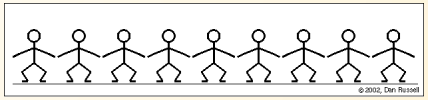
Physical properties in MTEX, current status and future developments

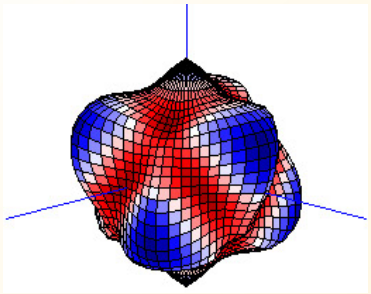
Chemnitz MTEX Workshop March 2019

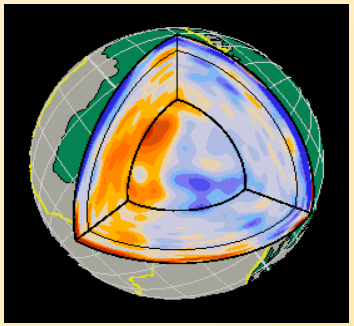
Technische Universität Chemnitz, Germnay

David Mainprice



(Géosciences Montpellier, Université de Montpellier, France)





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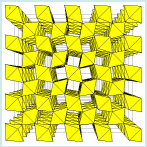
Plan of this talk, is there a plan ?

- 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

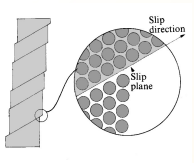
A brief resumé of what I do …sometimes

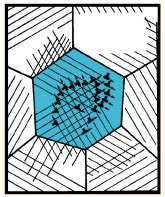
What do I do ?
Atomic Modelling & Experimentation at high P & T

Atomic Modelling *



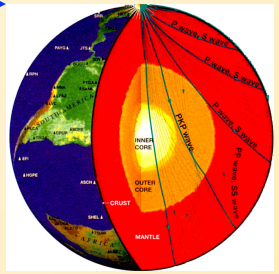
Slip Systems CRSS → Plasticity Modelling → Crystal Preferred Orientation → *Elastic Tensors* → Seismology





