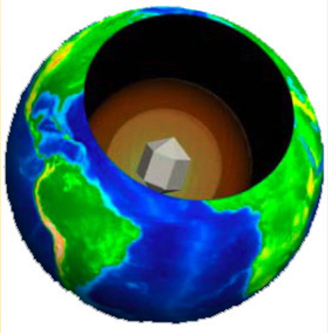
2011

- **Calculating anisotropic physical properties from texture data using the MTEX open source package**, D. Mainprice, R.Hielscher, H. Schaeben: in Prior, D.J., Rutter, E.H., Tatham, D. J. (eds) Deformation Mechanisms, Rheology and Tectonics: Microstructures, Mechanics and Anisotropy. Geological Society, London, Special Publications, 360, 175-192.

Single crystal introduction tensor basics – starting with 2nd rank tensors

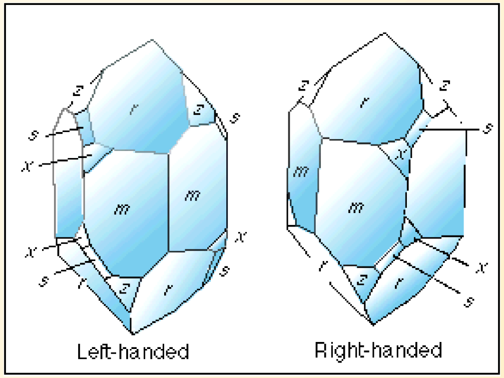
Why are we interested in Single Crystals ?

- To understand the anisotropic physical properties of poly-crystalline 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 …



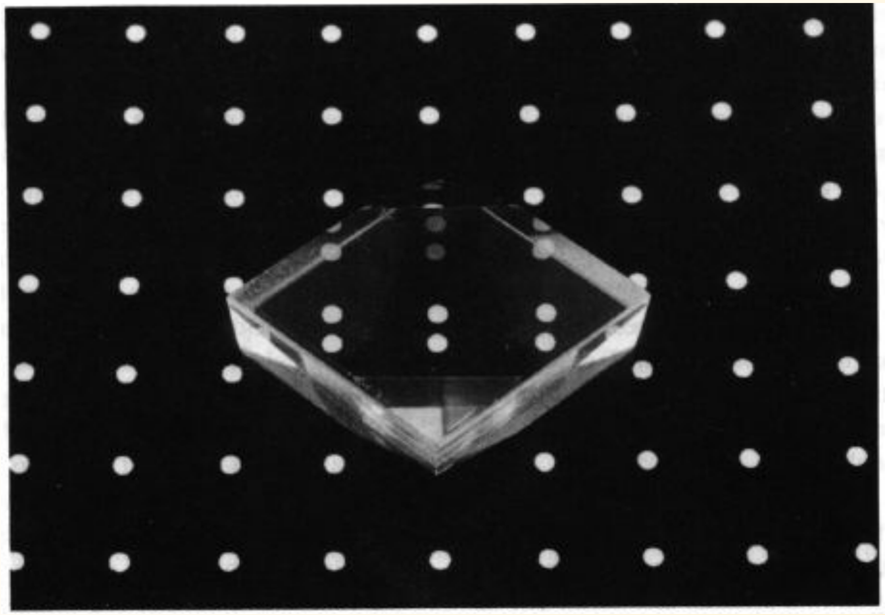
Physical properties of crystals

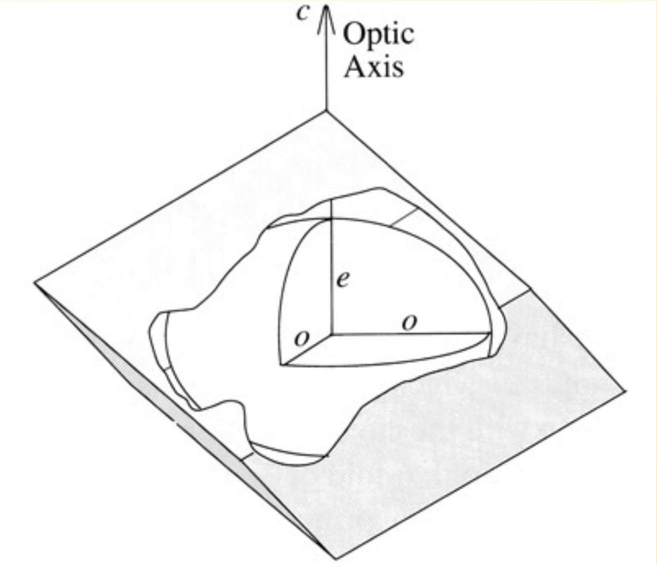
- Thermal conductivity and diffusivity (2th rank tensor) → can be calculated from CPO
- Thermal expansion (2th rank tensor) → can be calculated from CPO
- Electrical conductivity, electrical polarization and dielectric properties) → can be calculated from CPO, BUT may not be relevant if conductivity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



- Elasticity (4th rank tensor) → seismic (elastic) properties, can be calculated from CPO

Anisotropic Properties

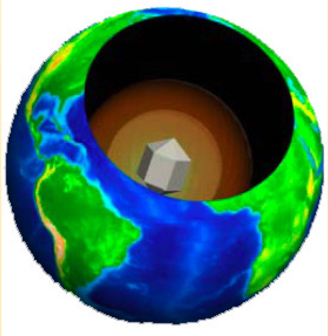




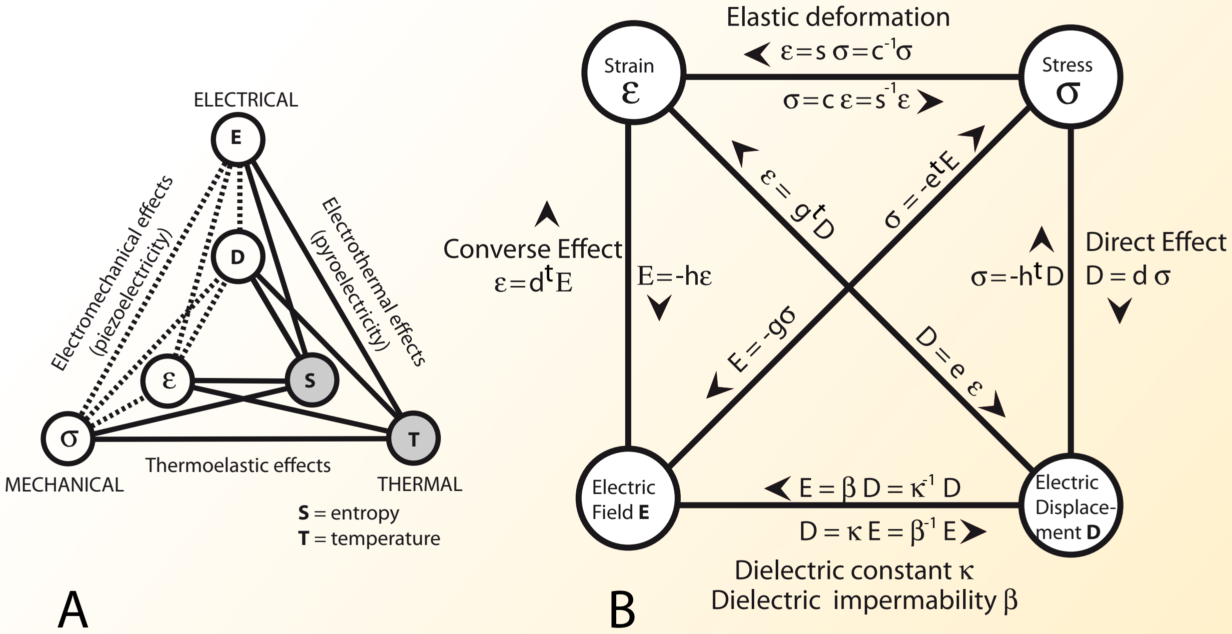
Calcite optical properties : 2nd Rank Tensor

Why are we interested in tensors of single Crystals ?

- To understand the anisotropic physical properties of poly-crystalline 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), **PF**s (pole figure) or **IPF**s (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



A) Heckmann (1925) introduced a triangular diagram

B) 4 variables choses from triangular diagram at constant entropy (s) and temperature (T)

For example, the elastic, thermal, electric and magnetic effects on strain (ε_{ij}), to first order can be written as a function of the independent variables (stress σ_{kl} , electric field E_k, magnetic field H_l and temperature gradient ΔT) 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 α_{ij} thermal expansion tensors.

Tensor rank of physical properties

Physical Property (rank)	**Driving Force (rank)**	**Response (rank)**
Density (0)	Mass (0)	Volume (0)
Pyroelectricity (1)	Temperature (0)	Electric Field (1)
Electric conductivity (2)	Electric Field (1)	Electric Current Density (1)
Electric Permitivity (2)	Electric Field (1)	Dielectric Displacement (1)
Dielectric Susceptibility (2)	Electric Field (1)	Polarization (1)
Chemical Diffusivity (2)	Potential Gradient –ve (1)	Chemical Flux (1)
Thermal Conductivity (2)	Temperature Gradient -ve (1)	Heat Flux (1)
Thermal Expansion (2)	Temperature (0)	Strain (2)
Magnetic Susceptibility (2)	Magnetic Field (1)	Magnetisation Intensity (1)
Magnetic Permeability (2)	Magnetic Field (1)	Magnetic Induction (1)
Piezolectricity (3)	Electric Field (1)	Strain (2)
Elastic Compliance (4)	Stress (2)	Strain (2)
Elastic Stiffness (4)	Strain (2)	Stress (2)

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

Crystal Symmetry	x	y	z
Orthorhombic, tetragonal, cubic	**a**	**b**	**c**
Trigonal, hexagonal	**a** **m**	**m** **-a**	**c** **c**
Monoclinic	**a*** **a**	**b** **b**	**c** **c***
Triclinic	**a*** **y** x **z** **y** x **z**	**z** x **x** **b*** **b**	**c*** **c** **c***

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

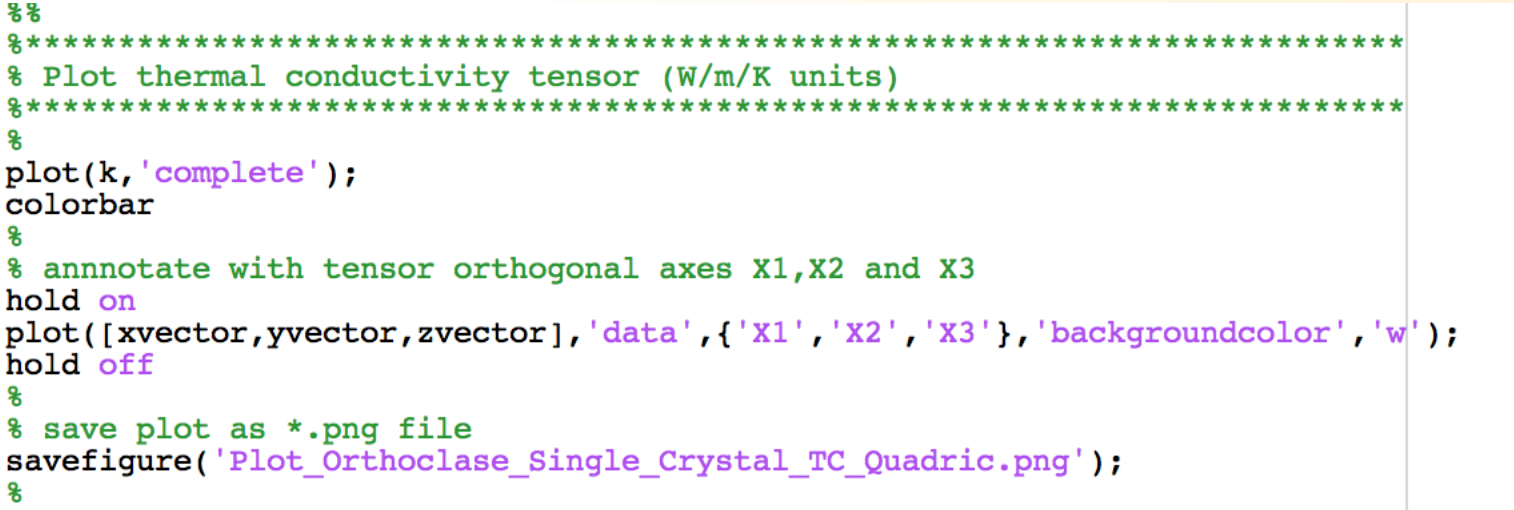
Name	Rank	New orientation in terms of old	Old orientation in terms of new
Scalar	0	$S' = S$	$S = S'$
Vector	1	$V'_i=R_{ij}V_j$	$V_i=R_{ji}V'_j$
2nd rank Tensor	2	$T'_{ij}=R_{ik}R_{jl}T_{kl}$	$T_{ij}=R_{ki}R_{lj}T'_{kl}$
3rd rank Tensor	3	$T'_{ijk}=R_{il}R_{jm}R_{kn}T_{lmn}$	$T_{ijk}=R_{li}R_{mj}R_{nk}T'_{lmn}$
4nd rank Tensor	4	$T'_{ijkl}=R_{im}R_{jn}R_{ko}R_{ip}T_{mnop}$	$T_{ijkl}=R_{mi}R_{nj}R_{ok}R_{pi}T'_{mnop}$

S = scalar, V=vector, T=tensor. T'_{ij} is the new orientation of the tensor and T_{ij} the old orientation.

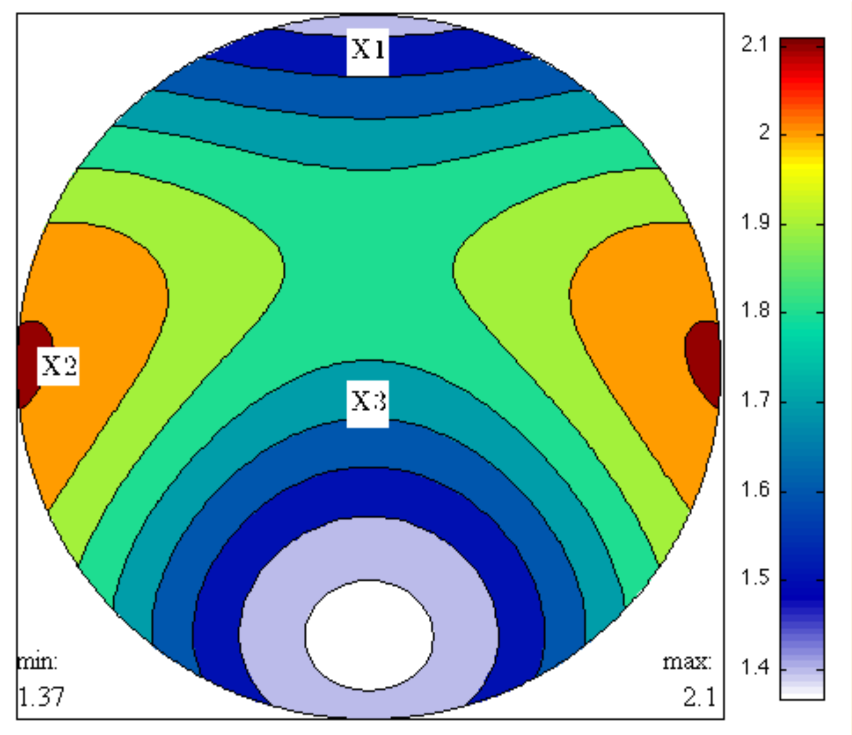
The rotation or transformation matrix R_{ij} used to calculate the tensor in new orientation is replaced by its transpose R_{ji} to calculate the old orientation.

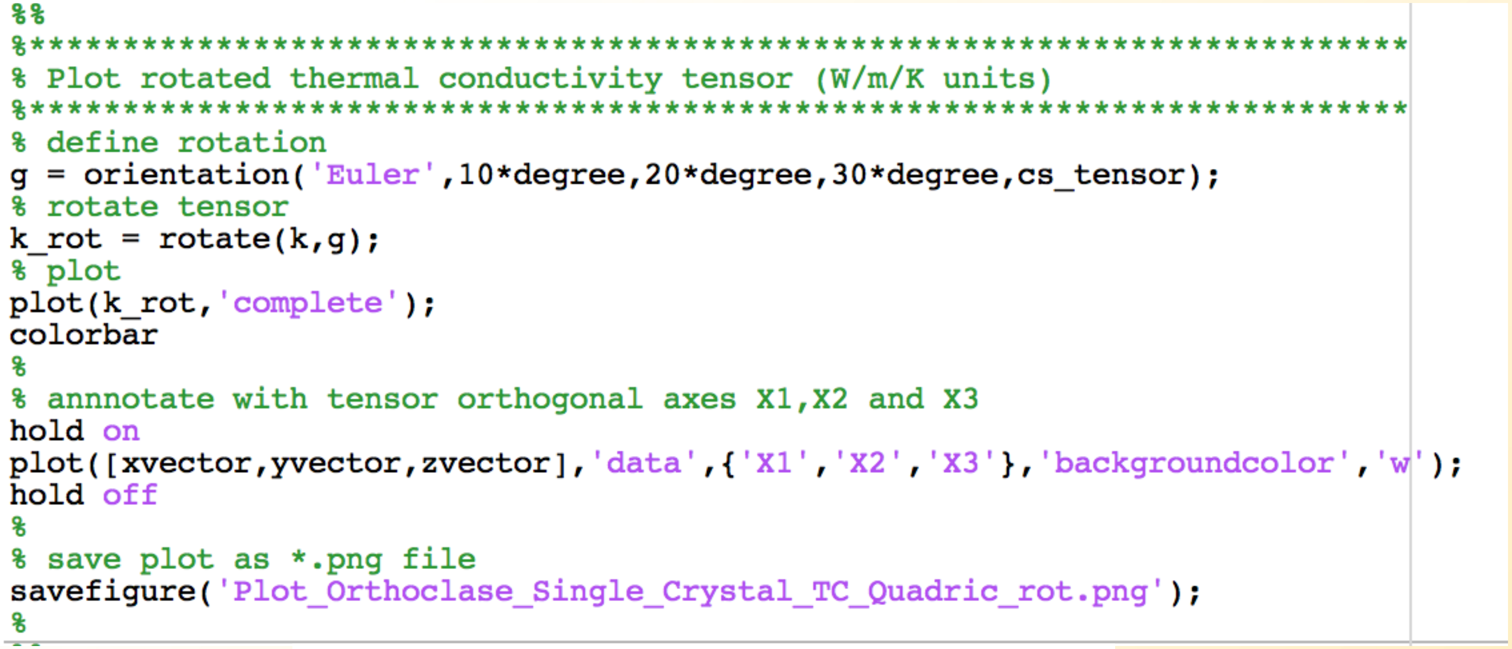
Cartesian tensors have orthogonal reference axes (labelled x, y and z in MTEX)

Representing single crystal properties

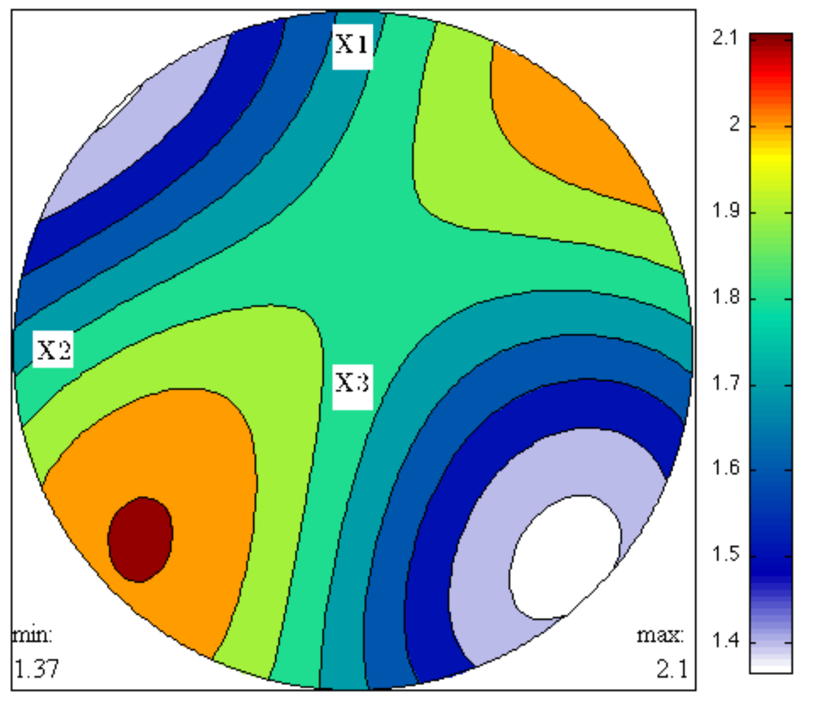


```
%%
%**************************************************************************
% Plot thermal conductivity tensor (W/m/K units)
%**************************************************************************
%
plot(k,'complete');
colorbar
%
% annnotate with tensor orthogonal axes X1,X2 and X3
hold on
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
%
% annnotate 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');
%
```



2nd 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).

$$\mathrm{T}_{\mathrm{ij}} = \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{bmatrix}$$

9 components

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

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

- In general the vectors **p** and **q** are not parallel.

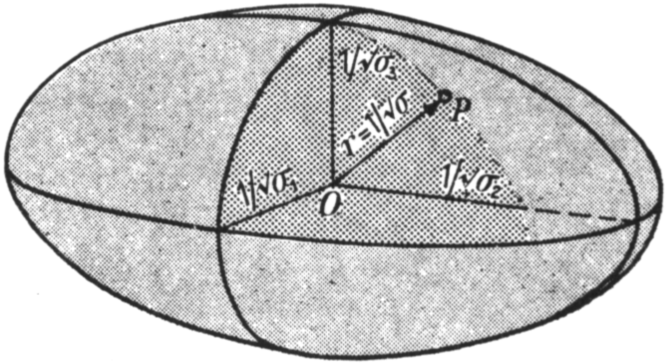
Difference between a transformation matrix ($\mathbf{R}_{ij}$) and a 2nd rank tensor ($\mathbf{T}_{ij}$)

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

$\mathbf{T}_{ij}$ is a physical quantity (e.g. 2nd rank tensor) that for a given set of reference axes is represented by 9 numbers (a 3 by 3 table).

The representation **quadric** for 2nd Rank Tensors

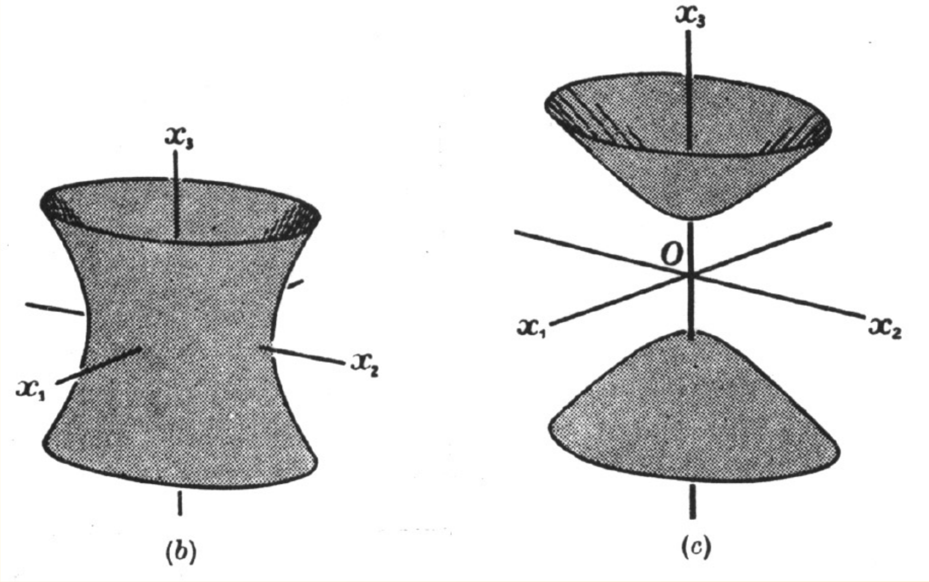
Geometrical representation of symmetrical second-rank tensors as a second-degree surface (called a **quadric**). The quadric may be an ellipsoid or a hyperboloid. Most common second-rank tensors are symmetric (Tij = Tji) and when the 3 principal coefficients are all positive then the property is represented by an ellipsoid with axes 1/√T1, 1/√T2 and 1/√T3, which is the case for electric polarization, electrical and thermal conductivity and optical properties.