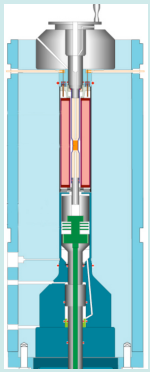
Orthorhombic
222, *mm2*, *mmm*

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



Experimentation

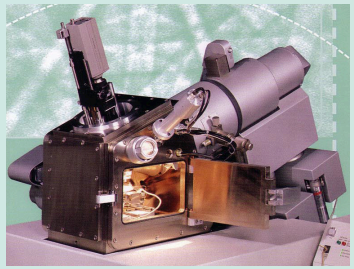
Multi-anvil 1400°C 16 GPa



Paterson Press * 0.3 GPa

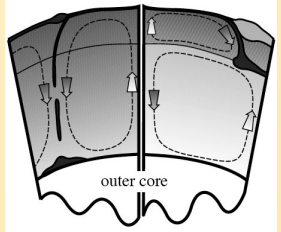
Sylvie Demouchy

EBSD *



P<10^{-4} GPa

Geodynamics



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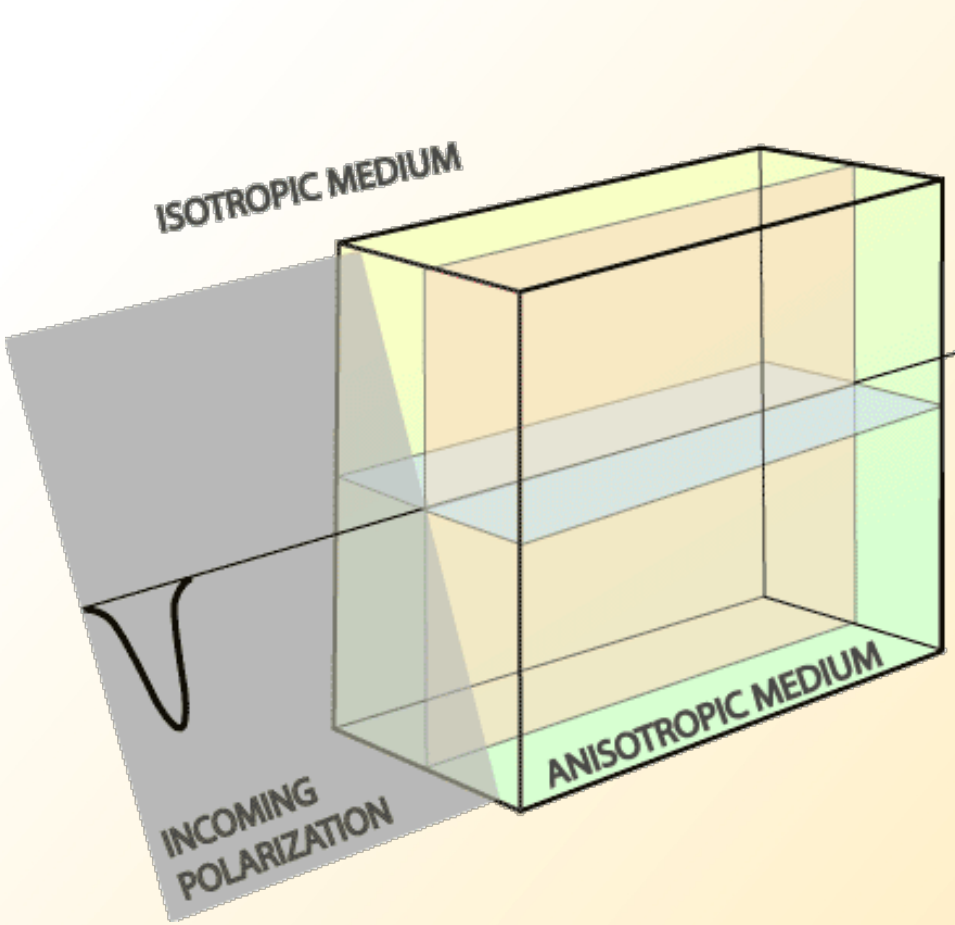
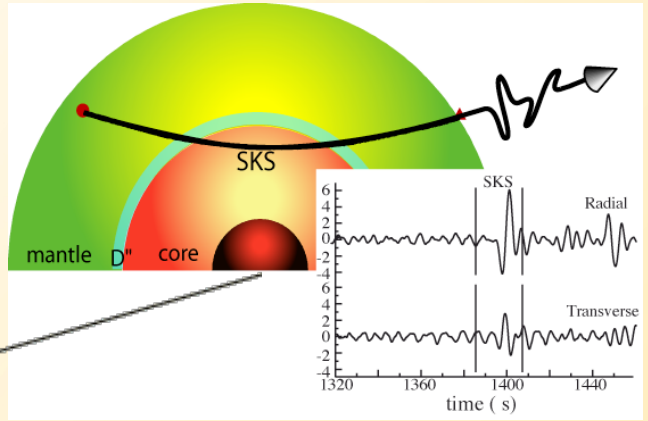
Shear Wave Splitting

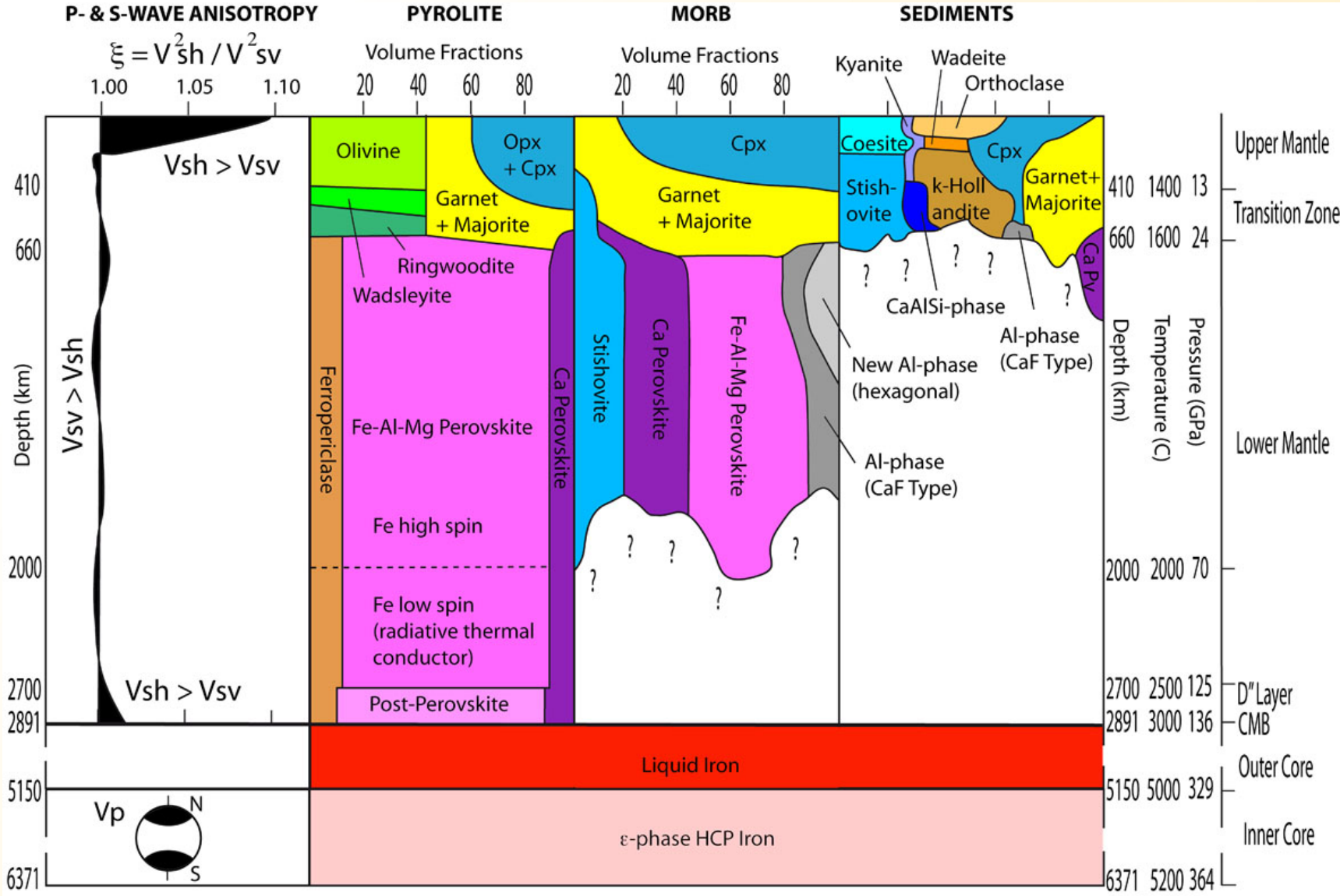




http://garnero.asu.edu

Mantle & Core : petrology & seismic anisotropy

Mainprice (2007)



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

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

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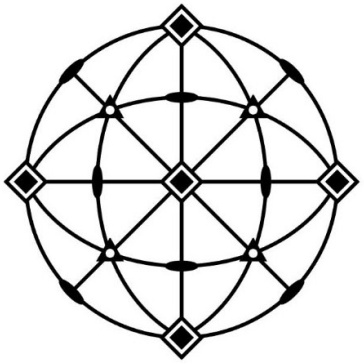
Getting Started

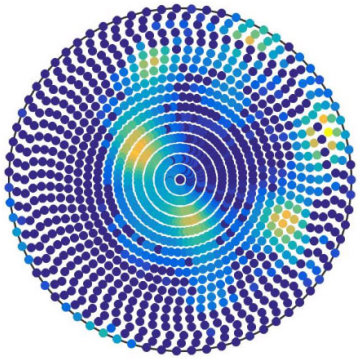
• Installation Guide • Configuration • Frequently Asked Questions • Release Notes • Function Overview • Matlab Basics •

Users Guide

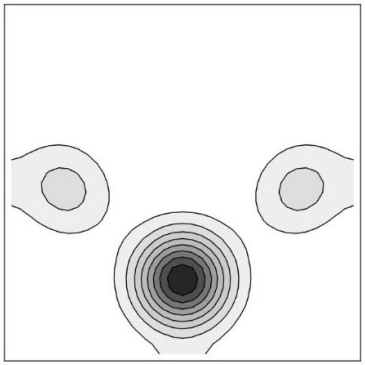
Crystal Geometry



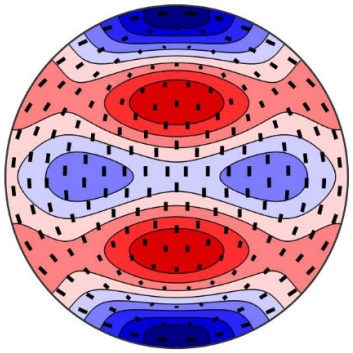
Pole Figures



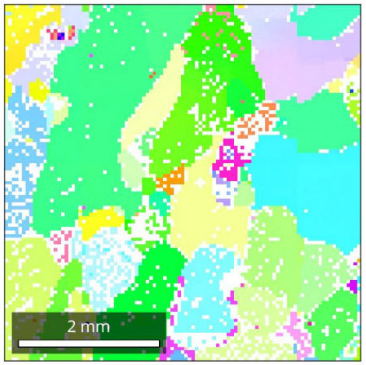
ODFs



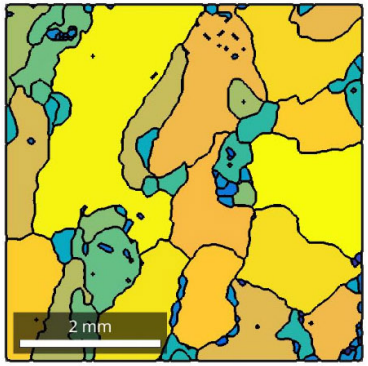
Tensors



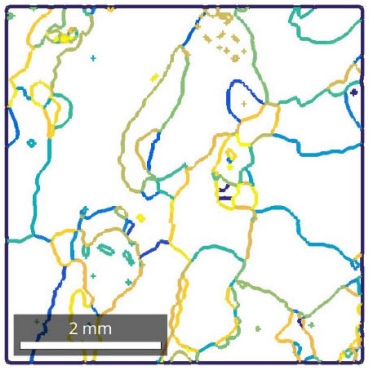
EBSD



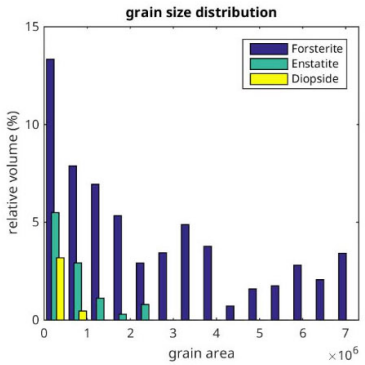
Grains



Grain Boundaries



Plotting



MTEX Reference papers on physical properties

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

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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,