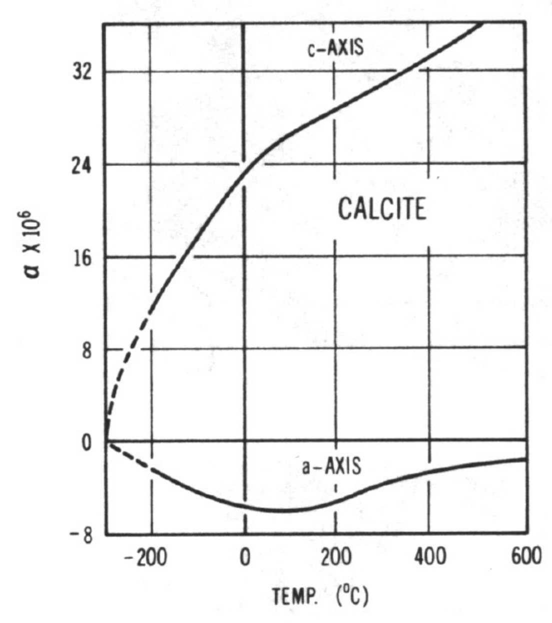


Illustrating the properties of the representation ellipsoid for conductivity: $\sigma_{ij}x_ix_j = 1$.

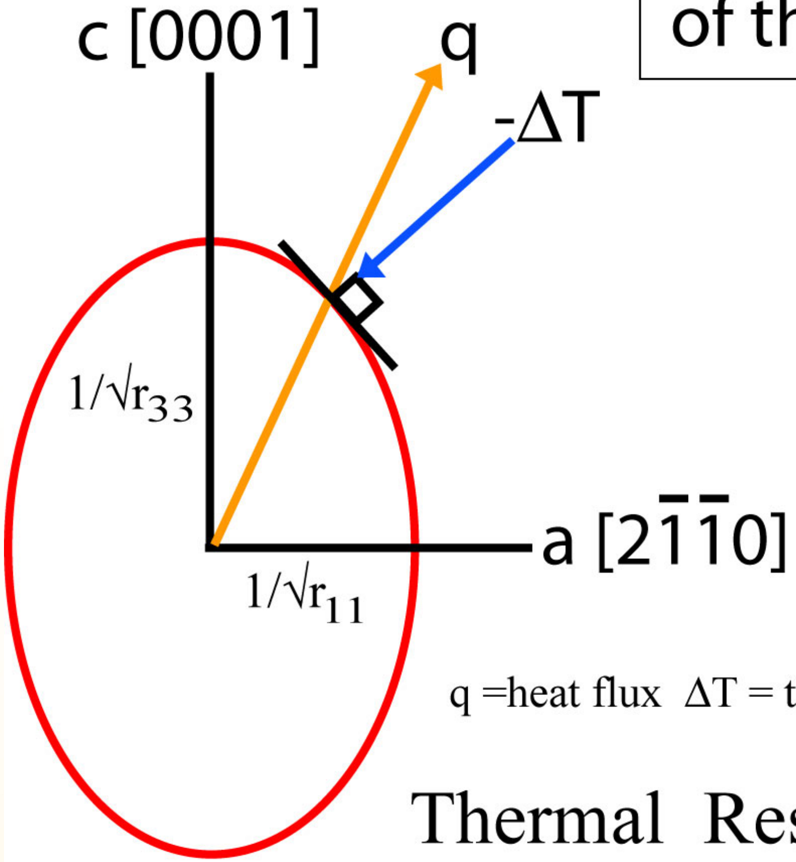
The representation **hyperboloid** for 2nd Rank Tensors

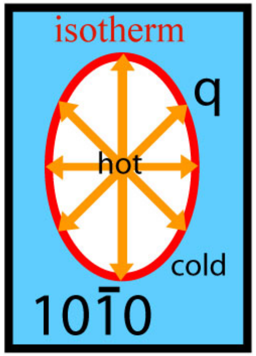
If one of the principal coefficients is negative then surface is a hyperboloid of one sheet (e.g. thermal expansion of plagioclase feldspar). If two of the principal coefficients are negative then surface is a hyperboloid of two sheets or caps, this the case for the thermal expansion of calcite with 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





Radial heat flux (q) (controlled by crystal properties not boundary conditions)

q =heat flux ΔT = thermal gradient

Thermal Resistivity (r)

$\Delta T_i = - r_{ij} q_j$

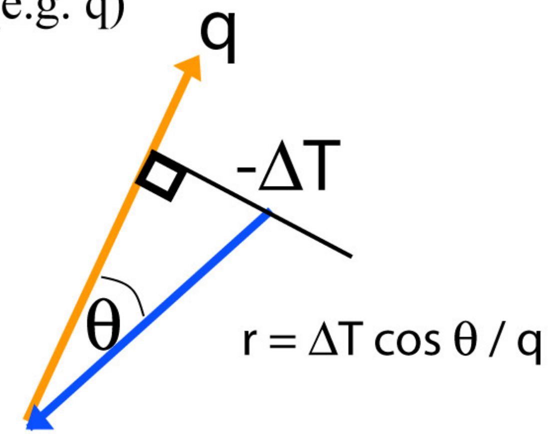
where $r_{11} = 1/k_{11}$ etc

Thermal Conductivity (k)

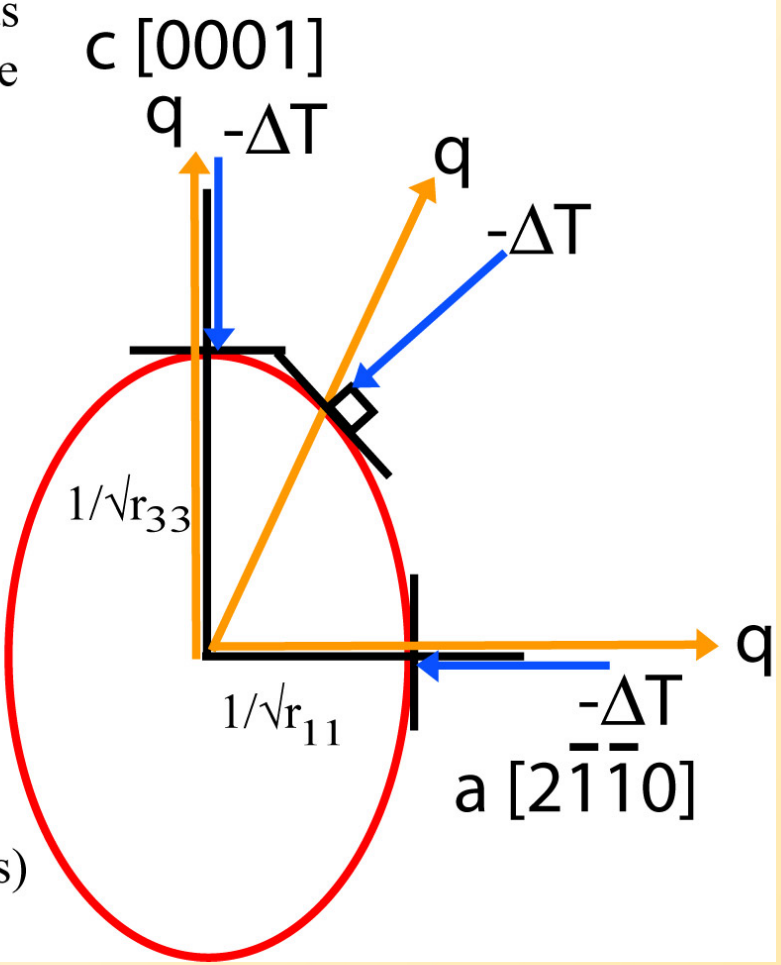
$q_i = - k_{ij} \Delta T_i$

The stimulus vector and response vectors for 2nd rank tensors

In general in anisotropic crystals the stimulus vector (e.g. ΔT) is not parallel to the response vector (e.g. 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)

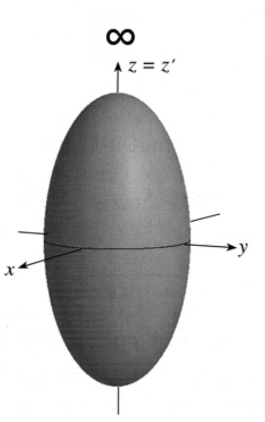


Fundamental concept for tensors

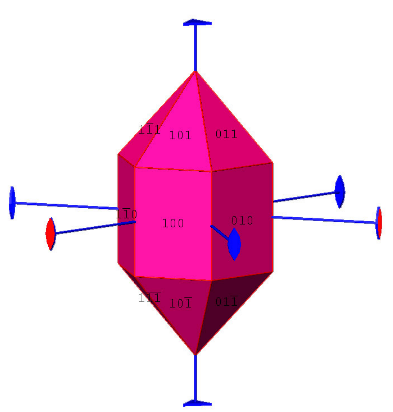
- Physical properties are anisotropic when the applied *tensor* is not aligned with resultant *tensor*
- Physical properties are isotropic when the applied *tensor* is aligned with resultant *tensor* for all directions
- In specific directions in an anisotropic crystal the applied and resultant tensor 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 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.



Physical property
higher symmetry

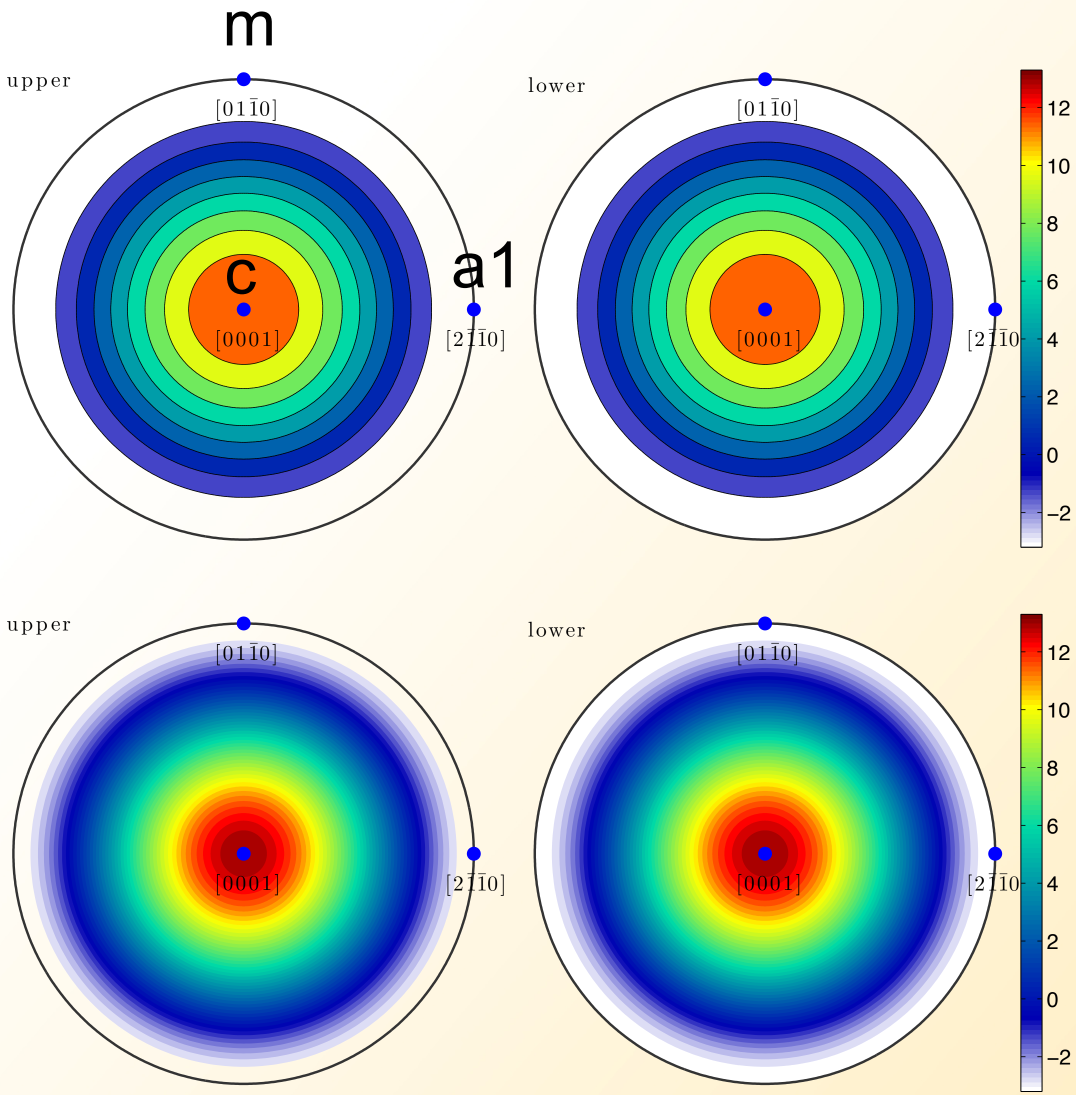


Crystal
lower symmetry

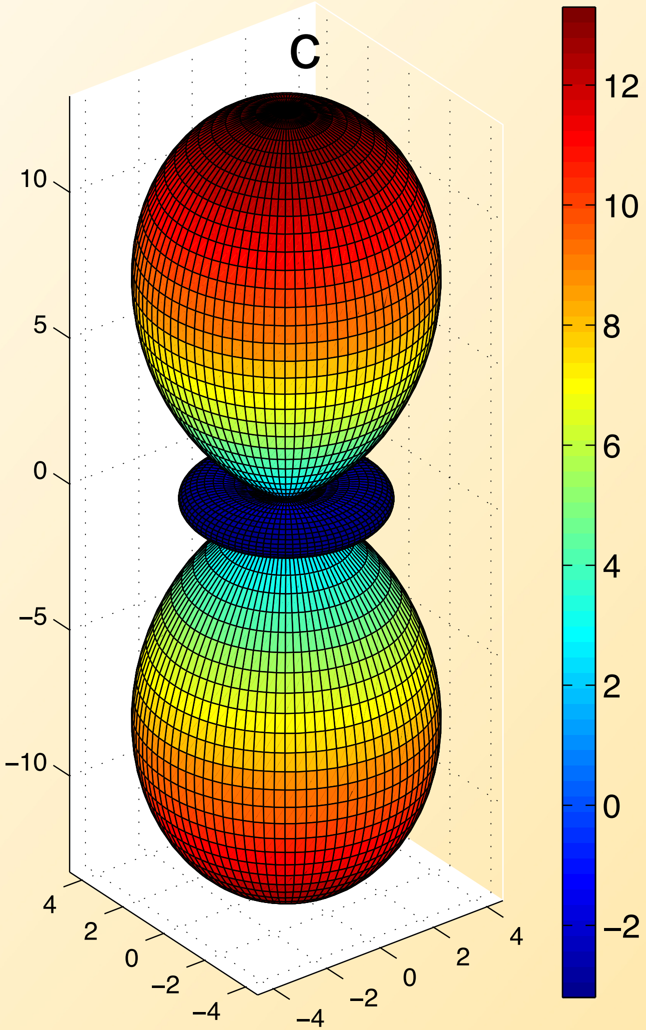
Symmetric 2nd rank tensors for all crystal symmetries

Crystal Symmetry (Independent constants)	Symmetry and tensor axes	Tensor
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** **2-fold // y** **2-fold // z**	$\begin{bmatrix} T_{11} & 0 & 0 \\ 0 & T_{22} & 0 \\ 0 & 0 & T_{33} \end{bmatrix}$
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