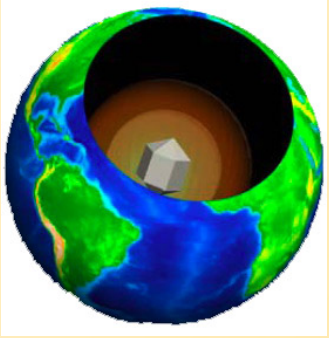
2011

- **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

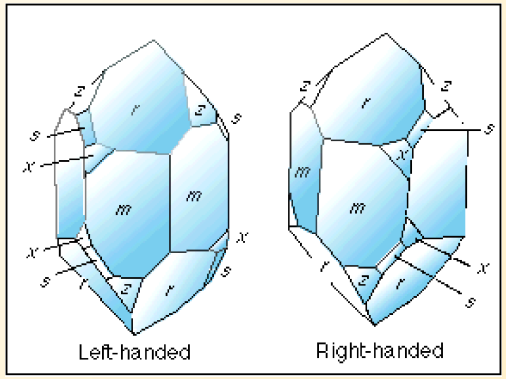
Why are we interested in Single Crystals ?

- 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

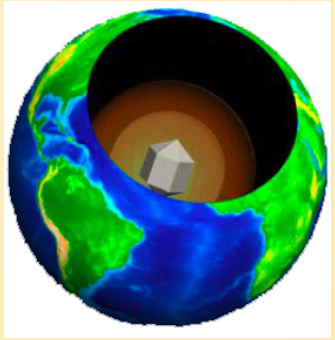
- Thermal conductivity and diffusivity (2th rank tensor) → can be calculated from CPO
- Thermal expansion (2th rank tensor) → can be calculated from CPO
- Electrical conductivity, electrical polarization and dielectric properties) → can be calculated from CPO, BUT may not be relevant if conductivity 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

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 …



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.

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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	$T'_{ijkl} = R_{im} R_{jn} R_{ko} R_{ip} T_{mnop}$	$T_{ijkl} = R_{mi} R_{nj} R_{ok} R_{pi} T'_{mnop}$

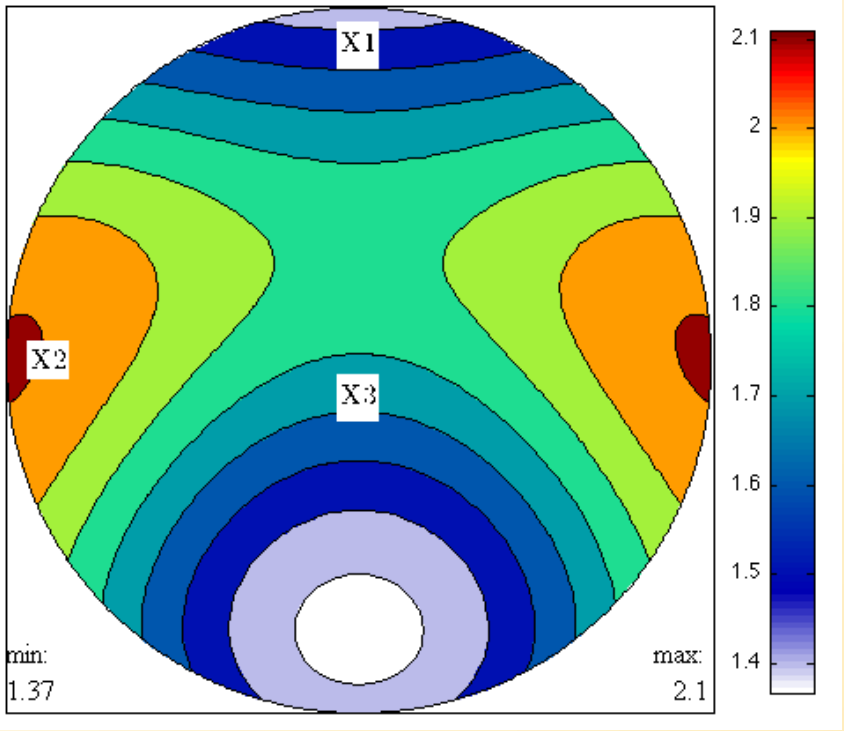
S = scalar, V=vector, T=tensor. T'_{ij} is the new orientation of the tensor and T_{ij} the old orientation.

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.

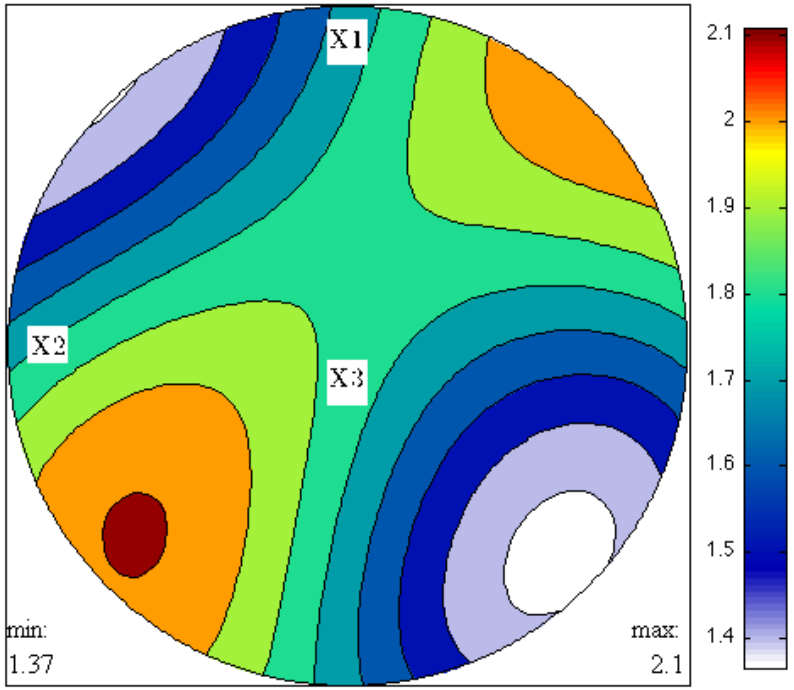
Cartesian tensors have orthogonal reference axes (labelled x, y and z in MTEX)