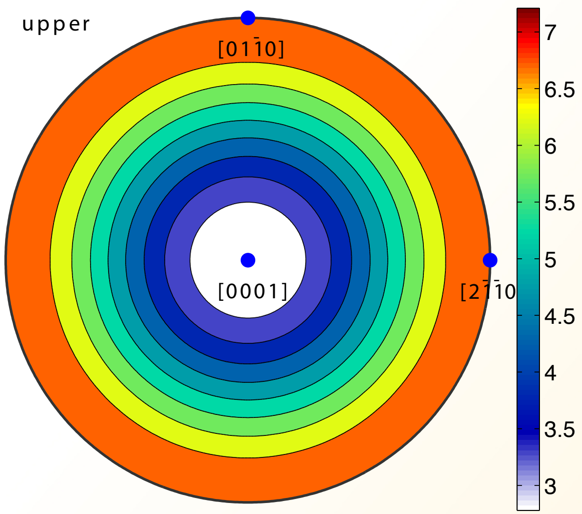


MTEX script

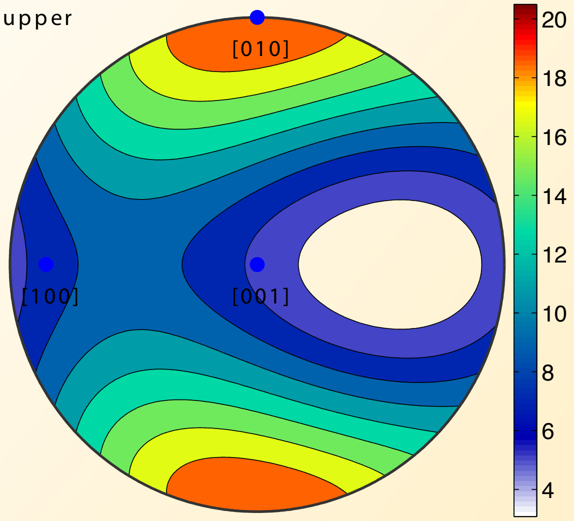
```
%**************************************************************************
% Step 1 : Define the tensor reference frame for Calcite
%**************************************************************************
cs_tensor = crystalSymmetry('-3m1',[4.9896, 4.9896, 17.0610],...
    [90, 90, 120]*degree,'mineral','calcite','x||a','z||c');
%**************************************************************************
% 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 tenor 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
% annnotate 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

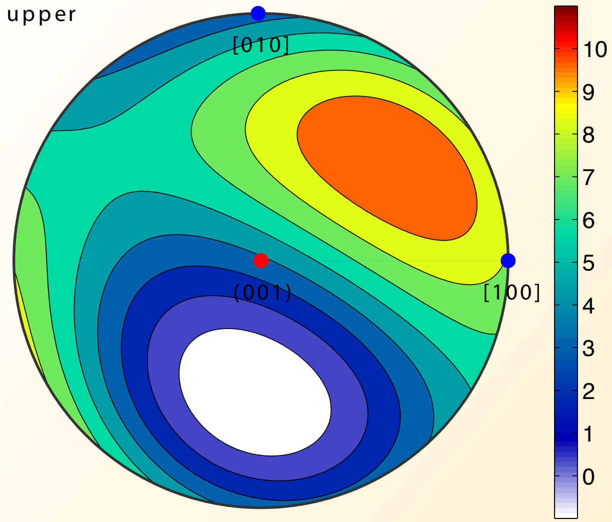
α-Quartz (trigonal -3m)



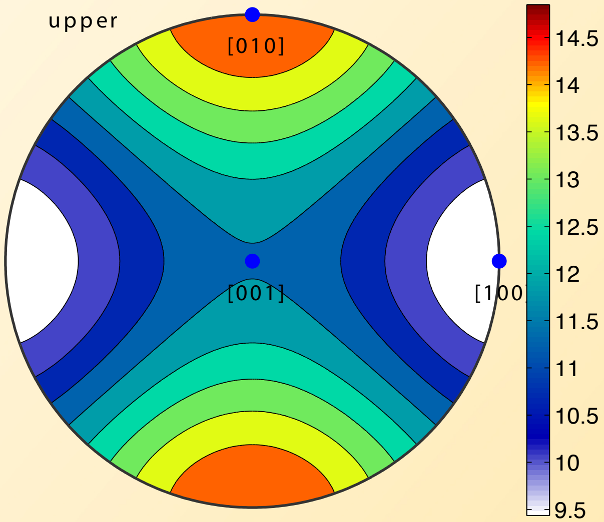
Diopside (monoclinic 12/m1)



Bytownite An76 (triclinic -1)



Forsterite (orthogonal mmm)



Optical properties - olivine

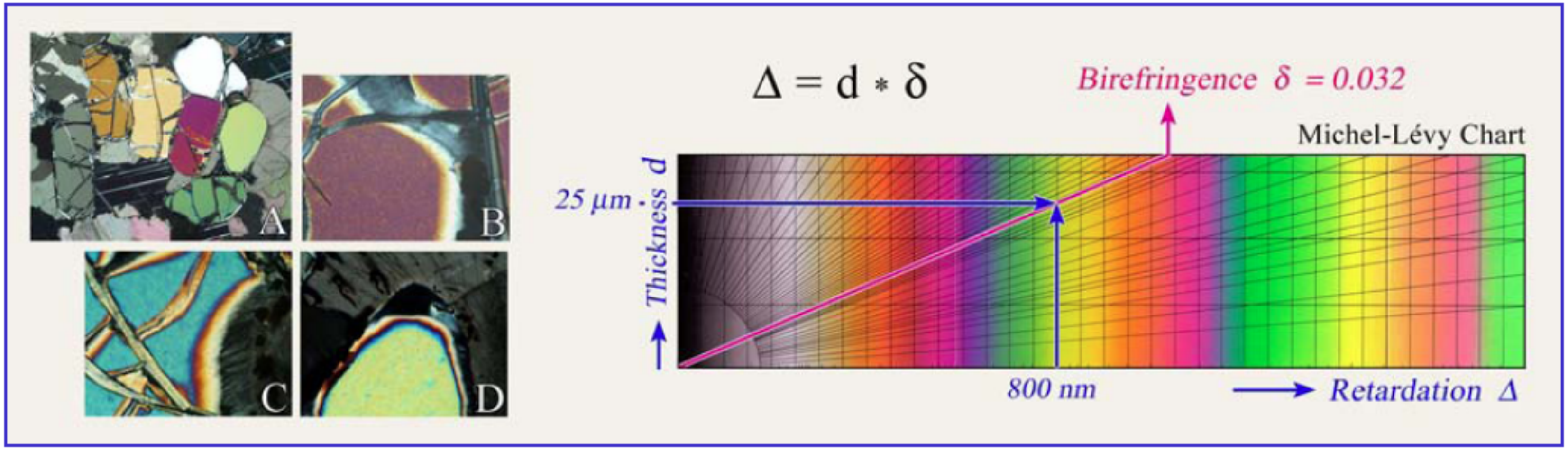
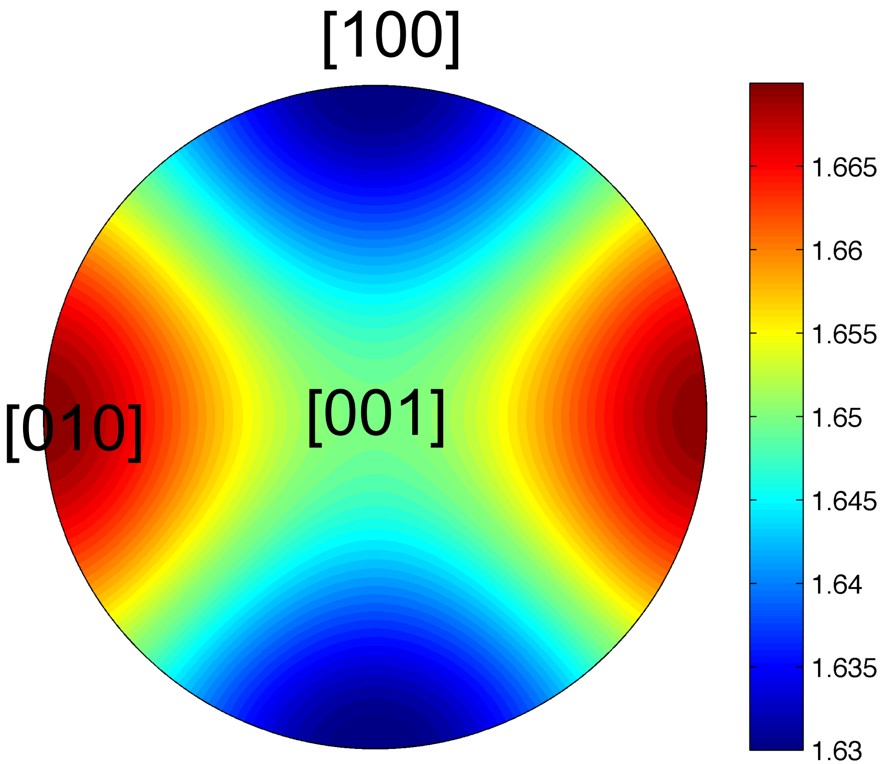


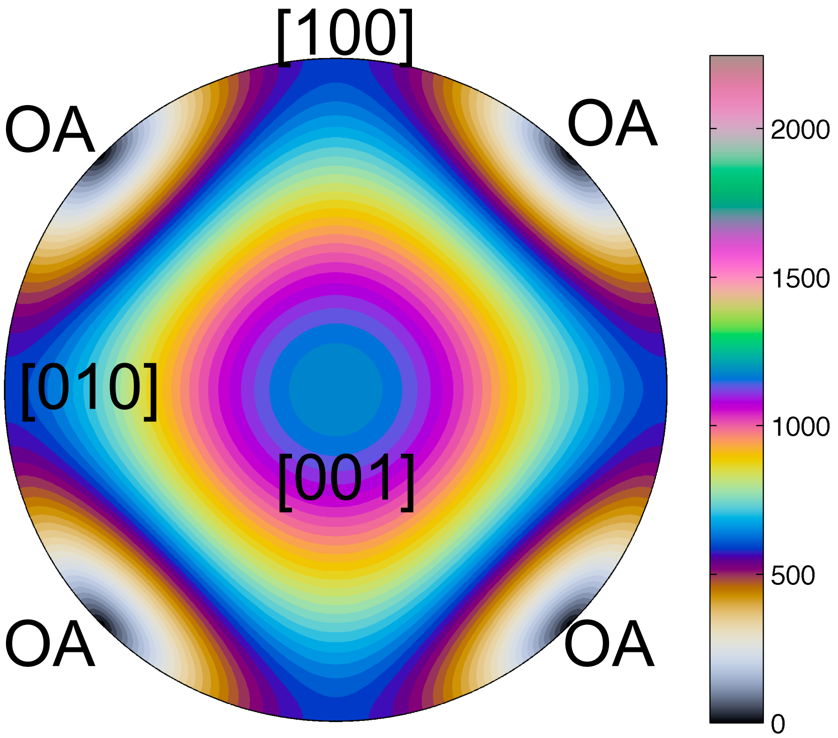
Figure 4.2.3-8: Left: (A) Variation of interference colour in differently oriented forsterite grains; (B) to (D) Decreasing interference colours at wedging-out edges of sections of forsterite grains that have different orientation in thin section. Right: Determination of birefringence using crystal thickness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



Refective index

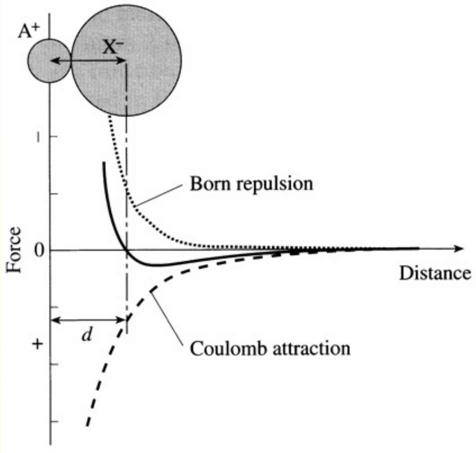


Retardation (nm): Michel Levy colours

Single crystal elasticity tensor basics – Young's modulus to wave propagation

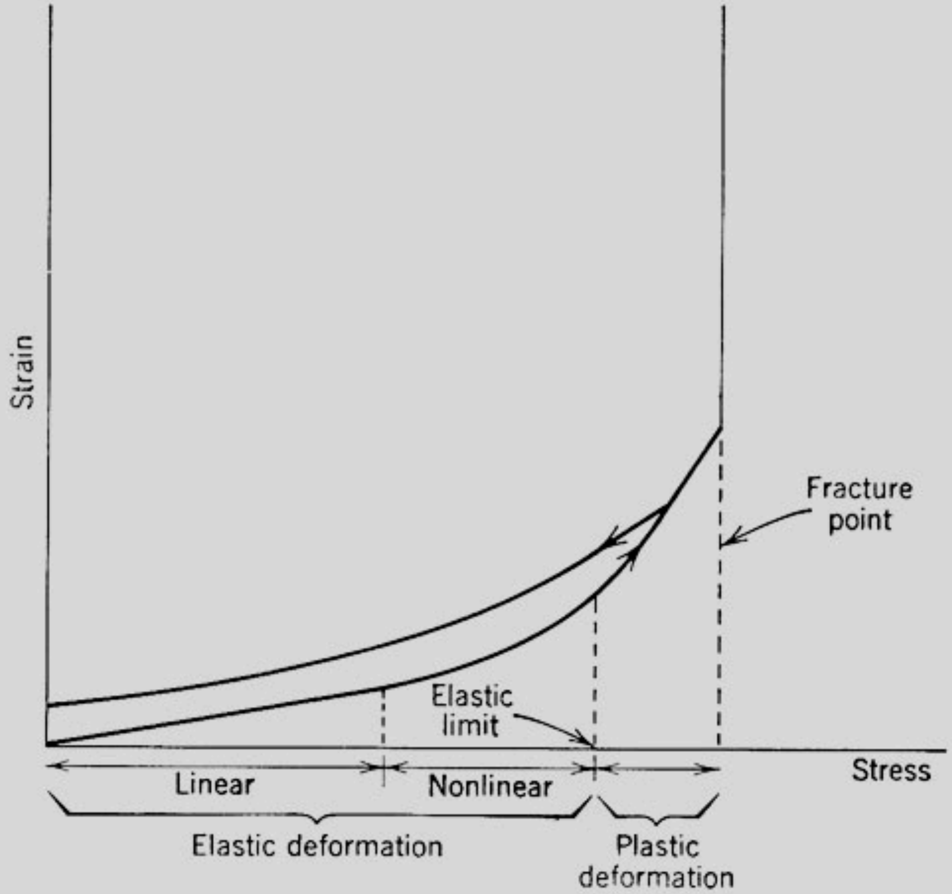
4th Rank Tensors - important for geophysics

- 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

$\sigma = \mathbf{c}\ \varepsilon$ and $\varepsilon = \mathbf{s}\ \sigma$

where $\mathbf{c}$ = stiffness coefficients (dimensions of stress)

$\mathbf{s}$ = compliance coefficients (dimensions of 1/stress)

σ = stress tensor (second order symmetric tensor)

ε = 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 where NOT symmetric
- 9 values of stress and strain

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{12} \\ \sigma_{32} \\ \sigma_{13} \\ \sigma_{21} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} & c_{24} & c_{25} & c_{26} \\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} & c_{34} & c_{35} & c_{36} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} & c_{46} & c_{56} & c_{66} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} & c_{46} & c_{56} & c_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \epsilon_{23} \\ \epsilon_{31} \\ \epsilon_{12} \\ \epsilon_{32} \\ \epsilon_{13} \\ \epsilon_{21} \end{bmatrix}$$

Stress and Strain Tensors

- Both symmetric for small linear elastic strains

$$\begin{bmatrix}\sigma_{11} & \sigma_{12} & \sigma_{31}\\ \sigma_{12} & \sigma_{22} & \sigma_{23}\\ \sigma_{31} & \sigma_{23} & \sigma_{33}\end{bmatrix} \qquad \begin{bmatrix}\epsilon_{11} & \epsilon_{12} & \epsilon_{31}\\ \epsilon_{12} & \epsilon_{22} & \epsilon_{23}\\ \epsilon_{31} & \epsilon_{23} & \epsilon_{33}\end{bmatrix}$$

- 6 Independent values ij = ji

  (not 9 because ij≠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 $C_{ijkl} = C_{klij}$

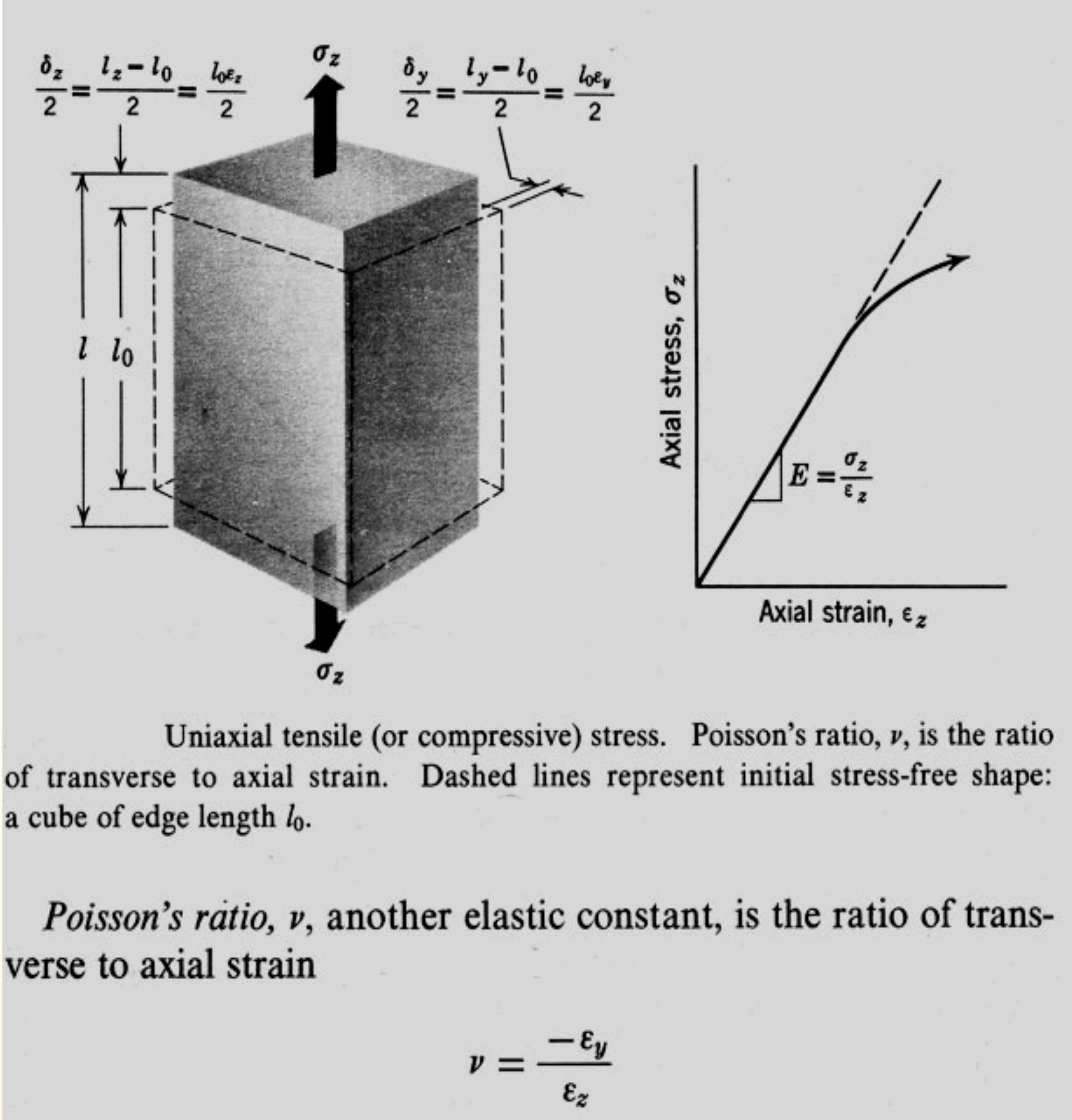
Life was not meant to be easy in elasticity !

21 independant 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

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ \gamma_{23} \\ \gamma_{31} \\ \gamma_{12} \end{bmatrix}$$

Young’s modulus & Poisson’s ratio



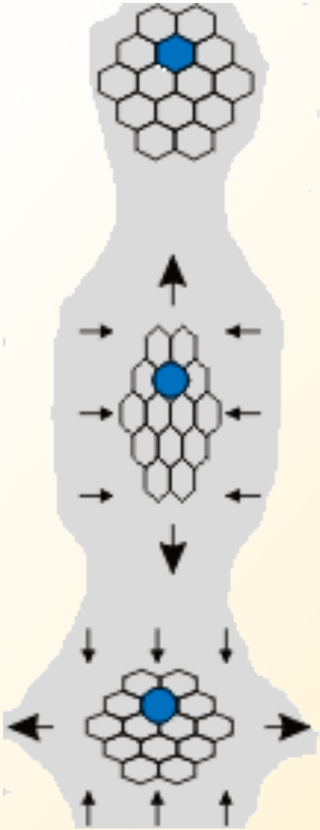
Uniaxial tensile (or compressive) stress. Poisson’s ratio, ν, is the ratio of transverse to axial strain. Dashed lines represent initial stress-free shape: a cube of edge length l_0.

Poisson’s ratio, ν, another elastic constant, is the ratio of transverse to axial strain

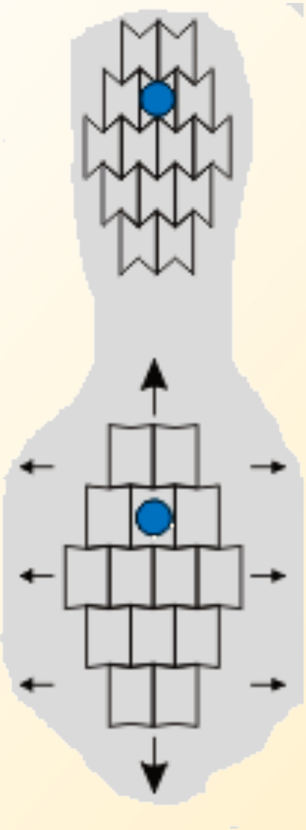
$$\nu = \frac{-\varepsilon_y}{\varepsilon_z}$$

Auxetic behaviour – negative Poission’s ratio

Poisson’s ratio +ve



Poisson’s ratio –ve



The case of cork ?

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 !

M.A. Fortes , M. Teresa Nogueria (1989) The poisson effect in cork, Materials Science and Engineering: A 122, 227-232.

The Voigt Notation 1

Voigt	Tensors
p,q = 1 to 6	i,j,k,l = 1 to 3

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

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

$$\varepsilon_{ij} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix} \dashrightarrow \varepsilon_i = \begin{bmatrix} \varepsilon_1 & \varepsilon_6/2 & \varepsilon_5/2 \\ \varepsilon_6/2 & \varepsilon_2 & \varepsilon_4/2 \\ \varepsilon_5/2 & \varepsilon_4/2 & \varepsilon_3 \end{bmatrix}$$

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 ε -> shear strain matrix $\varepsilon/2$.

$Sijkl = Spq$ for $p=1,2,3$ and $q = 1,2,3$

$2Sijkl = Spq$ for either p= or $q = 4,5,6$

$4Sijkl = Spq$ for either p= and $q = 4,5,6$

However

$Cijkl = Cpq$

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

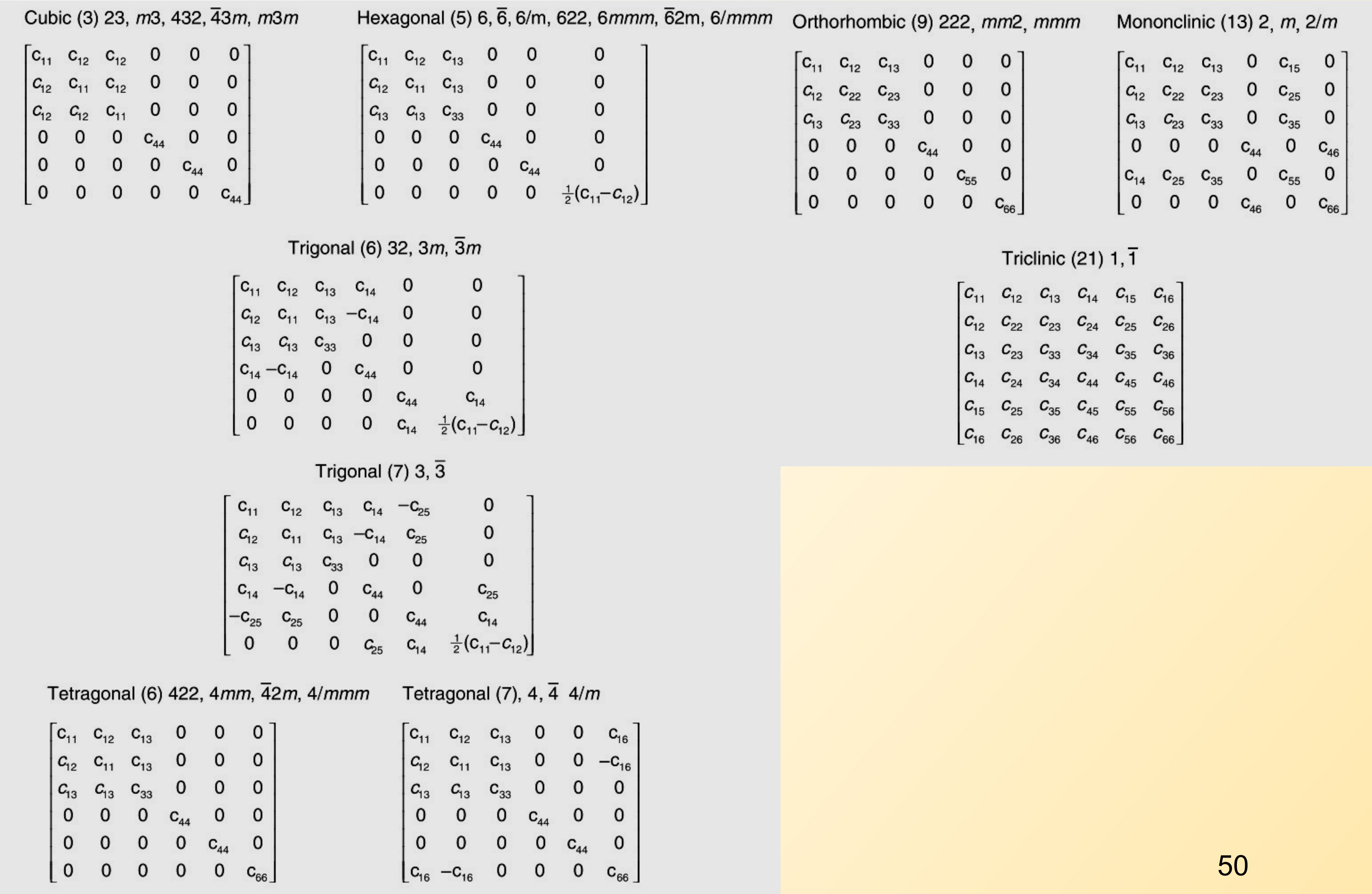
$p = \delta ij.i + (1-\delta ij)(9-i-j)$

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

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



Cubic (3) 23, *m*3, 432, $\bar{4}3m$, *m*3*m*

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

Hexagonal (5) 6, $\bar{6}$, 6/m, 622, 6*mmm*, $\bar{6}$2m, 6/*mmm*

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(c_{11}-c_{12}) \end{bmatrix}$$

Orthorhombic (9) 222, *mm*2, *mmm*

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

Mononclinic (13) 2, *m*, 2/*m*

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & c_{15} & 0 \\ c_{12} & c_{22} & c_{23} & 0 & c_{25} & 0 \\ c_{13} & c_{23} & c_{33} & 0 & c_{35} & 0 \\ 0 & 0 & 0 & c_{44} & 0 & c_{46} \\ c_{14} & c_{25} & c_{35} & 0 & c_{55} & 0 \\ 0 & 0 & 0 & c_{46} & 0 & c_{66} \end{bmatrix}$$

Trigonal (6) 32, 3*m*, $\bar{3}m$

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & 0 & 0 \\ c_{12} & c_{11} & c_{13} & -c_{14} & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & 0 & c_{14} & \frac{1}{2}(c_{11}-c_{12}) \end{bmatrix}$$

Triclinic (21) 1, $\bar{1}$

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

Trigonal (7) 3, $\bar{3}$

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & -c_{25} & 0 \\ c_{12} & c_{11} & c_{13} & -c_{14} & c_{25} & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & c_{25} \\ -c_{25} & c_{25} & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & c_{25} & c_{14} & \frac{1}{2}(c_{11}-c_{12}) \end{bmatrix}$$

Tetragonal (6) 422, 4*mm*, $\bar{4}2m$, 4/*mmm*

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

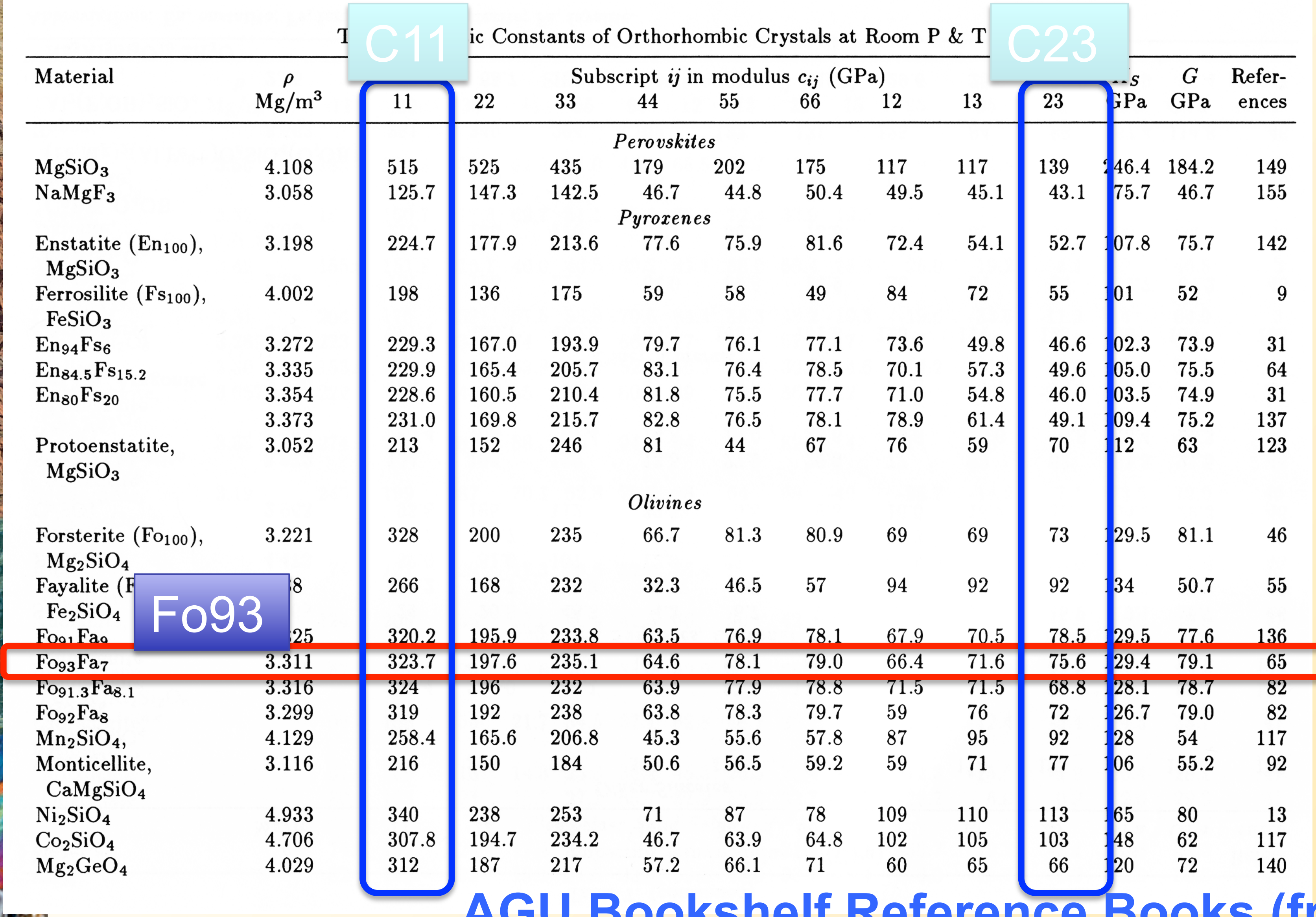
Tetragonal (7), 4, $\bar{4}$ 4/*m*

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\ c_{12} & c_{11} & c_{13} & 0 & 0 & -c_{16} \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ c_{16} & -c_{16} & 0 & 0 & 0 & c_{66} \end{bmatrix}$$

Orthorhombic Crystals
Elastic Stiffness Cij

J.D.Bass (1995)

$(Mg,Fe)_2SiO_4$



C11

C23

Fo93

T ic Constants of Orthorhombic Crystals at Room P & T

Material	ρ Mg/m³	11	22	33	44	55	66	12	13	23	K_S GPa	G GPa	References
Perovskites													
$MgSiO_3$	4.108	515	525	435	179	202	175	117	117	139	246.4	184.2	149
$NaMgF_3$	3.058	125.7	147.3	142.5	46.7	44.8	50.4	49.5	45.1	43.1	75.7	46.7	155
Pyroxenes													
Enstatite (En_{100}), $MgSiO_3$	3.198	224.7	177.9	213.6	77.6	75.9	81.6	72.4	54.1	52.7	107.8	75.7	142
Ferrosilite (Fs_{100}), $FeSiO_3$	4.002	198	136	175	59	58	49	84	72	55	101	52	9
$En_{94}Fs_6$	3.272	229.3	167.0	193.9	79.7	76.1	77.1	73.6	49.8	46.6	102.3	73.9	31
$En_{84.5}Fs_{15.2}$	3.335	229.9	165.4	205.7	83.1	76.4	78.5	70.1	57.3	49.6	105.0	75.5	64
$En_{80}Fs_{20}$	3.354	228.6	160.5	210.4	81.8	75.5	77.7	71.0	54.8	46.0	103.5	74.9	31
	3.373	231.0	169.8	215.7	82.8	76.5	78.1	78.9	61.4	49.1	109.4	75.2	137
Protoenstatite, $MgSiO_3$	3.052	213	152	246	81	44	67	76	59	70	112	63	123
Olivines													
Forsterite (Fo_{100}), Mg_2SiO_4	3.221	328	200	235	66.7	81.3	80.9	69	69	73	129.5	81.1	46
Fayalite (F Fe_2SiO_4	8	266	168	232	32.3	46.5	57	94	92	92	134	50.7	55
$Fo_{91}Fa_9$	25	320.2	195.9	233.8	63.5	76.9	78.1	67.9	70.5	78.5	129.5	77.6	136
$Fo_{93}Fa_7$	3.311	323.7	197.6	235.1	64.6	78.1	79.0	66.4	71.6	75.6	129.4	79.1	65
$Fo_{91.3}Fa_{8.1}$	3.316	324	196	232	63.9	77.9	78.8	71.5	71.5	68.8	128.1	78.7	82
$Fo_{92}Fa_8$	3.299	319	192	238	63.8	78.3	79.7	59	76	72	126.7	79.0	82
Mn_2SiO_4,	4.129	258.4	165.6	206.8	45.3	55.6	57.8	87	95	92	128	54	117
Monticellite, $CaMgSiO_4$	3.116	216	150	184	50.6	56.5	59.2	59	71	77	106	55.2	92
Ni_2SiO_4	4.933	340	238	253	71	87	78	109	110	113	165	80	13
Co_2SiO_4	4.706	307.8	194.7	234.2	46.7	63.9	64.8	102	105	103	148	62	117
Mg_2GeO_4	4.029	312	187	217	57.2	66.1	71	60	65	66	120	72	140

Subscript *ij* in modulus c_{ij} (GPa)

AGU Bookshelf Reference Books (free !)

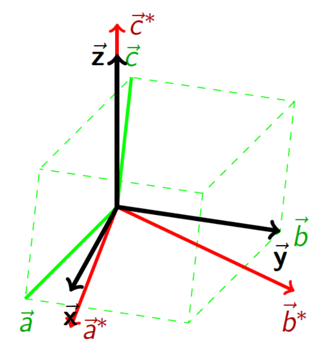
http://www.agu.org/reference/minphys.html

Defining a single crystal elastic tensor in MTEX

Editor Window

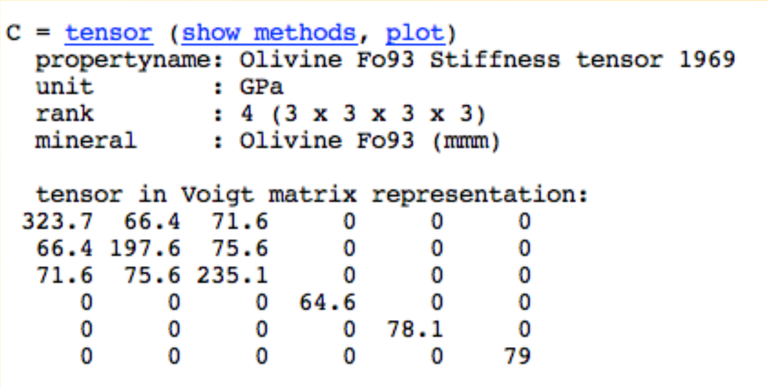
```
%************************************************
% Define elastic stiffness tensor (GPa)
%************************************************
%
% Reference Elastic constants
% Kumazawa, M., Anderson, O.L., 1969. Elastic moduli,
% pressure derivatives, and temperature derivatives of
% single-crystal olivine and single-crystal forsterite.
% J. Geophys. Res., 74, 5961-5972.
%
% 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')
%
```

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



Cartesian Tensor frame **x**,**y**,**z**

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 (mmm)

  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
```