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');
%
```



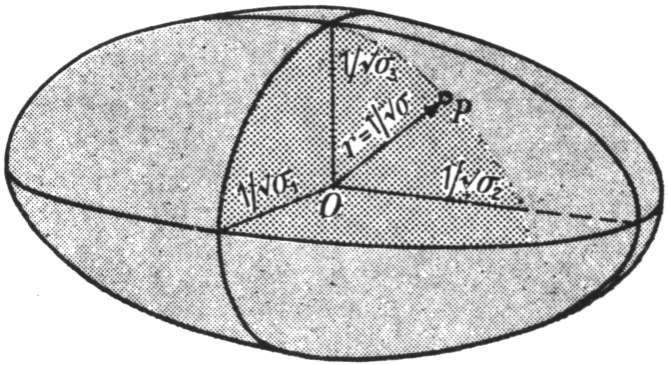
Difference between a transformation matrix (R_{ij}) and a 2nd rank tensor (T_{ij})

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 Det(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(R)=-1.

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

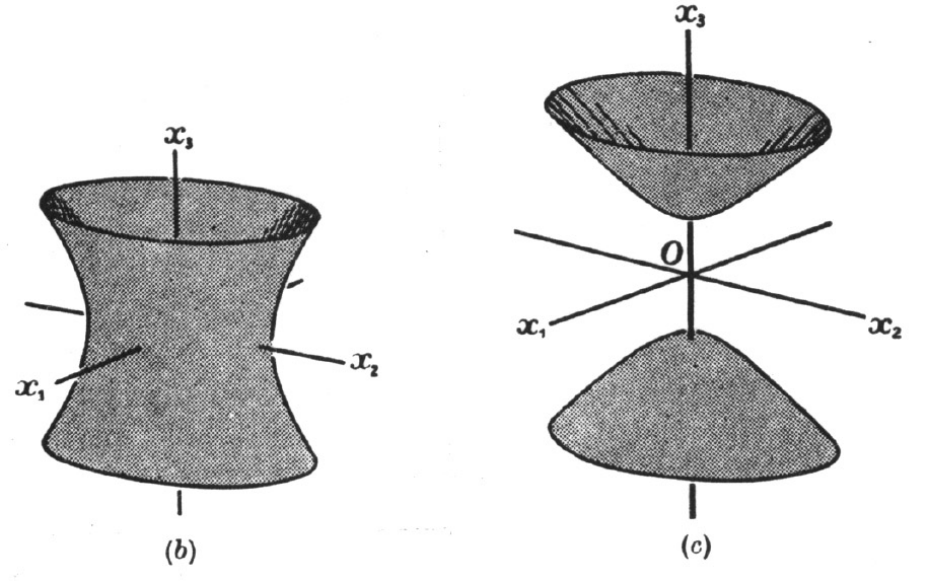
Geometrical representation of symmetrical second-rank tensors as a second-degree surface (called a **quadric**). The quadric may be an ellipsoid or a hyperboloid. Most common second-rank tensors are symmetric (Tij = Tji) and when the 3 principal coefficients are all positive then the property is represented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

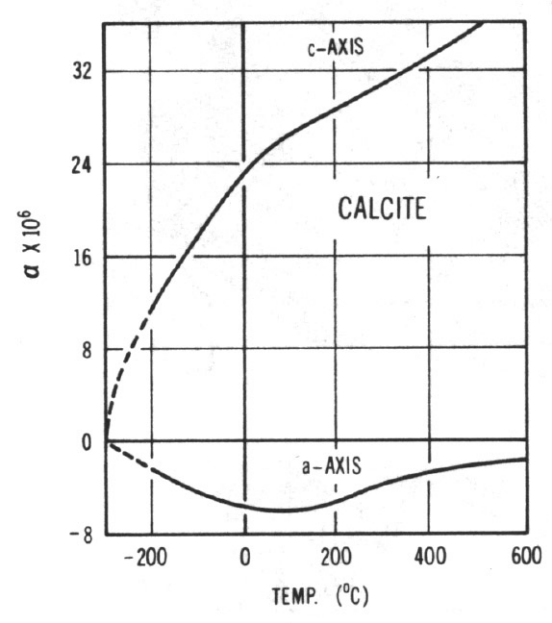


Illustrating the properties of the representation ellipsoid for conductivity: $\sigma_{ij} x_i x_j = 1$.

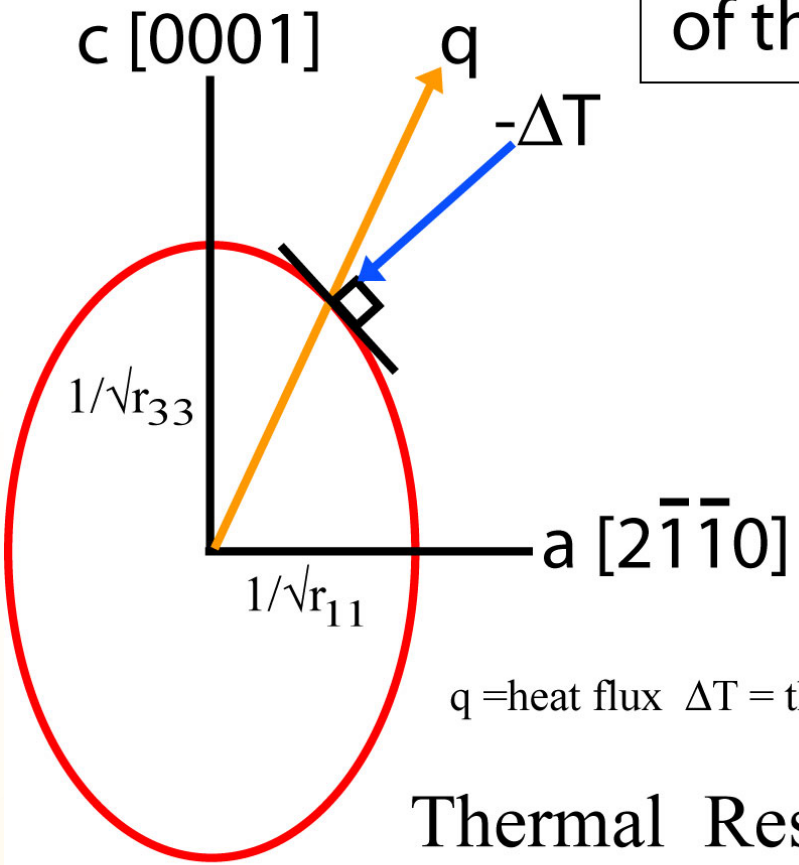
The representation **hyperboloid** for 2nd Rank Tensors

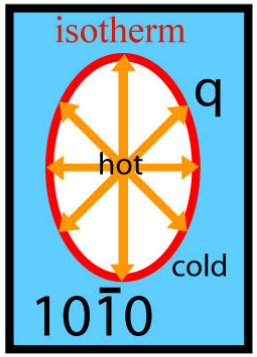
If one of the principal coefficients is negative then surface is a hyperboloid of one sheet (e.g. thermal expansion of plagioclase feldspar). If two of the principal coefficients are negative then surface is a hyperboloid of two sheets or caps, this the case for the thermal expansion of calcite with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

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

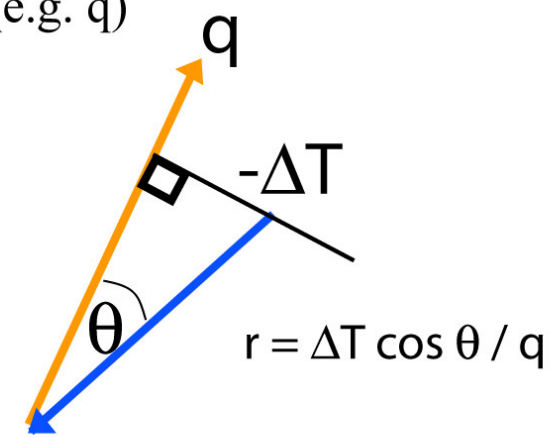
where $r_{11} = 1/k_{11}$ etc

Thermal Conductivity (k)

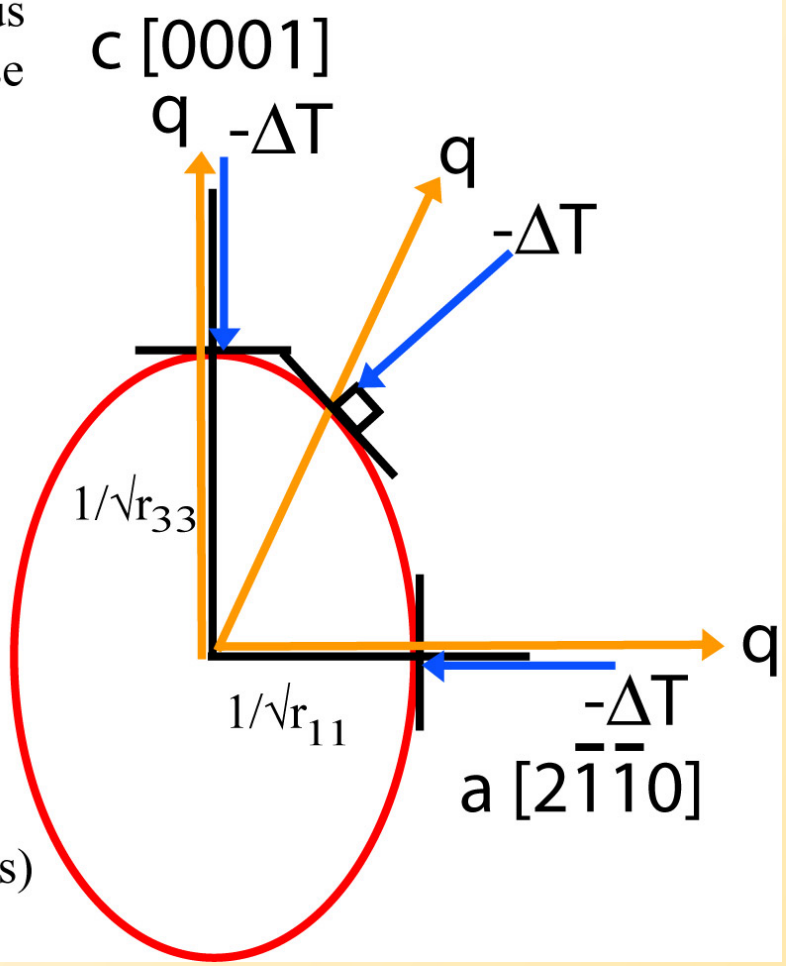
$q_i = - k_{ij} \Delta T_i$

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)

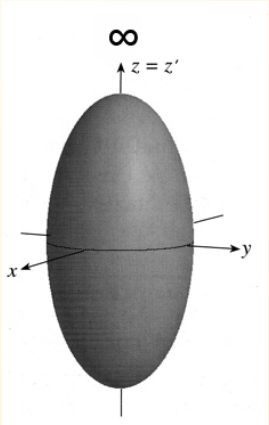


Fundamental concept for tensors

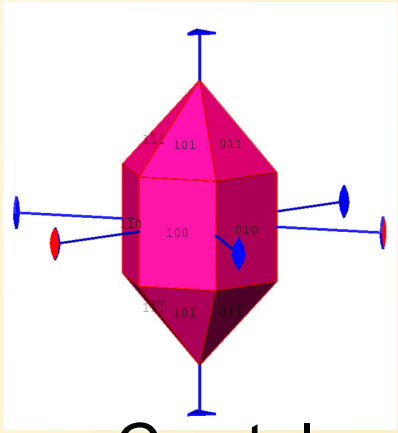
- Physical properties are anisotropic when the applied *tensor* is not aligned with resultant *tensor*
- Physical properties are isotropic when the applied *tensor* is aligned with resultant *tensor* for all directions