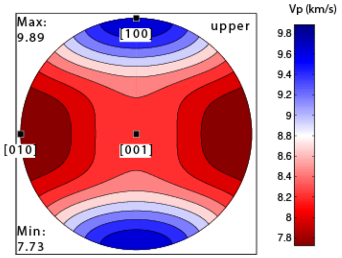
Single crystal velocity calculation

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

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

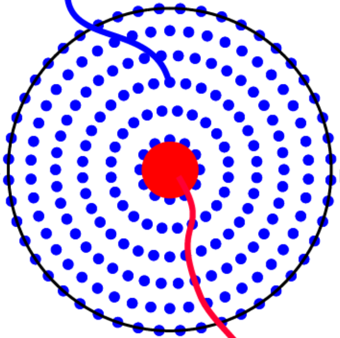
$$V_p = \sqrt{\frac{\lambda_1}{\rho}}, \quad V_{s1} = \sqrt{\frac{\lambda_2}{\rho}}, \quad V_{s2} = \sqrt{\frac{\lambda_3}{\rho}}$$

Single Crystal Cij for Olivine
(orthorhombic)

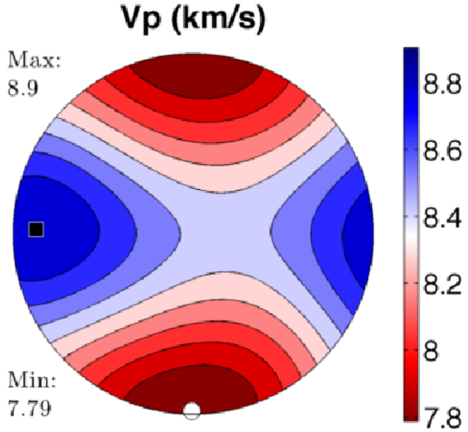


crystal coordinates

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



pcrystal coordinates



```
plot(C_Crystal ,'density',rho_Crystal,
'PlotType','velocity','vp','complete','contourf')
```

Plot and rotate a tensor of any rank

```
%% Plot elastic tensor property Vp in km/s with density rho
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');
```

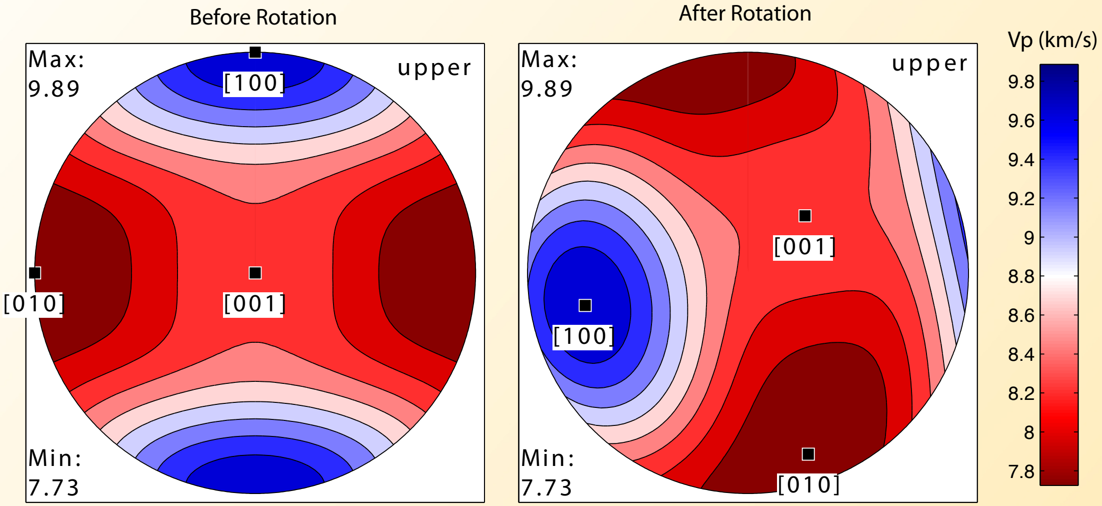
Rotate a 4th rank tensor

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

Plot(C,’density’,rho,’PlotType’,’velocity’,’vp’,’complete’,’contourf’)

r=rotation(’Euler’,45*degree,30*degree,60*degree)

C_rotated = rotate(C,r)   x_rotated = rotate(xvector,r)



In MTEX the reference frames are defined

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

```
CS = crystalSymmetry('triclinic',[5.2957,9.1810,9.4228]...
   ,[90.372,98.880,90.110]*degree,'xlla*','zllc','mineral','Talc’)
```

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

```
CS_tensor = crystalSymmetry('triclinic',[5.2957,9.1810,9.4228]...
   ,[90.372,98.880,90.110]*degree,'xlla','zllc*','mineral','Talc')
```

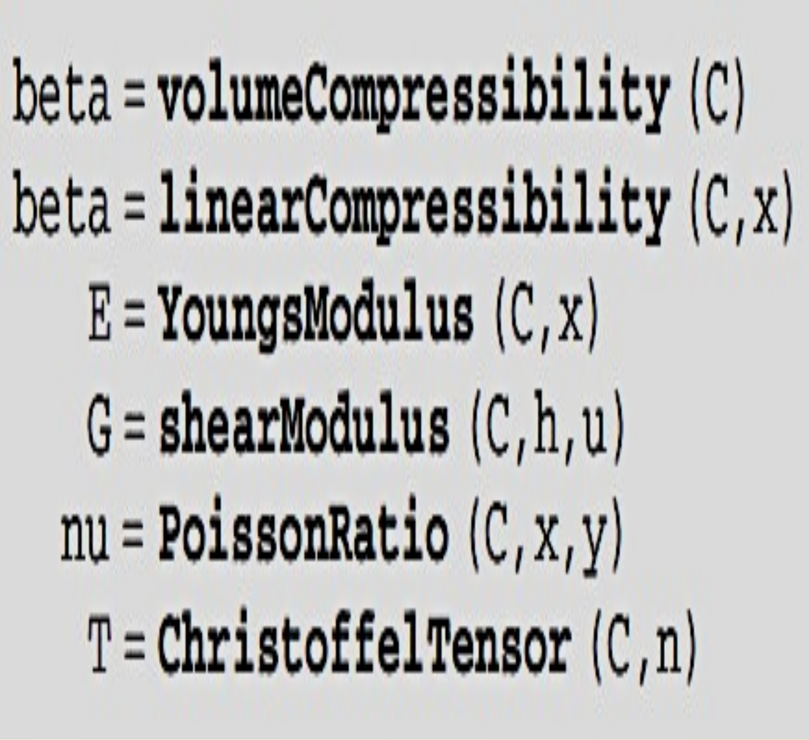
N.B. in **Euler frame** 'xlla*','zllc and in the **Tensor frame** 'xlla','zllc*’

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 compressiblity
- Linear compressiblity
- Young’s modulus
- Shear modulus
- Poission’s ratio
- Christoffel Tensor
- Etc…

MTEX commands

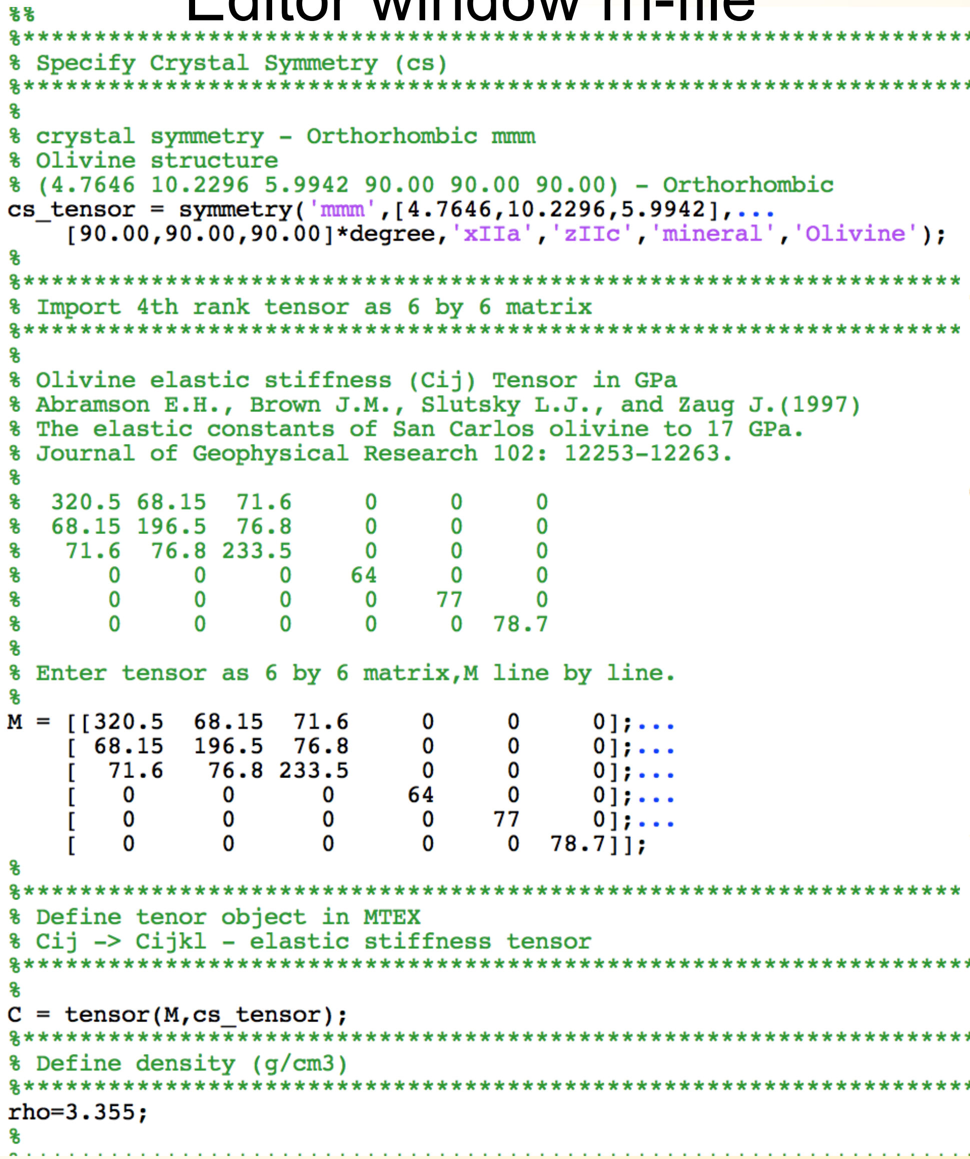


```
beta = volumeCompressibility (C)
beta = linearCompressibility (C,x)
   E = YoungsModulus (C,x)
   G = shearModulus (C,h,u)
  nu = PoissonRatio (C,x,y)
   T = ChristoffelTensor (C,n)
```

Life was not meant to be easy in elasticity! **But there is MTEX!**

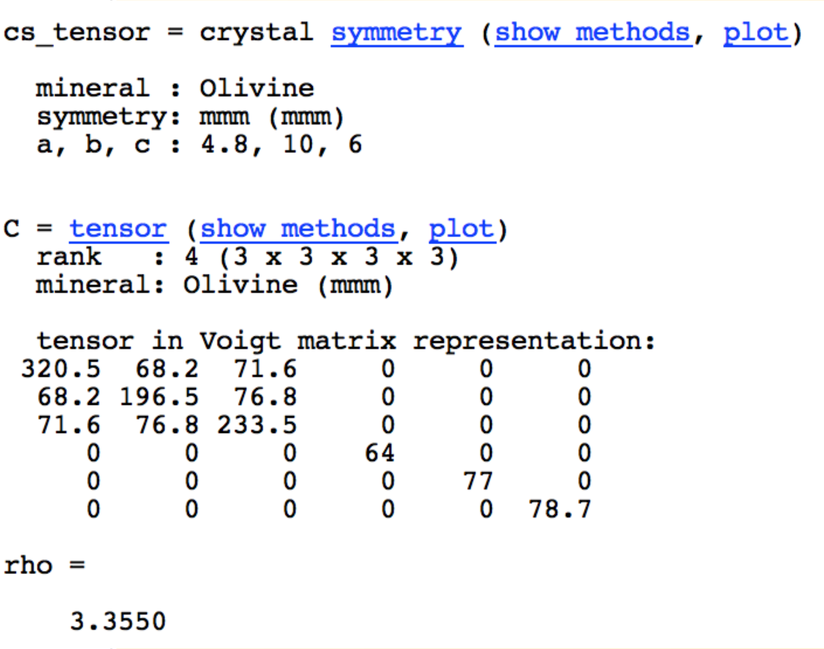
Define Elastic tensor in MTEX

Editor window m-file



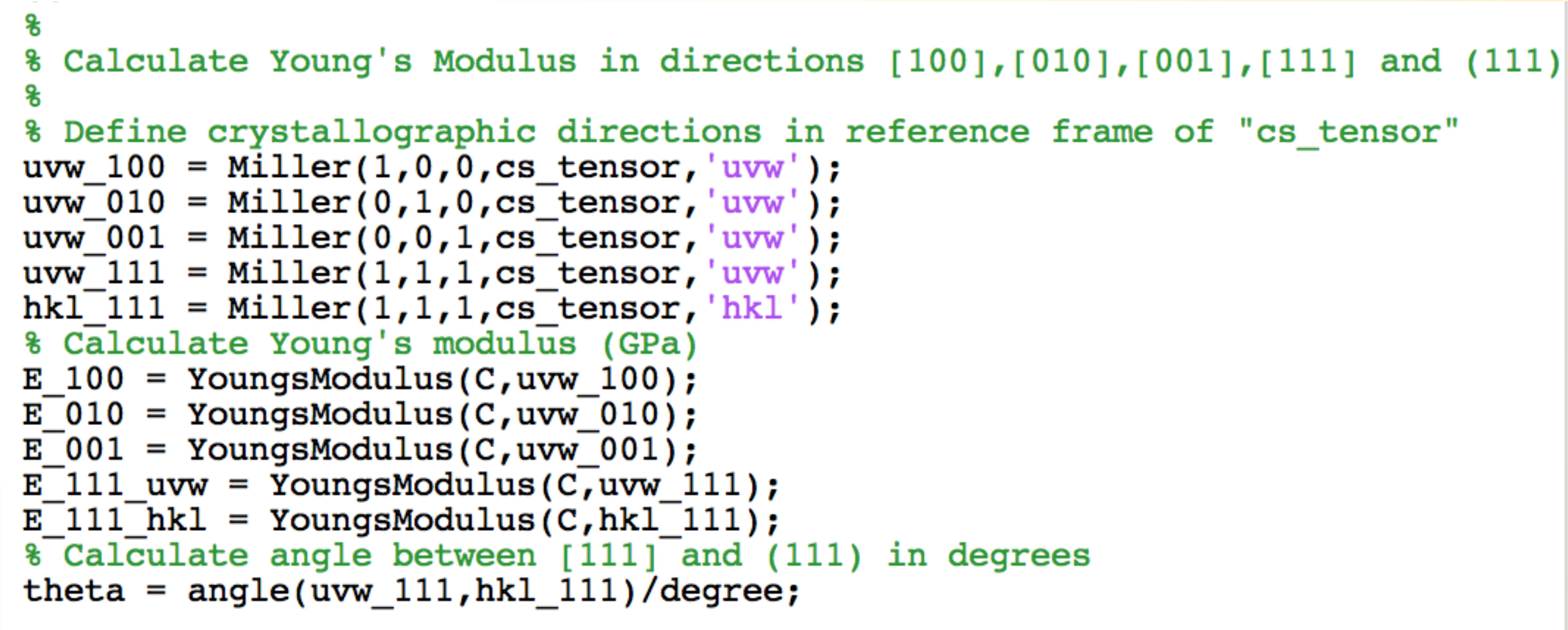
```
%%
%*************************************************************************
% Specify Crystal Symmetry (cs)
%*************************************************************************
%
% crystal symmetry - Orthorhombic mmm
% Olivine structure
% (4.7646 10.2296 5.9942 90.00 90.00 90.00) - Orthorhombic
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
% Abramson E.H., Brown J.M., Slutsky L.J., and Zaug J.(1997)
% The elastic constants of San Carlos olivine to 17 GPa.
% Journal of Geophysical Research 102: 12253-12263.
%
%  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 tenor object in MTEX
% Cij -> Cijkl - elastic stiffness tensor
%*************************************************************************
%
C = tensor(M,cs_tensor);
%*************************************************************************
% Define density (g/cm3)
%*************************************************************************
rho=3.355;
%
```

Command window



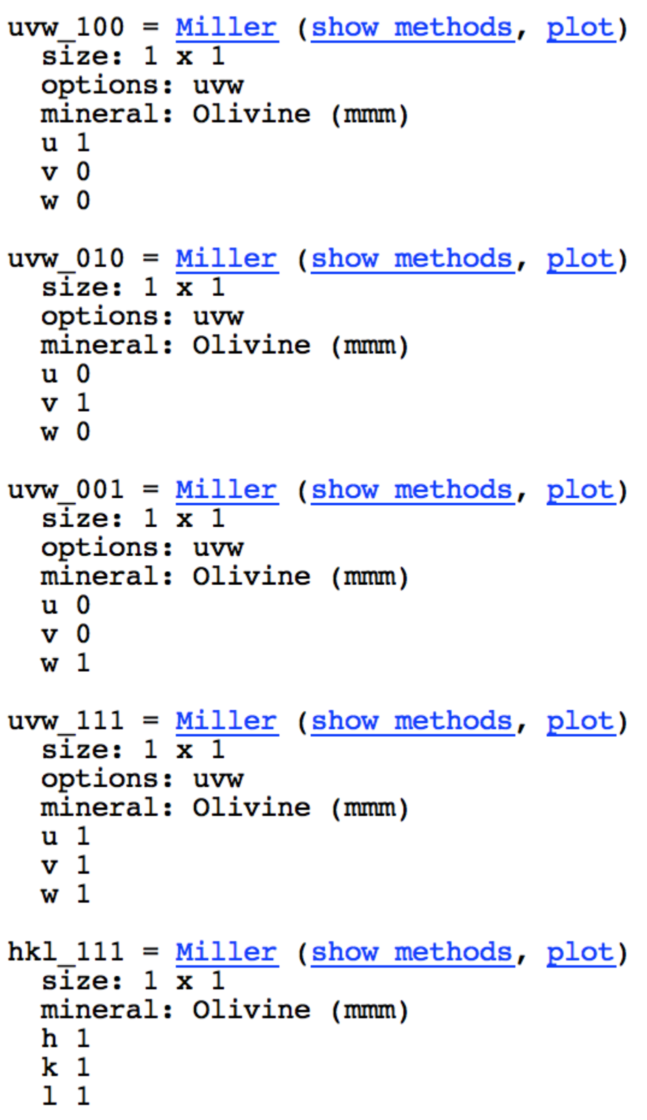
```
cs_tensor = crystal symmetry (show methods, plot)

  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

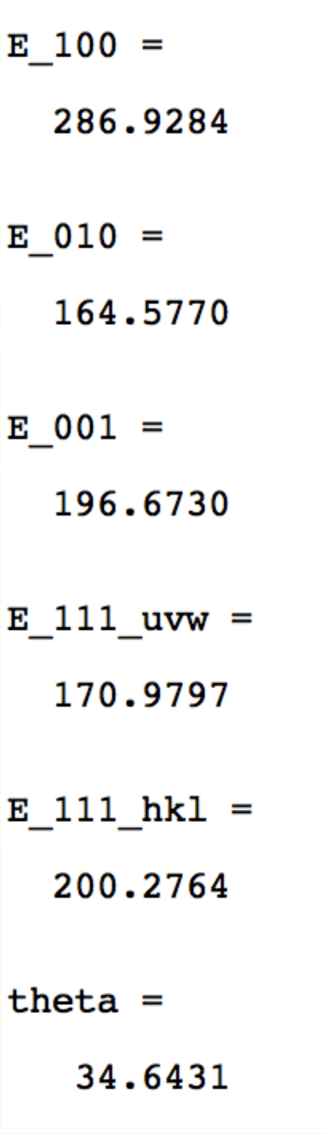


```
%
% Calculate Young's Modulus in directions [100],[010],[001],[111] and (111)
%
% Define crystallographic directions in reference frame of "cs_tensor"
uvw_100 = Miller(1,0,0,cs_tensor,'uvw');
uvw_010 = Miller(0,1,0,cs_tensor,'uvw');
uvw_001 = Miller(0,0,1,cs_tensor,'uvw');
uvw_111 = Miller(1,1,1,cs_tensor,'uvw');
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

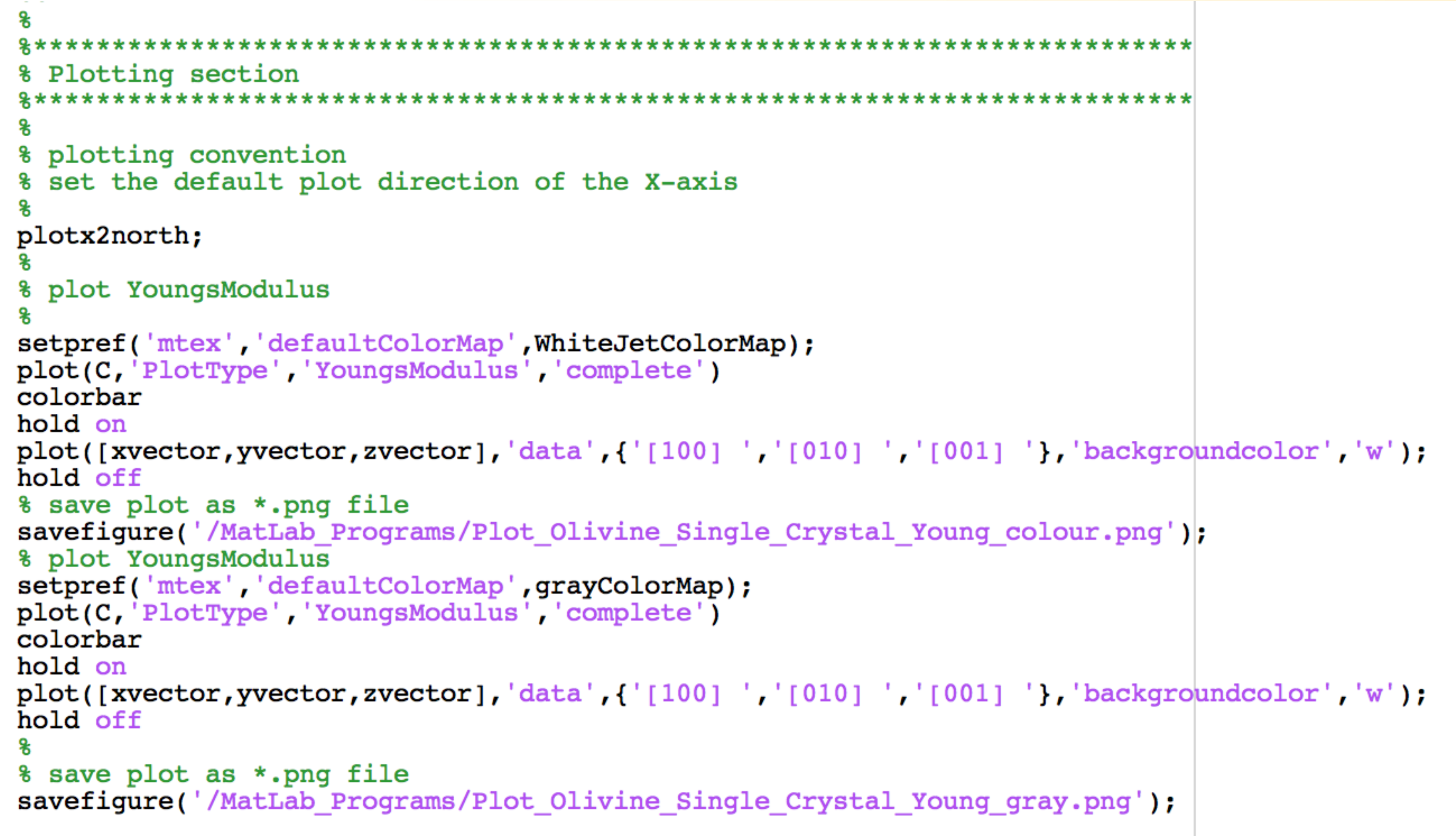


```
uvw_100 = Miller (show methods, plot)
  size: 1 x 1
  options: uvw
  mineral: Olivine (mmm)
  u 1
  v 0
  w 0

uvw_010 = Miller (show methods, plot)
  size: 1 x 1
  options: uvw
  mineral: Olivine (mmm)
  u 0
  v 1
  w 0

uvw_001 = Miller (show methods, plot)
  size: 1 x 1
  options: uvw
  mineral: Olivine (mmm)
  u 0
  v 0
  w 1

uvw_111 = Miller (show methods, plot)
  size: 1 x 1
  options: uvw
  mineral: Olivine (mmm)
  u 1
  v 1
  w 1

hkl_111 = Miller (show methods, plot)
  size: 1 x 1
  mineral: Olivine (mmm)
  h 1
  k 1
  l 1
```



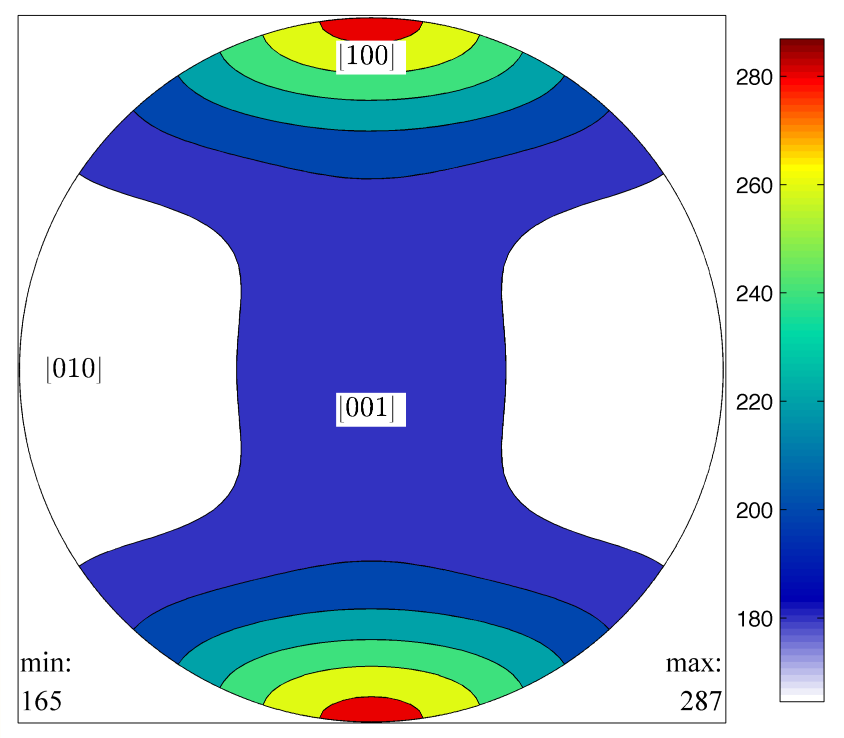
```
E_100 =

   286.9284


E_010 =

   164.5770


E_001 =

   196.6730


E_111_uvw =

   170.9797


E_111_hkl =

   200.2764


theta =

    34.6431
```

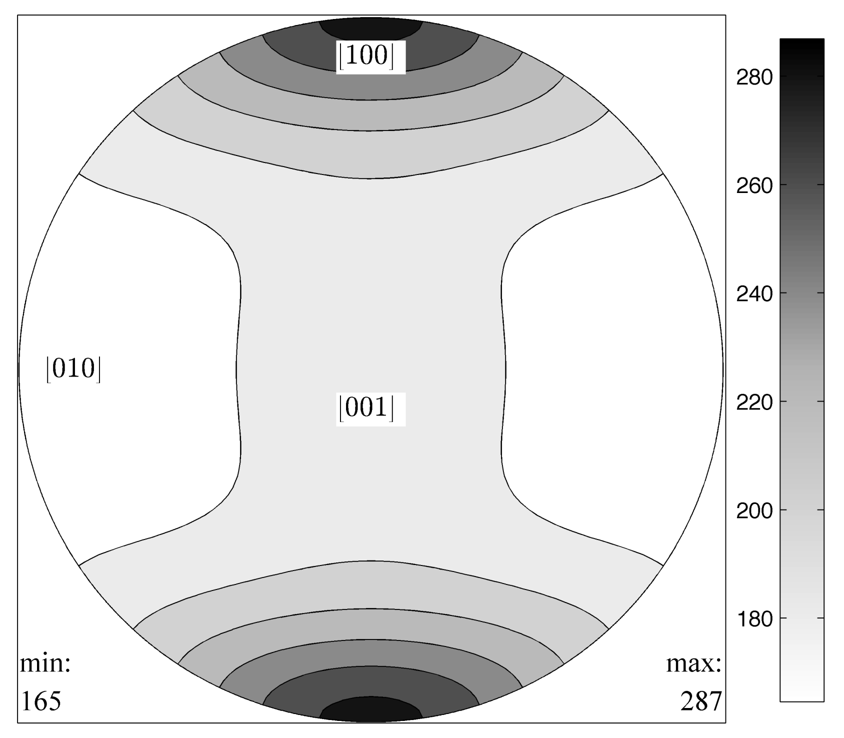
MTEX : Plotting Young’s modulus



```
%
%**************************************************************************
% 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

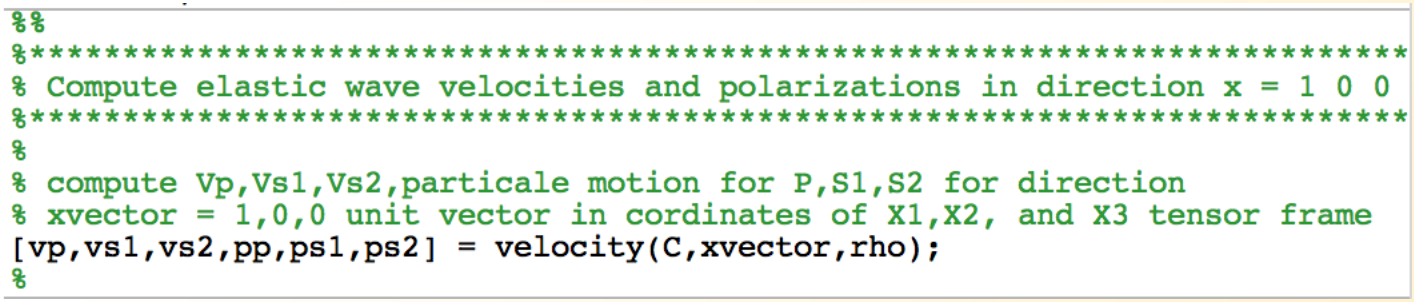




`setMTEXpref('defaultColorMap',WhiteJetColorMap)`

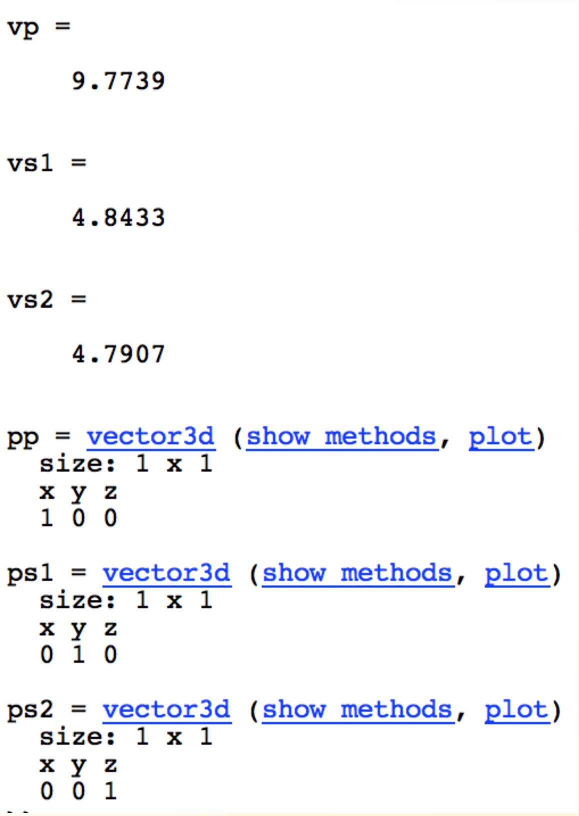
`setMTEXpref('defaultColorMap',white2blackColorMap)`

MTEX – calculate velocities (plotx2north)



```
%%
%***************************************************************************
% 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 cordinates of X1,X2, and X3 tensor frame
[vp,vs1,vs2,pp,ps1,ps2] = velocity(C,xvector,rho);
%
```

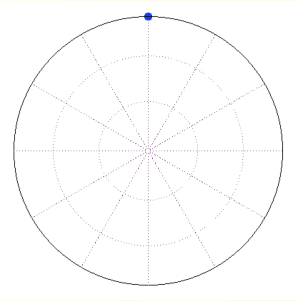
Velocities in km/s



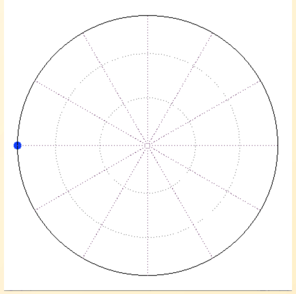
```
vp =

    9.7739


vs1 =

    4.8433


vs2 =

    4.7907


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

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

ps2 = vector3d (show methods, plot)
  size: 1 x 1
  x y z
  0 0 1
```

plot

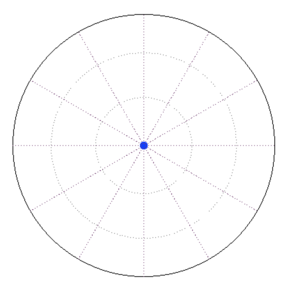
pp polarization vp



ps1 polarization vs1



ps2 polarization vs2



show methods

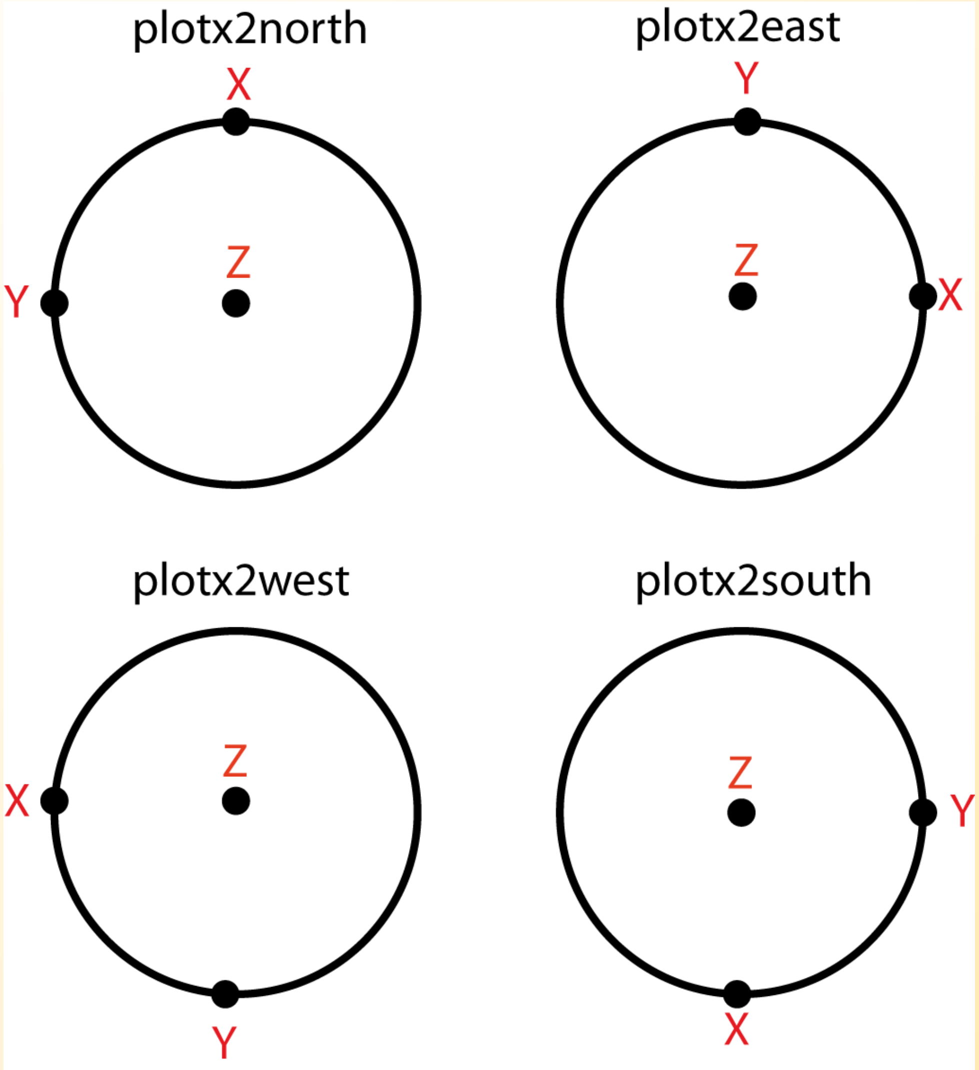
```
Methods for class vector3d:

  abs                             angle
  angle_outer                     char
  check_option                    cross
  ctranspose                      delete_option
  display                         dot
  dot_outer                       double
  end                             eq
  extract_option                  find
  get                             getx
  gety                            getz
  horzcat                         kernelDensityEstimation
  length                          mean
  minus                           mtimes
  ne                              norm
  normalize                       numel
  orth                            plot
  plus                            polar
  project2FundamentalRegion       rdivide
  repmat                          reshape
  rotate                          SchmidTensor
  set                             set_option
  size                            subsasgn
  subsref                         sum
  symmetrise                      times
  transpose                       uminus
  unique                          vector3d
  vertcat
```

Sample co-ordinates for plotting in MTEX

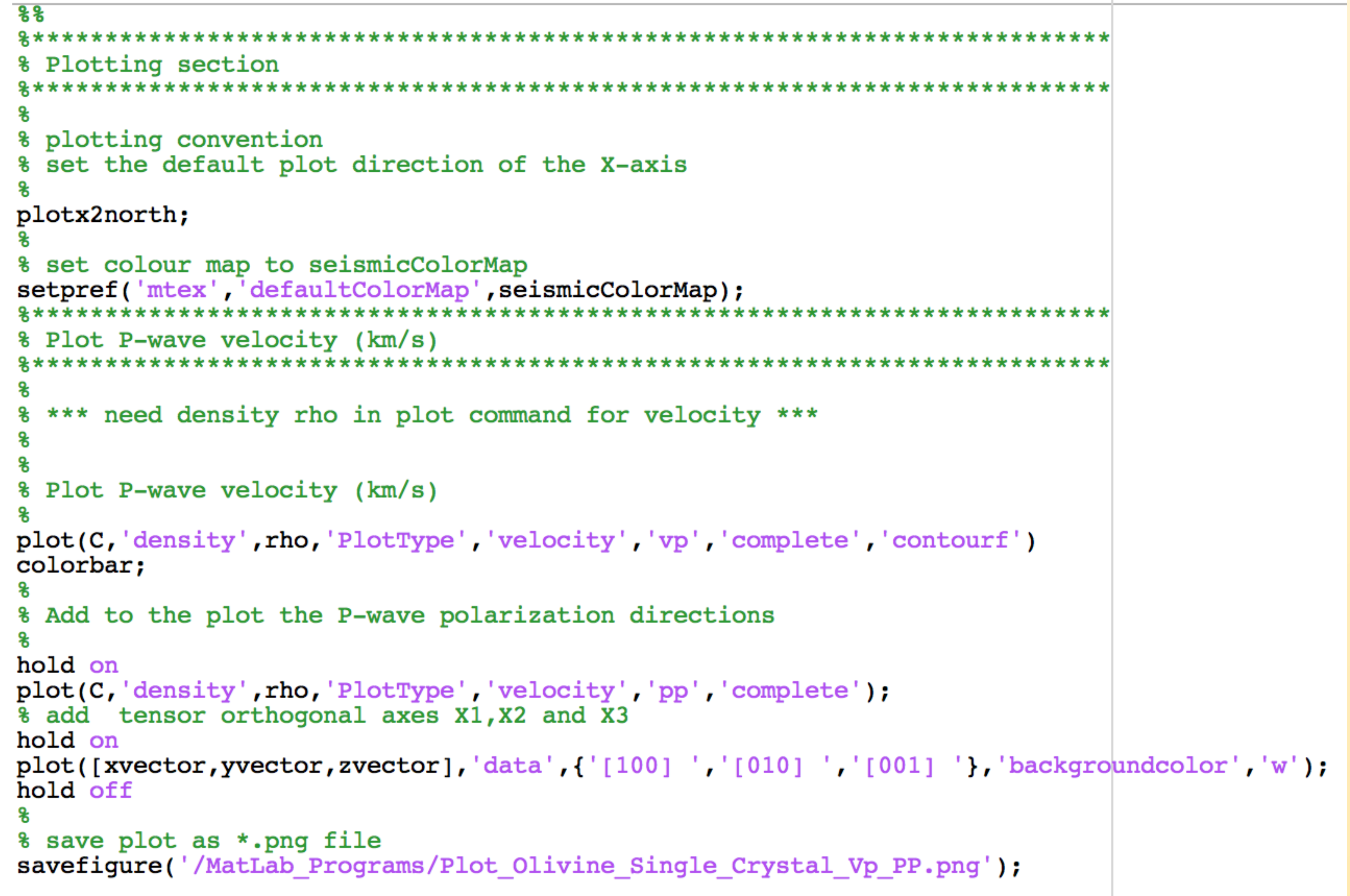
Default
plotx2north

Defined in
upper hemisphere

N.B. only rotates Plots, does not affect numerical results

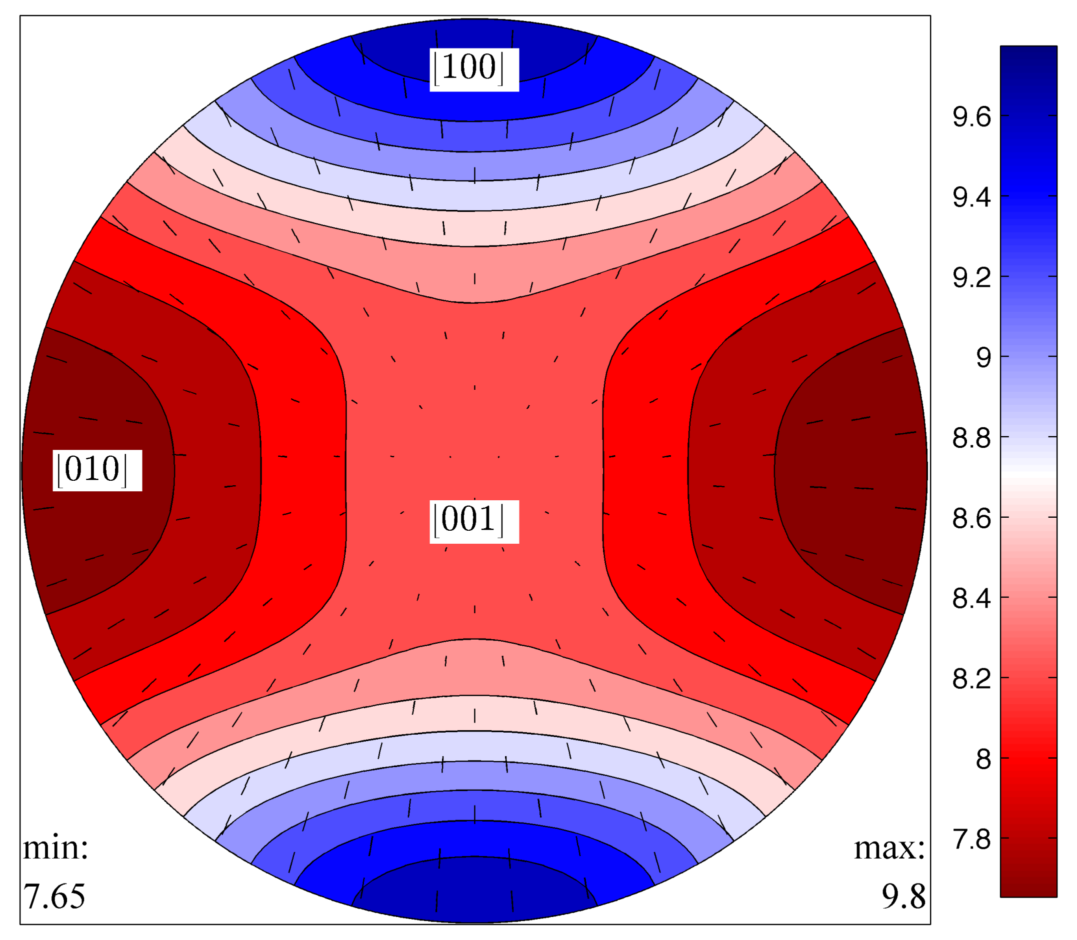


MTEX – plot velocities



```
%%
%**************************************************************************
% Plotting section
%**************************************************************************
%
% plotting convention
% set the default plot direction of the X-axis
%
plotx2north;
%
% set colour map to seismicColorMap
setpref('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)**
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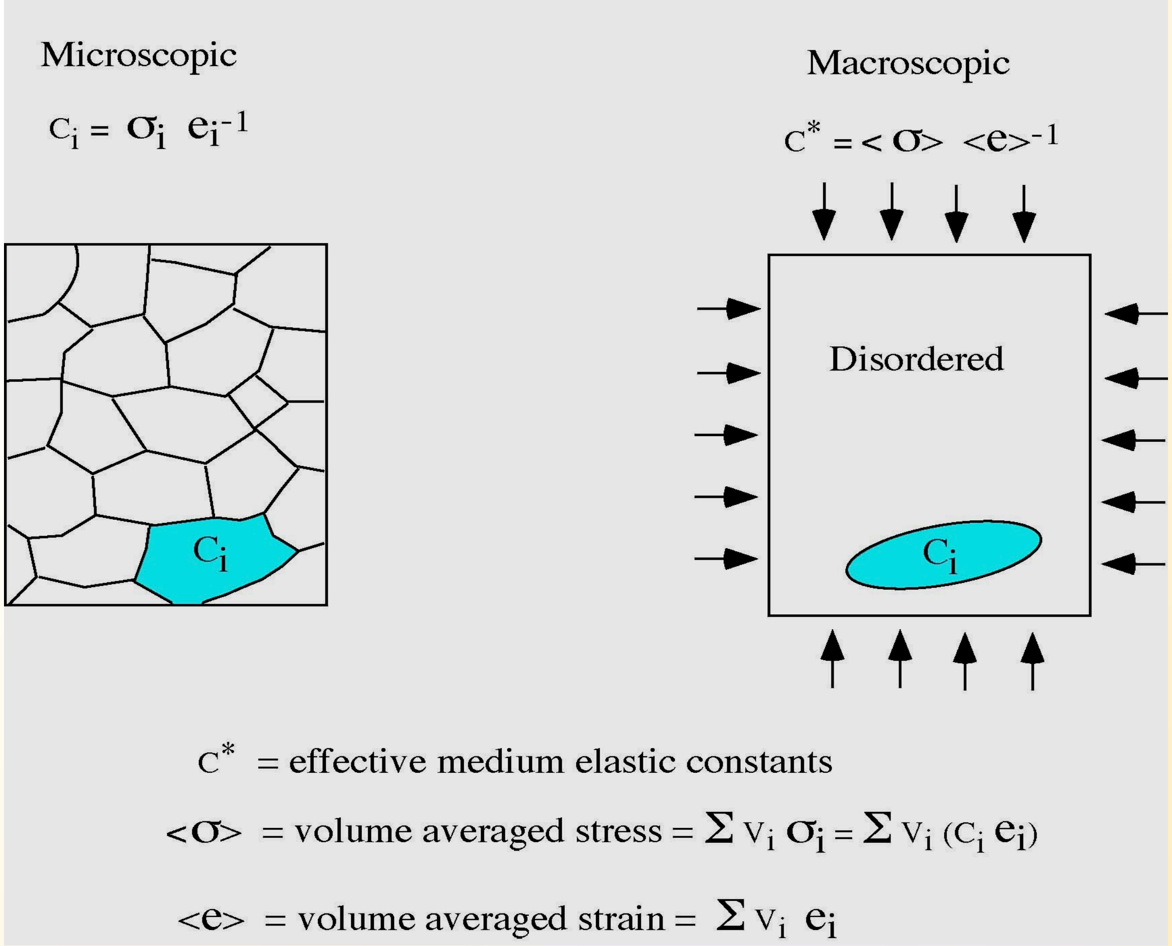
- Cady, W. G. Piezoelectricity: An Introduction to the Theory and Applications of Electromechanical Phenomena in Crystals, New rev. ed., 2 vols. New York: Dover, 1964.
- Bhagavantam, S., Crystal Symmetry and Physical Properties , London, New York, Academic Press (1966)
- D.McKie and C.McKie Crystalline Solids Nelson, 1974 (Chapter 11)
- *Nye, J. F., Physical Properties of Crystals , Oxford, Clarendon Press (1957,1985 2nd Edition)*
- *Sirotin, Yu. I. & Shakolskaya, M. P. 1982. Fundamentals of Crystal Physics. Mir, Moscow, 654.*
- **Putnis, A. 1992. Introduction to Mineral Sciences, Cambridge University Press (Chapter 2)**
- **Wenk, H.-R. and Bulakh,A., 2004. Minerals Their Constitution and Origin, Cambridge University Press. (Chapter 8)**
- **Newnham, R.E., 2005. Properties of materials Anisotropy, Symmetry, Structure. Oxford University Press,Oxford**.
- **Mainprice, D. (2007) Seismic anisotropy of the deep Earth from a mineral and rock physics perspective. Schubert, G. '*Treatise in Geophysics*' Volume 2 pp437-492. Oxford: Elsevier. (I have a PDF of this chapter)**

Effective media : average properties for polycrystalline aggregates, Voigt, Reuss and Hill…

2 Germans & 1 Englishman

Microscopic and Macroscopic



c^* = effective medium elastic constants

$<\sigma>$ = volume averaged stress = $\Sigma \, v_i \, \sigma_i = \Sigma \, v_i \, (c_i \, e_i)$

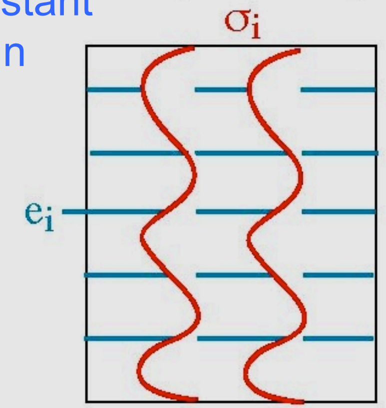
$<e>$ = volume averaged strain = $\Sigma \, v_i \ e_i$

Homogeneous
Effective
Media
(H.E.M.)

Simple volume averages

Voigt Average

Constant strain

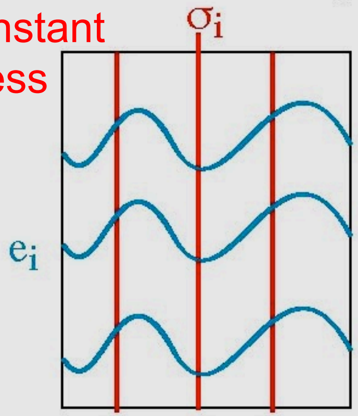


$e_i = \text{constant}: C^* \langle \sigma \rangle = \Sigma v_i (C_i \ e_i)$

$\boxed{C^* \approx C^{Voigt} = \Sigma v_i C_i}$

Reuss Average

Constant stress

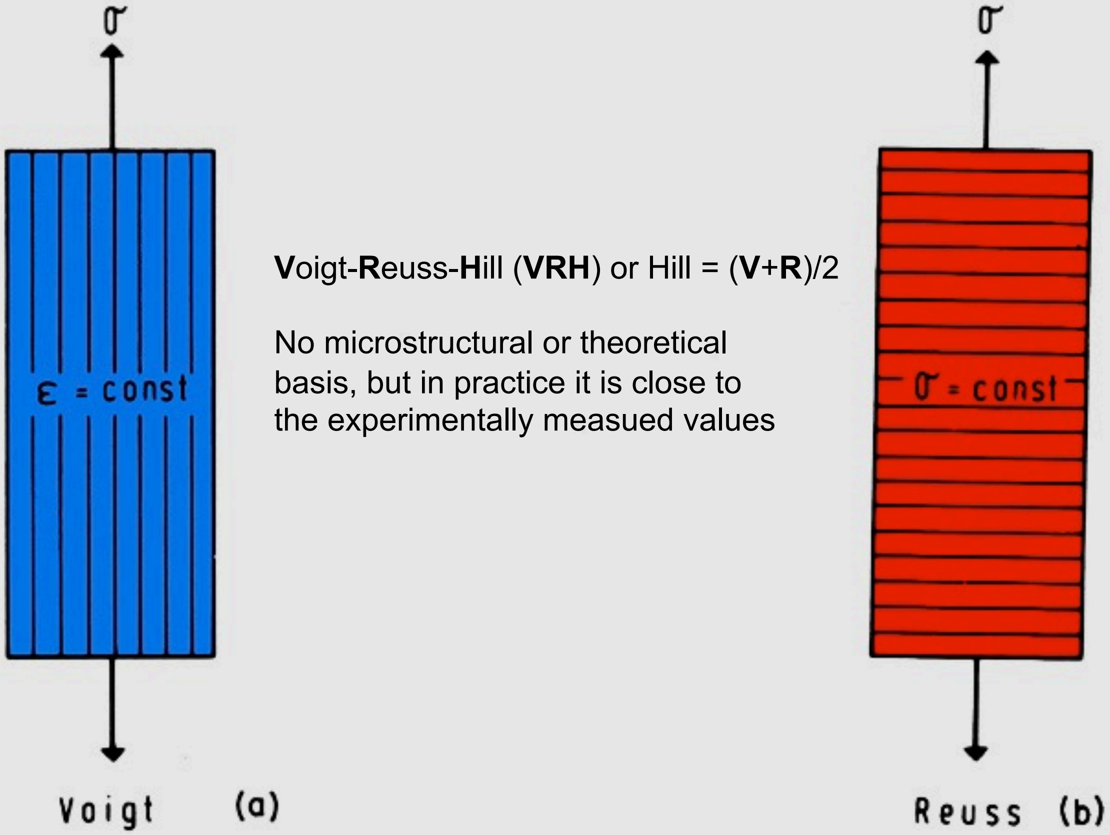


$\sigma_i = \text{constant}: C^* \ \langle e \rangle^{-1} = (\Sigma v_i \ e_i)^{-1} = (\Sigma v_i \ (S_i \sigma_i)))^{-1}$

$\boxed{C^* \approx C^{Reuss} = (\Sigma v_i \ S_i)^{-1}}$

- 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

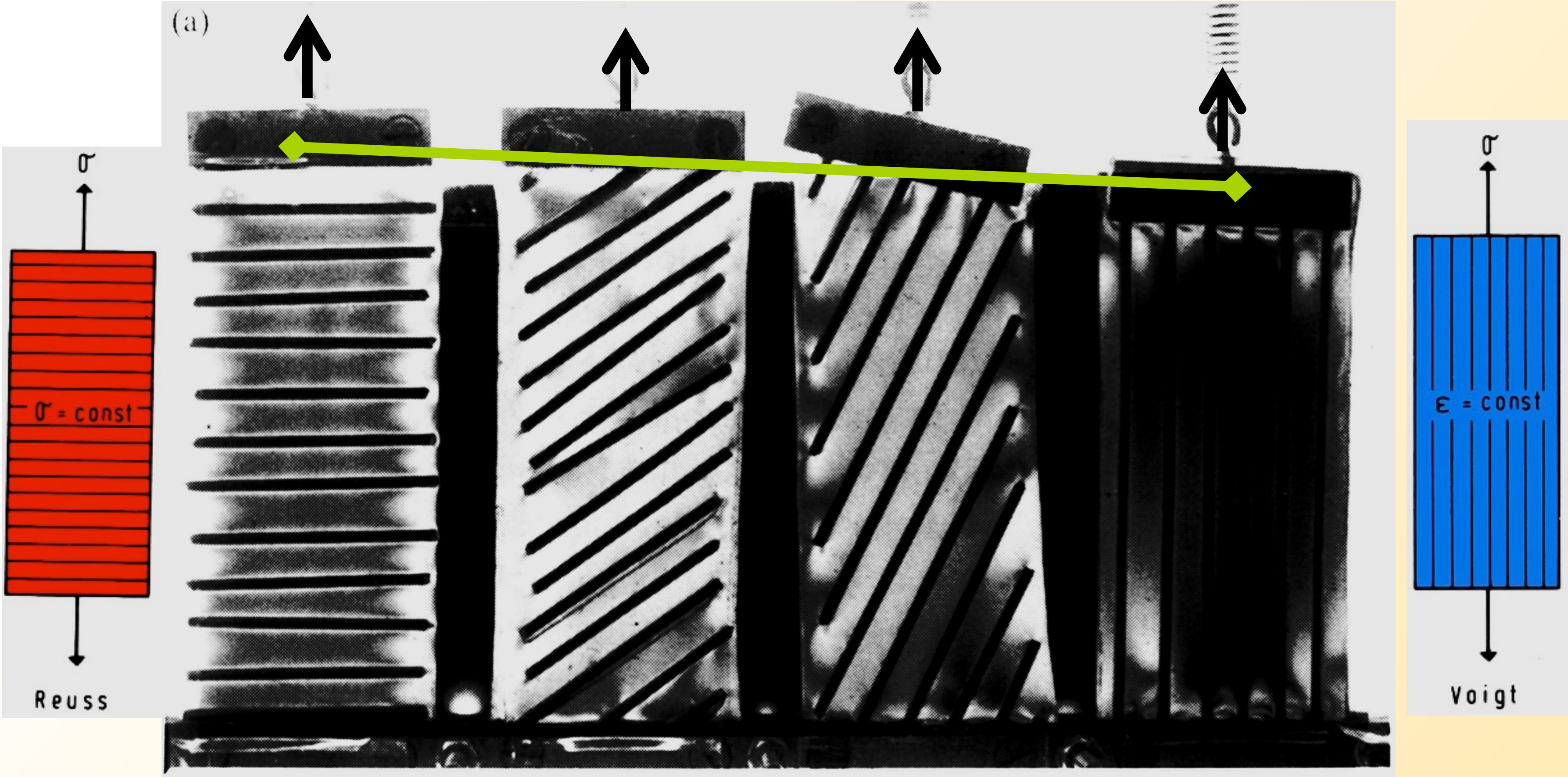


Voigt-**R**euss-**H**ill (**VRH**) or Hill = (**V**+**R**)/2

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

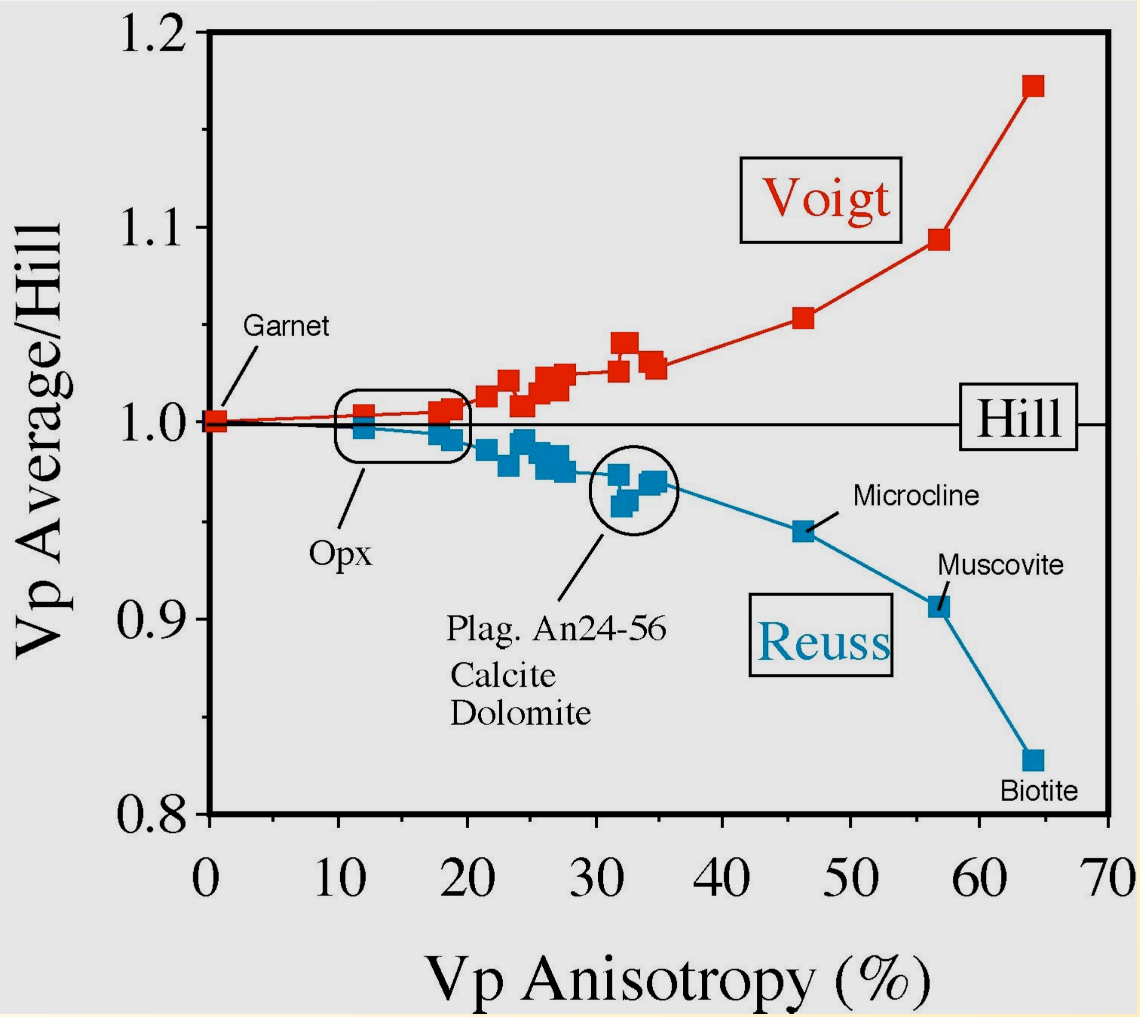
(a) Grain structure of a polycrystal for which Voigt's assumption is valid. (b) Grain structure of a polycrystal for which Reuss's assumption is valid.

Macromodel composite laminates



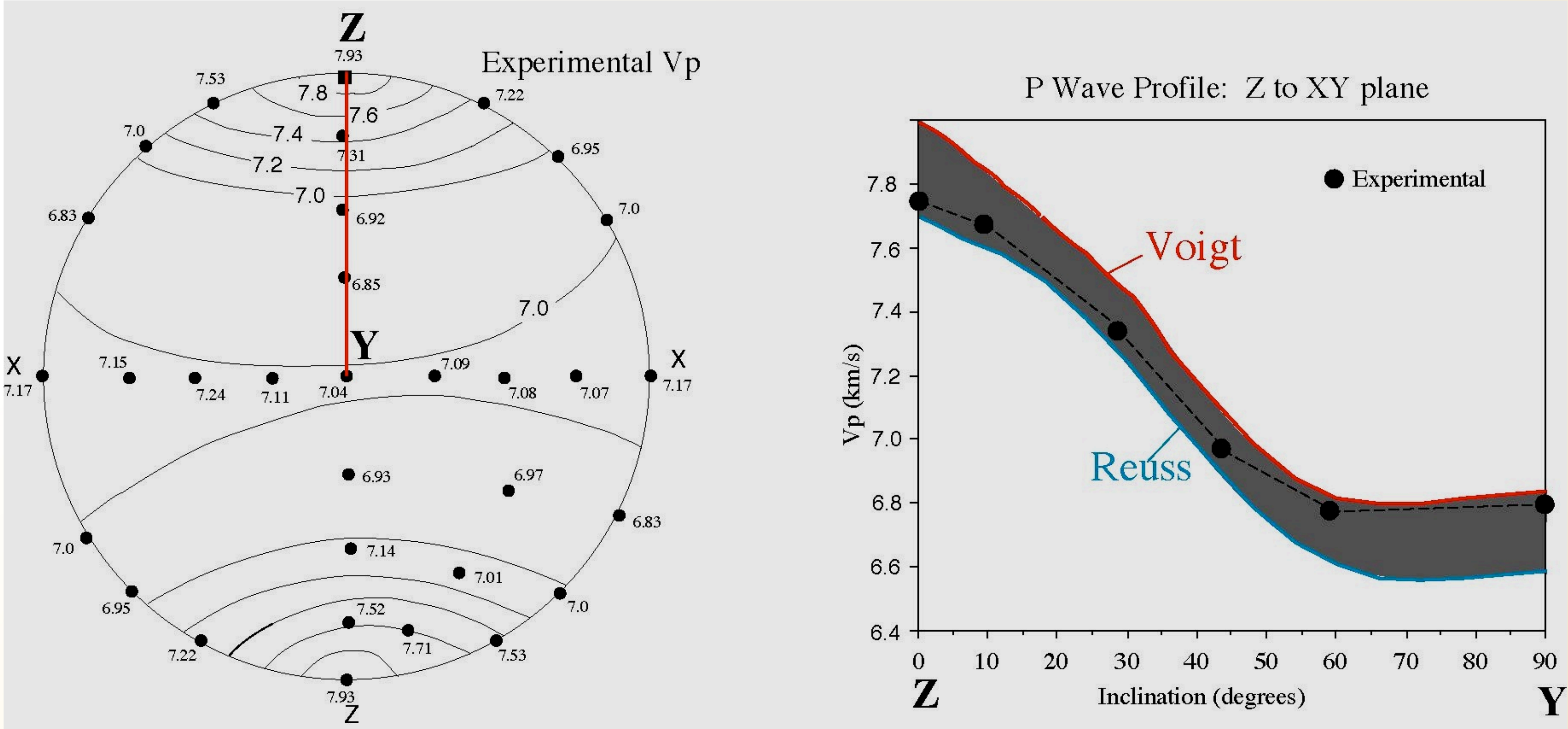
Aligned metal rods(black) in polyurethane matrix grey where lighter greys - larger shear strains

Vp Polycrystal Averages



MAINPRICE, D. and HUMBERT M. (1994) Surveys in Geophysics 15, 575-592.

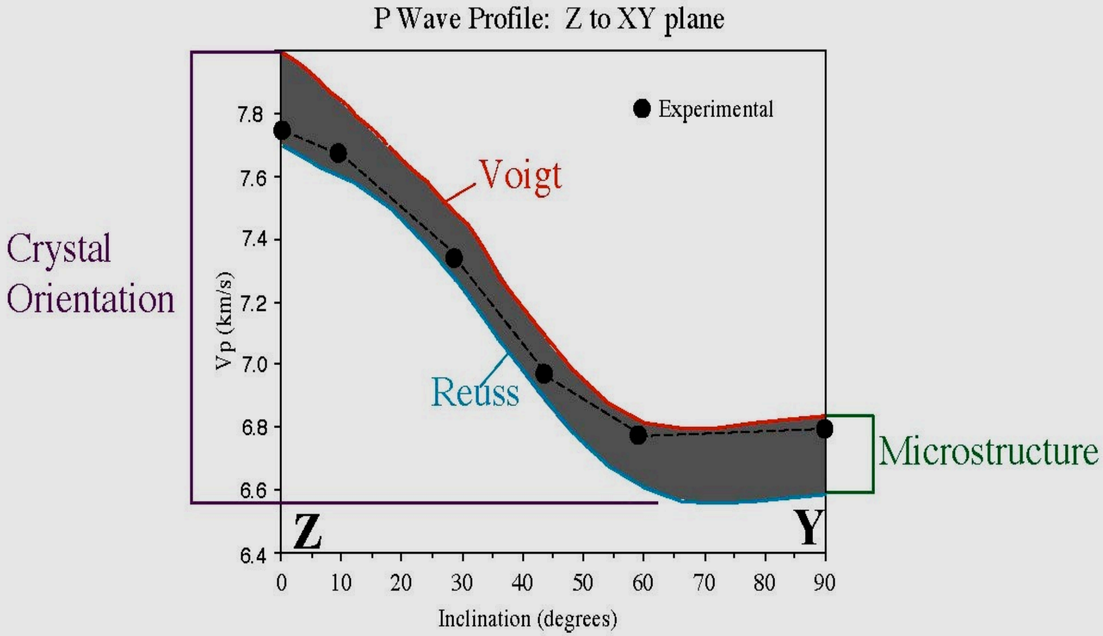
Oklahoma Gabbro
Stereo & Vp YZ profile



Confining pressure = 800 MPa

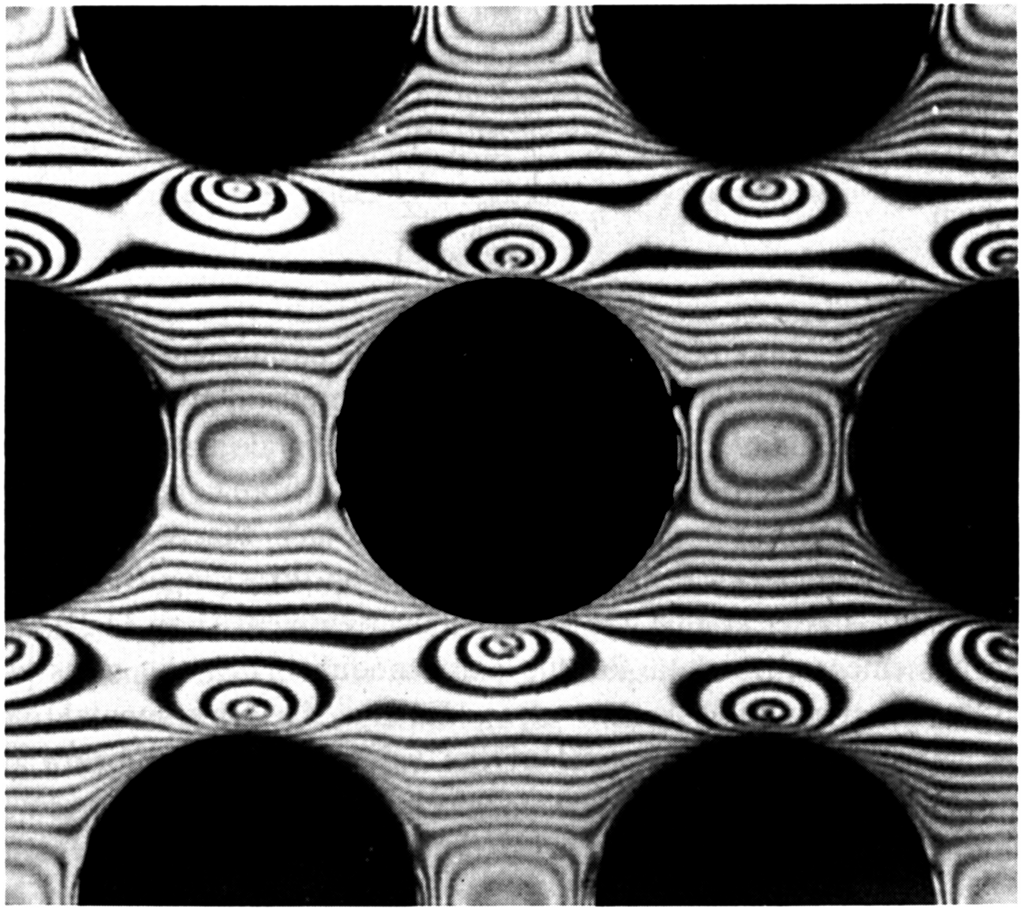
SERONT, B., MAINPRICE, D. AND CHRISTENSEN, N.I. (1993)
J. Geophy. Res. 98: 2209-2221.

Physical Properties & Microstructure - Composite materials approach



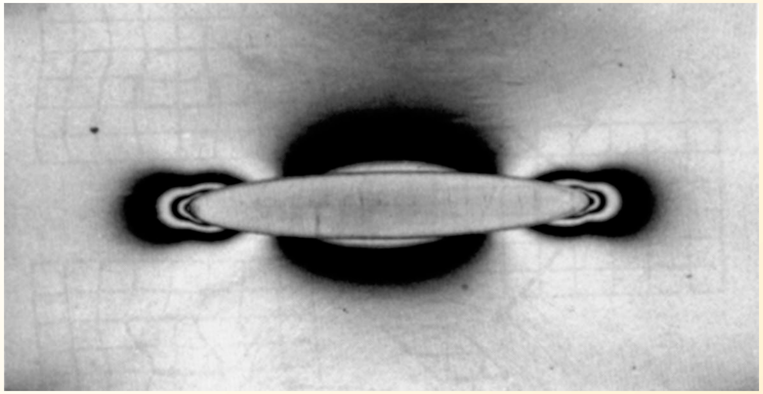
Crystal Orientation "signal" = 5 x Microstructure "signal"

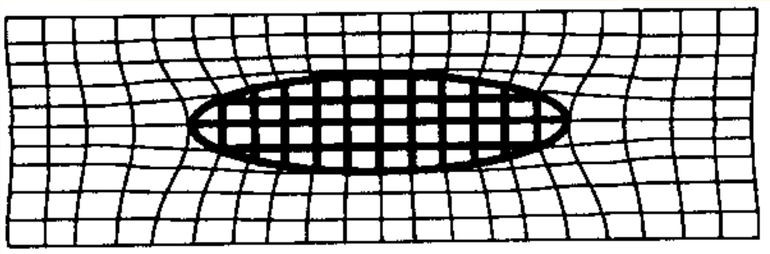
Interaction between inclusions



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

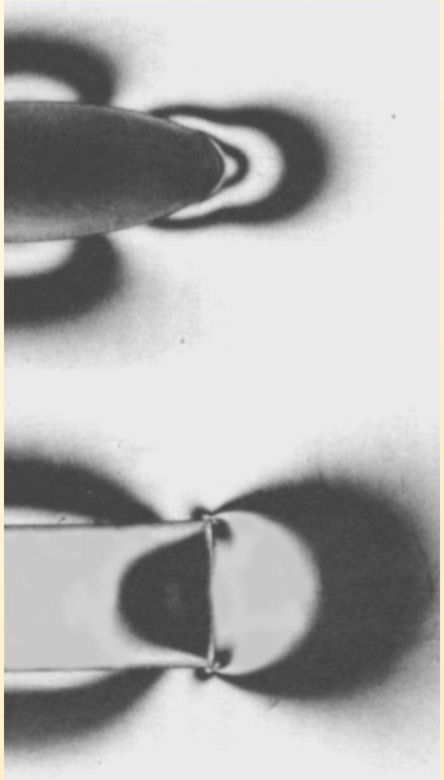
Ellipsoidal inclusion - special properties





Uniform stress and strain field within the inclusion

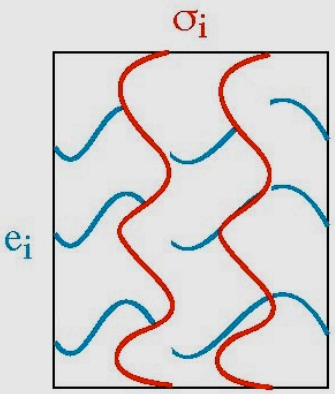
Ellipsoid and Cylinder



homogeneous stress & strain fields

heterogeneous stress & strain fields

Self Consistent (SC) Method

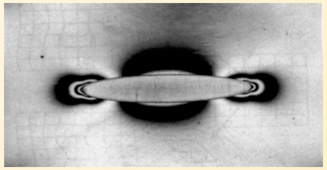


$e_i \neq$ constant $\sigma_i \neq$ constant : $C^* = <\sigma> \; <e>^{-1}$

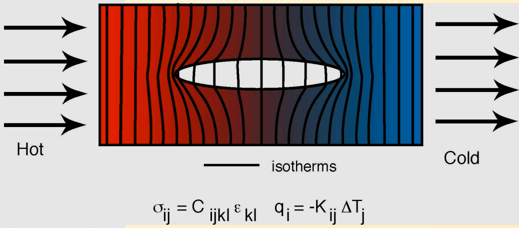
$$C^* = <\sigma> \; <e>^{-1}$$

$$<\sigma> = \Sigma V_i (C_i e_i) \qquad <e> = \Sigma V_i e_i$$

$$\boxed{C^* \approx C^{SC} = <\sigma> . <e>^{-1} = [\Sigma V_i (C_i e_i)] . [\Sigma V_i e_i]^{-1}}$$



The value of e_i is found using a generalization of Eshelby's inclusion theory to anisotropic inclusions in anisotropic back ground media.

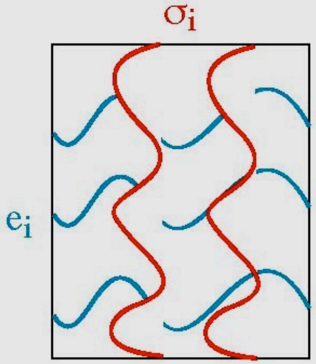


$$e_i = [\mathbf{I} + \mathbf{G} (C_i - C^*)]^{-1}$$

Where **I** is the 4th rank idenity tensor and **G** is a Green's tensor involving ellipitical intergrals 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 ellipsiodal inclusion
- "best" bounds for mixtures with very different stiffnesses e.g. solids,liquids and voids
- treats every object (grain, void, fracture) in an identical manor
- further information about neighbour interaction could be introduced via two-point correlation functions

DEM Method

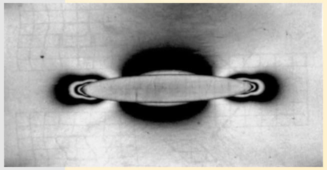


$e_i \neq$ constant $\sigma_i \neq$ constant : $C^* = \langle\sigma\rangle \langle e\rangle^{-1}$

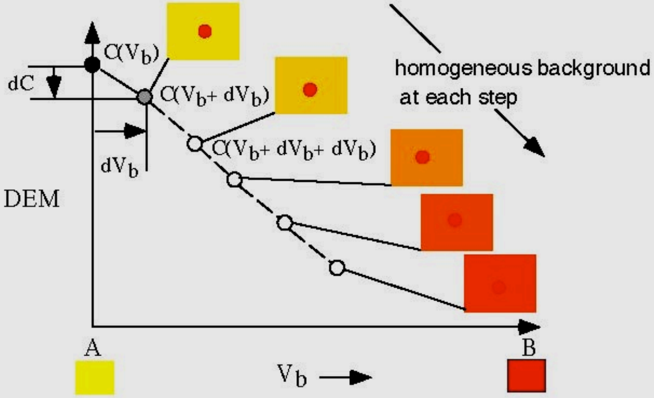
$$C^* = \langle\sigma\rangle \langle e\rangle^{-1}$$

$$\langle\sigma\rangle = \Sigma V_i (C_i e_i) \qquad \langle e\rangle = \Sigma V_i e_i$$

$$\boxed{dC^* \approx dC^{DEM} = \frac{dV_b}{(1-V_b)} (C_i - C^{DEM}) e_i}$$

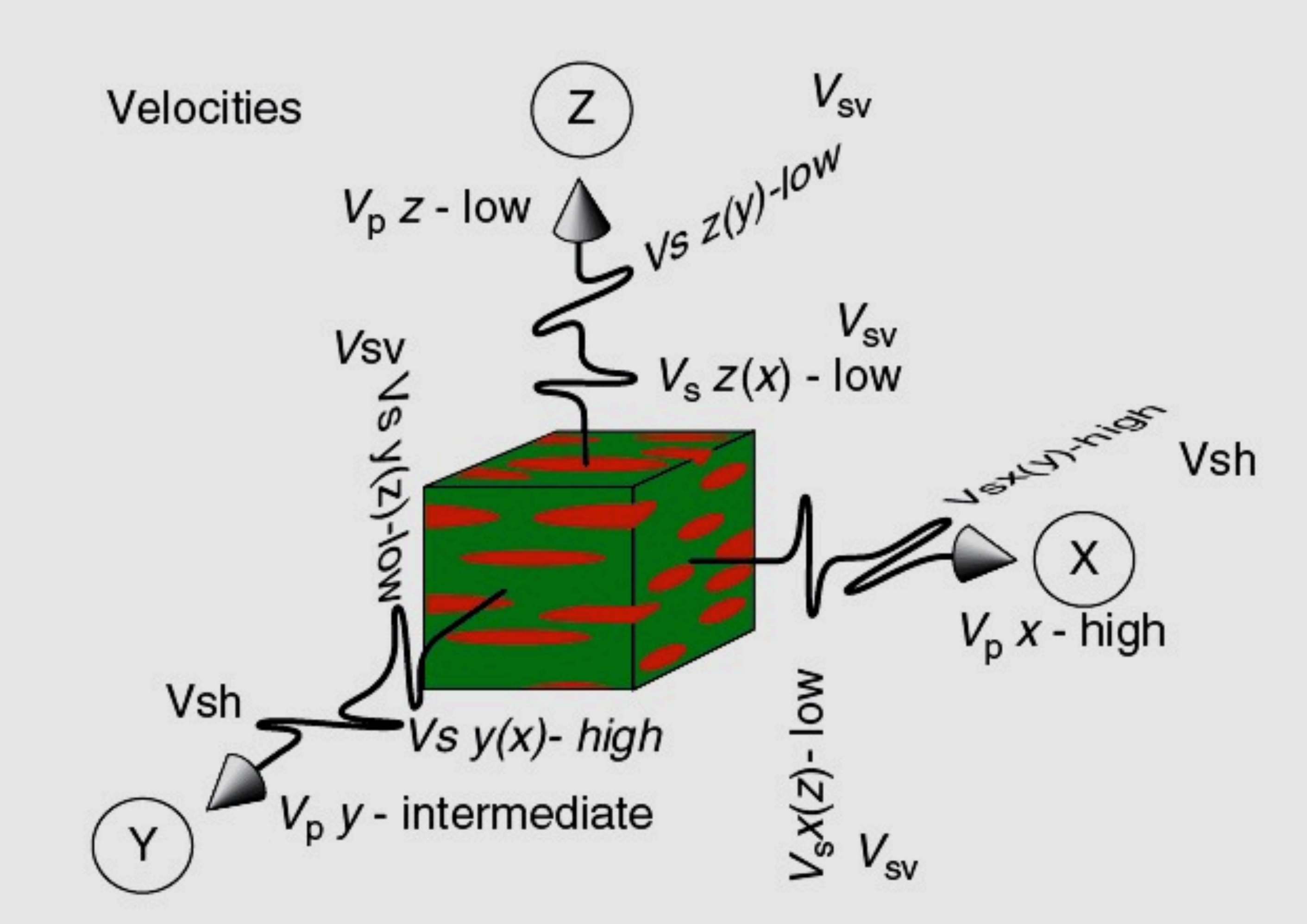


Developed for two phase aggregates type AB (McLaughlin,1977) where Vb = 1-Va. The phase B is the included phase and phase A is the host phase. Requires some inital value of C* at a compostion Vb - this may be a pure end member.The incremental nature of the differential approch preserves the percolating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

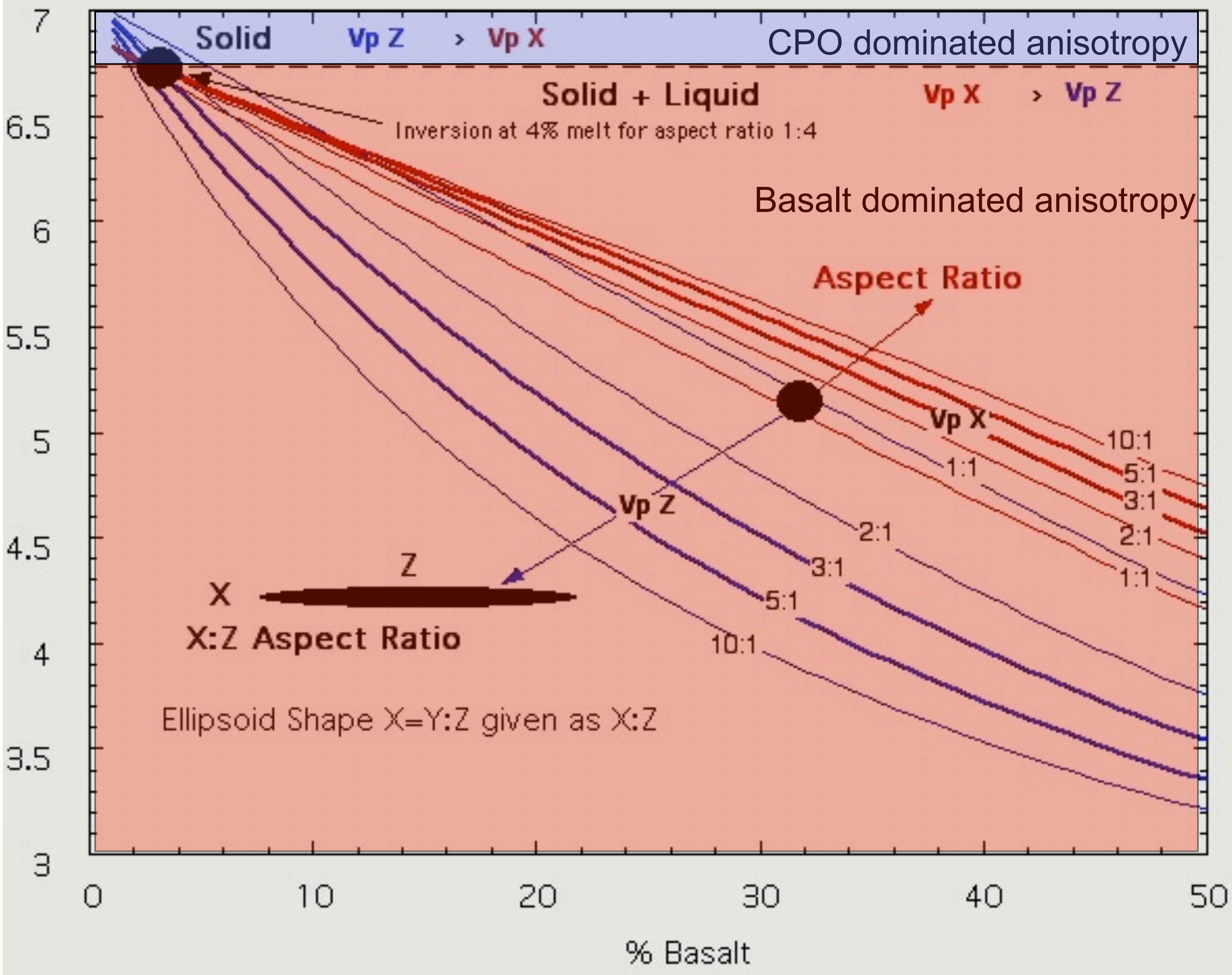


- now phases A and B are microstructurally different (A=Host, B= Inclusion)
- preserves connectivity of initial estimate

Velocity Cube – with melt inclusions

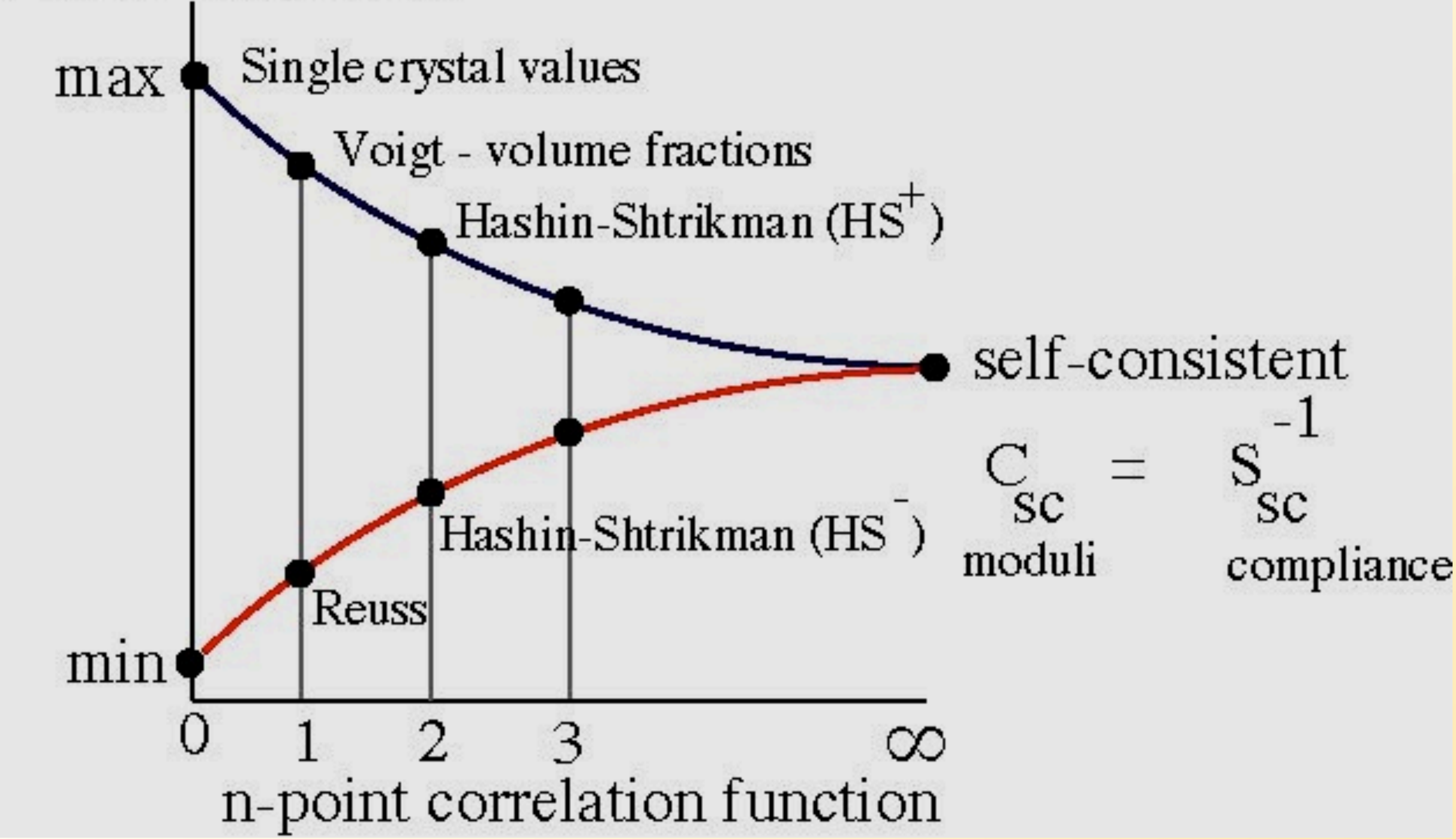


VpX and VpZ Gabbro - Basalt : Effect of Aspect Ratio



MAINPRICE, D. (1997) Tectonophysics 279,161-179.

Elastic Properties

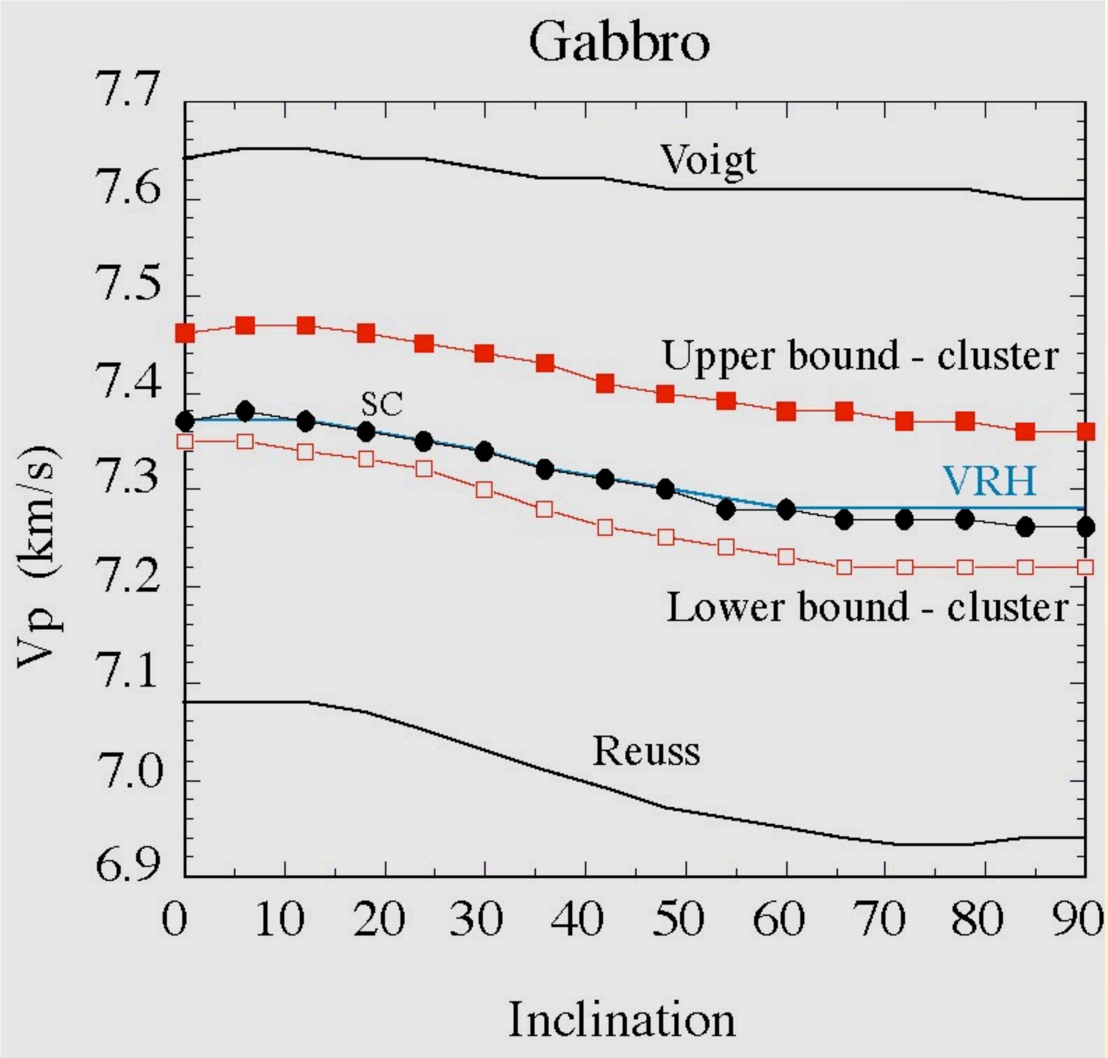


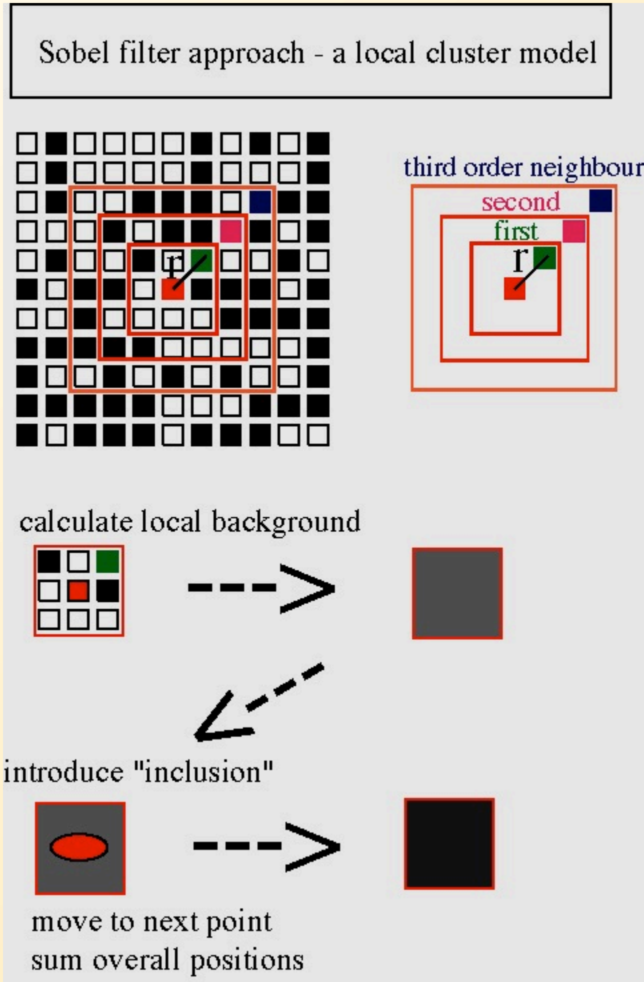
$$C_{sc} = S_{sc}^{-1}$$

moduli

compliance

Cluster method



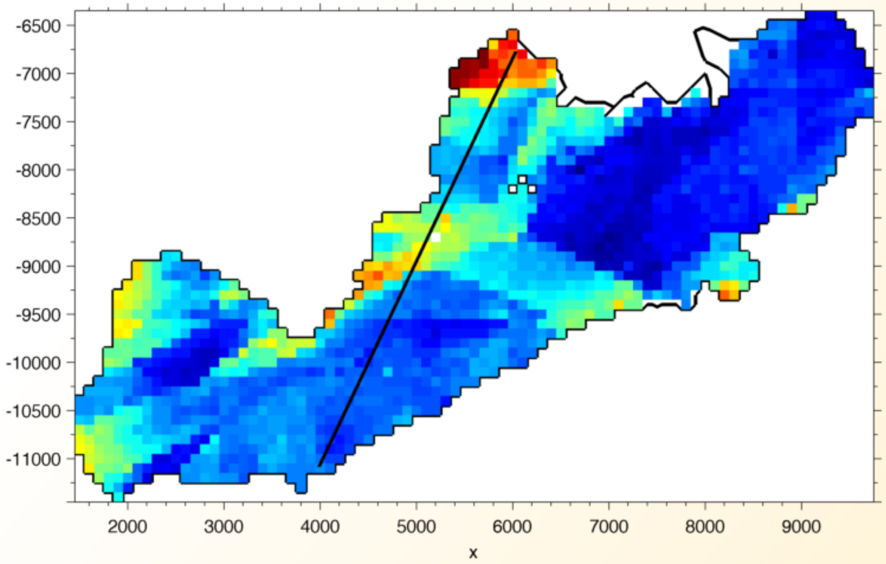


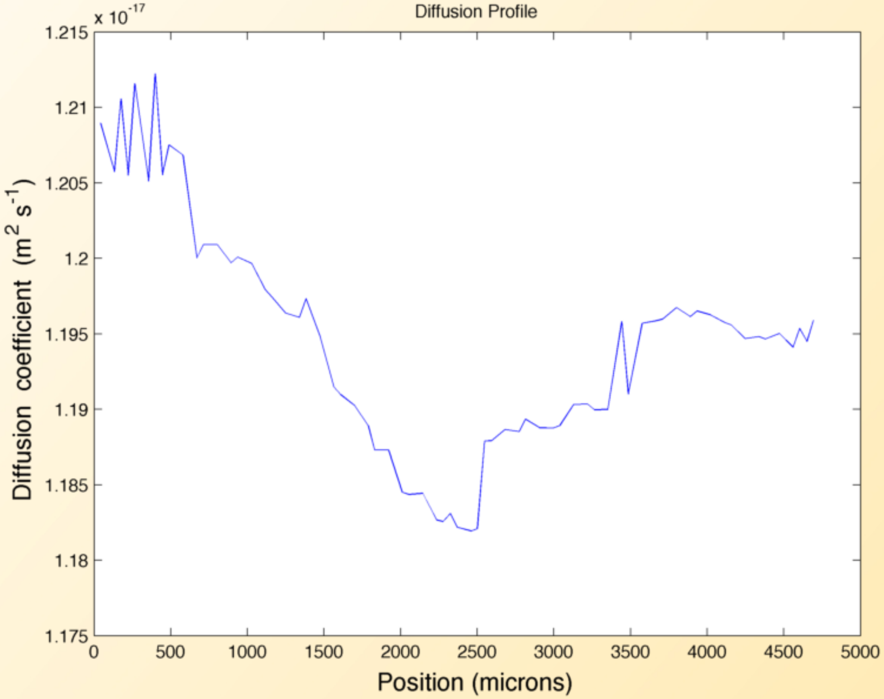
MAINPRICE, D. (2000) Physics and Chemistry of the Earth, 25,155-161.

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 : 2nd rank tensors *e.g.* chemical diffusivity
- Properties : 3rd rank tensors *e.g.* piezoelectricity
- Properties : 4th 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 you own color scales
- And any thing else you care to add !

Ca-diffusion in olivine





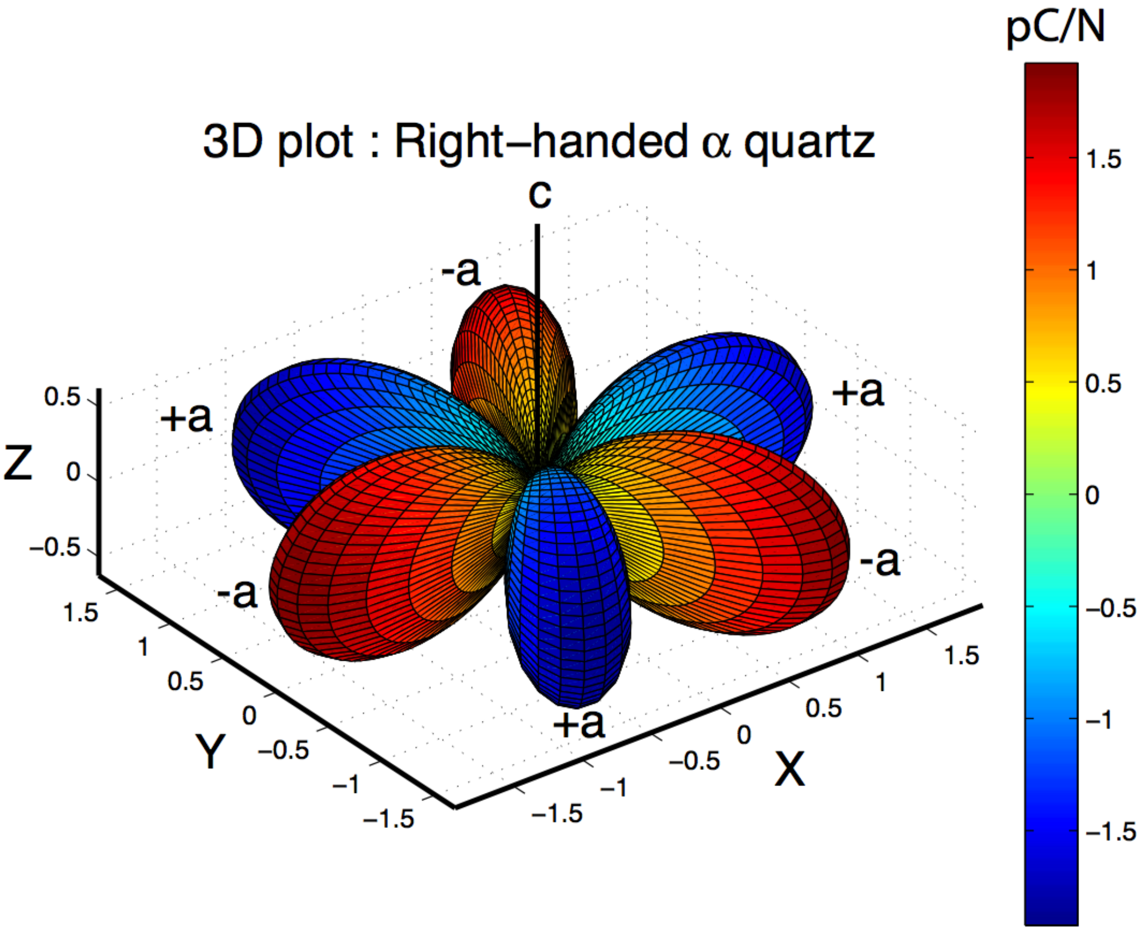
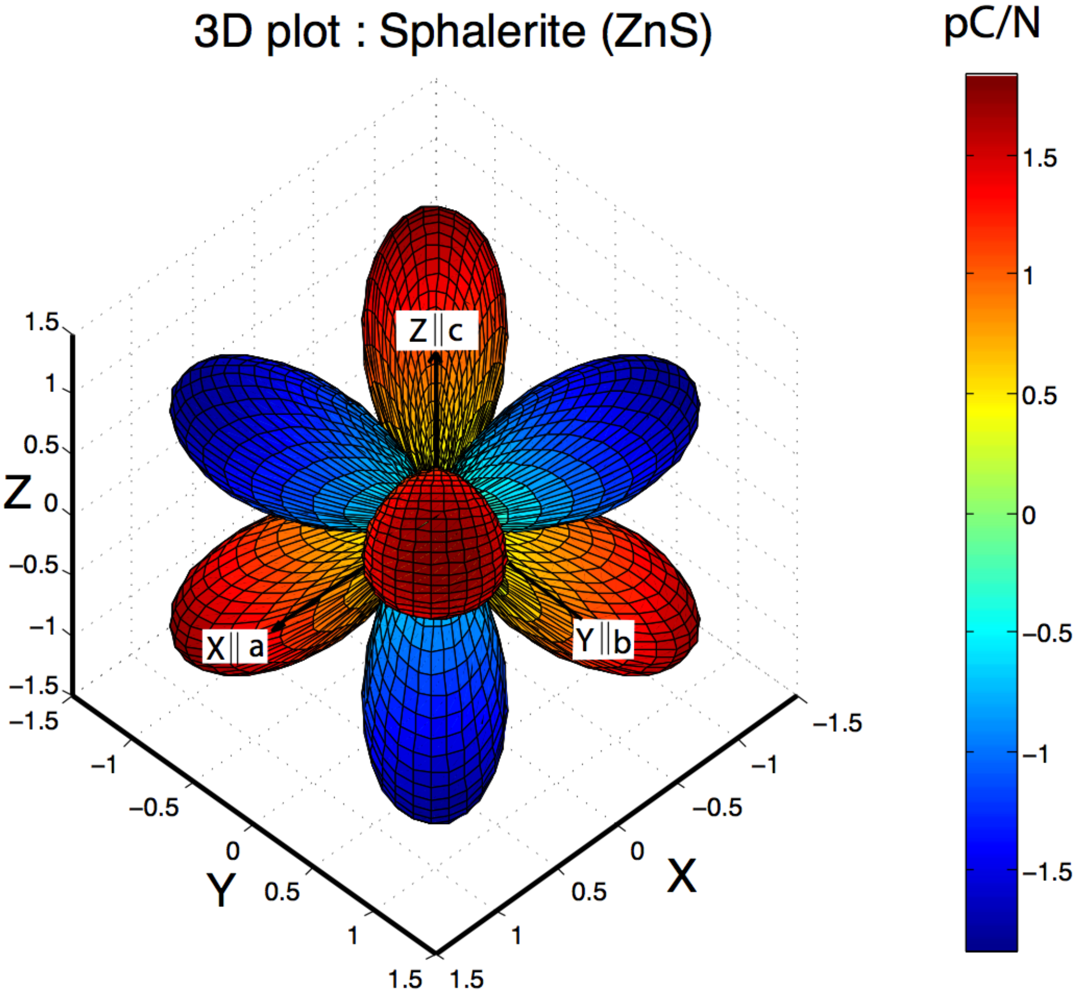


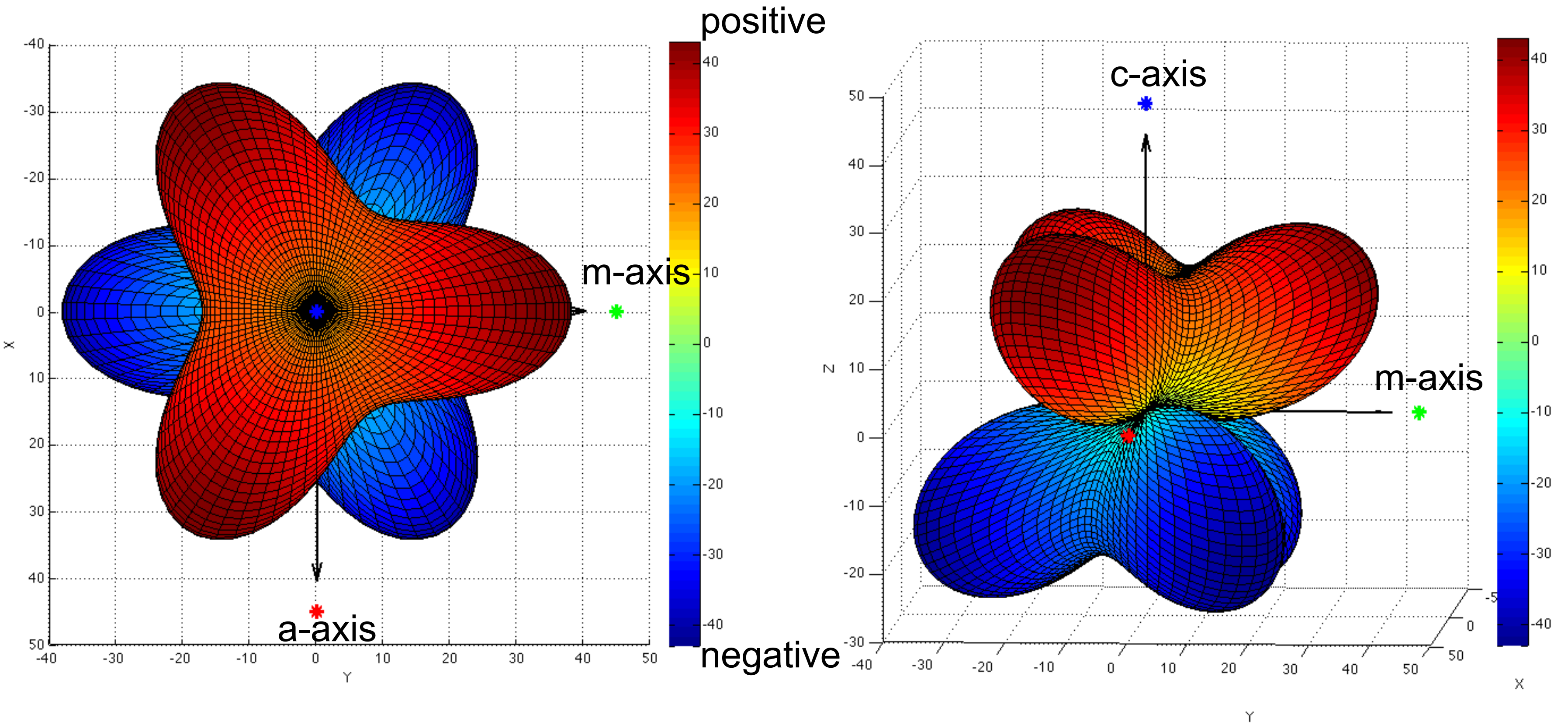
Figure 4: 3D plot of the piezoelectric tensor ***d*** for right-handed α-quartz **32** using plot(d,'3D'). Note the 3-fold *c*-axis repeating the red (positive) and blue (negative) lobes, 2-fold *a*-axes, +*a*-axes have negative values, and the zero value along the *c*-axis.



3D plot : Sphalerite (ZnS)

Figure 5: 3D plot of the piezoelectric tensor ***d*** Sphalerite $\bar{4}3\mathbf{m}$ 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)

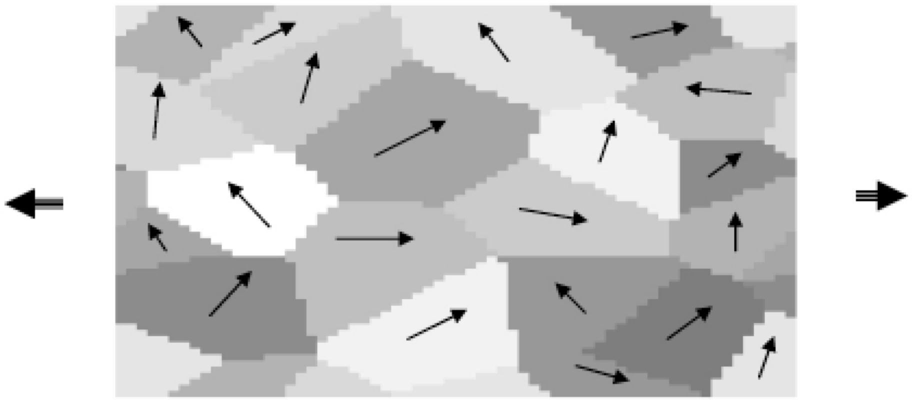
Future developments 1; Self-consistent (SC) and Differential Effective Media (DEM), FFT methods

- 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.

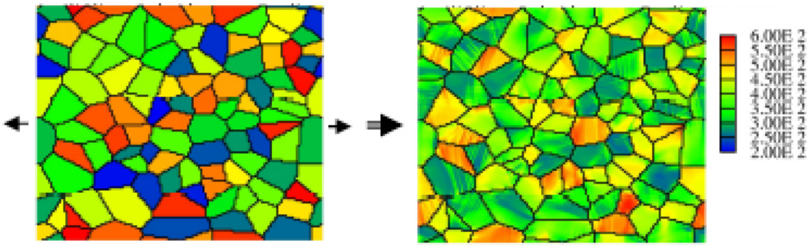
Polycrystal models: full-field vs. mean-field (statistical) approaches

Lebensohn, Tome & Ponte Castaneda, Phil Mag 87, 4287 (2007)

Full-field solution



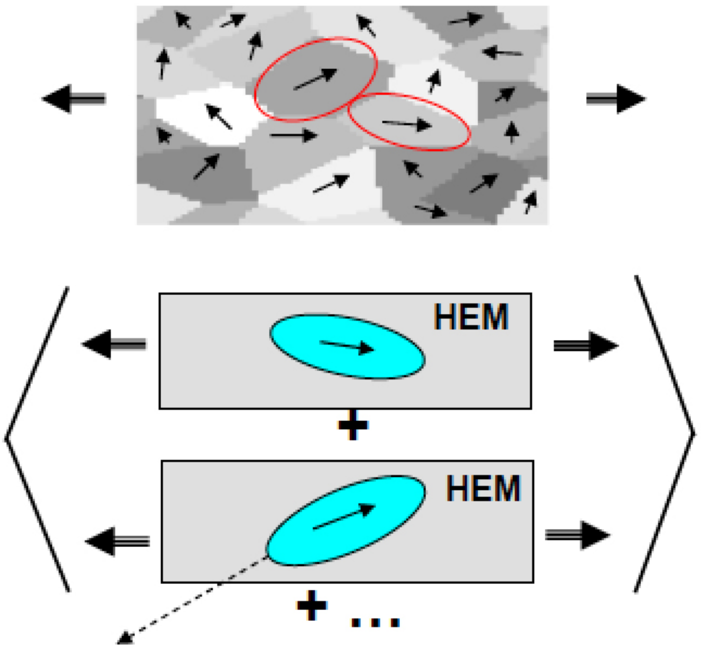
Solving equilibrium + compatibility:



grain structure

stress field

Mean-field statistical solution



Solving Eshelby inclusion problem

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 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 (α) in 4 directions determine the α_{11}, α_{22}, α_{33} and α_{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

- 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