- In specific directions in an anisotropic crystal the applied and resultant tensor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



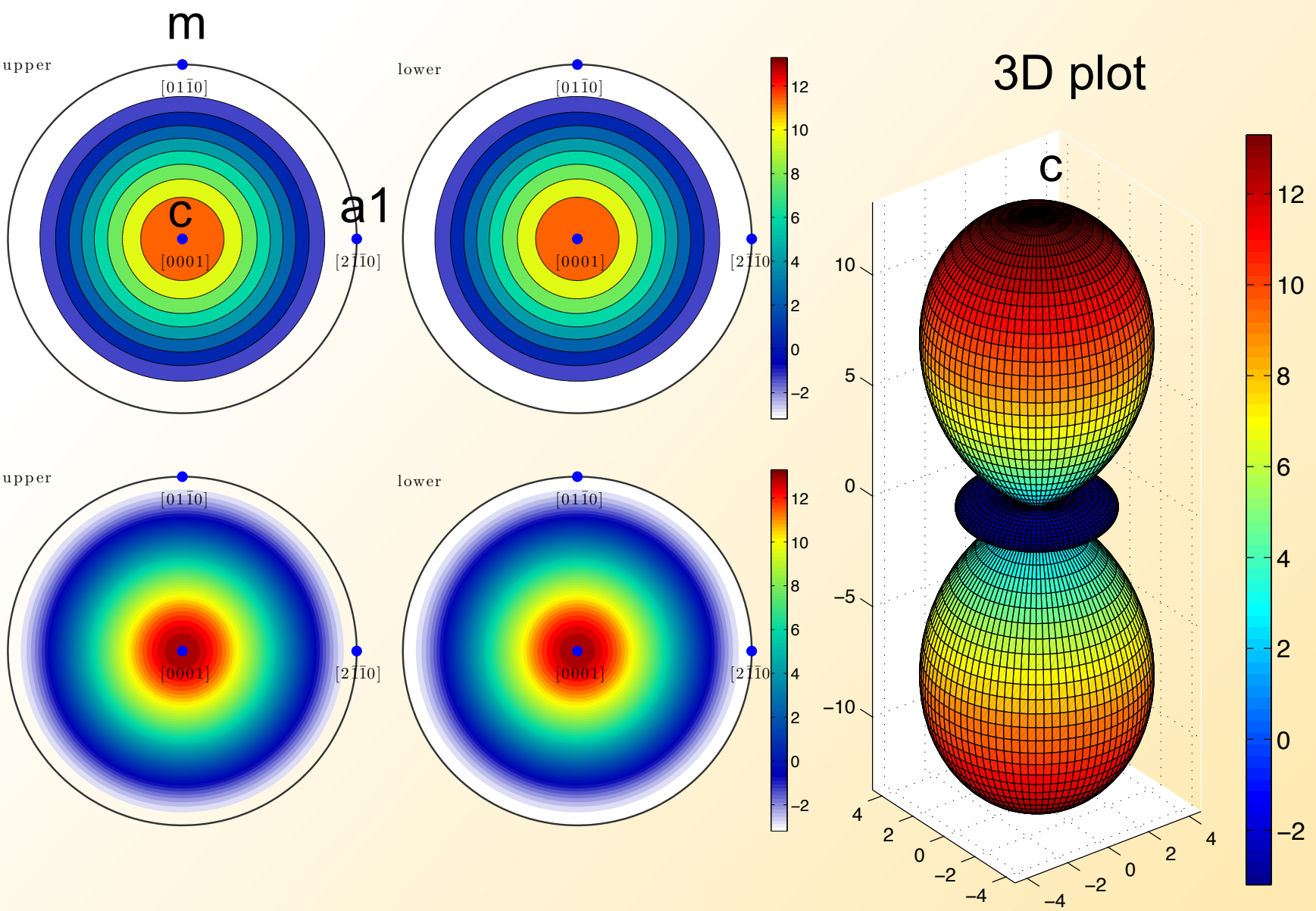
Crystal
lower symmetry

Symmetric 2nd rank tensors for all crystal symmetries

Crystal Symmetry (Independent constants)	Symmetry and tensor axes	Tensor
Cubic (1)	Isotropic $T_{11} = T_{22} = T_{22}$	$\begin{bmatrix} T_{11} & 0 & 0 \\ 0 & T_{11} & 0 \\ 0 & 0 & T_{11} \end{bmatrix}$
Hexagonal (2) Trigonal on hexagonal axes (2) Tetragonal (2)	6-fold ‖ **z** 3-fold ‖ **z** 4-fold ‖ **z** $T_{11} = T_{22} \neq T_{33}$	$\begin{bmatrix} T_{11} & 0 & 0 \\ 0 & T_{11} & 0 \\ 0 & 0 & T_{33} \end{bmatrix}$
Orthorhombic (3)	2-fold ‖ **x** 2-fold ‖ **y** 2-fold ‖ **z** $T_{11} \neq T_{22} \neq T_{33}$	$\begin{bmatrix} T_{11} & 0 & 0 \\ 0 & T_{22} & 0 \\ 0 & 0 & T_{33} \end{bmatrix}$
Mononclinic (4)	2-fold ‖ **y** $T_{13} = T_{31}$ 2-fold ‖ **z** $T_{12} = T_{21}$ 2-fold ‖ **x** $T_{23} = T_{32}$ & $T_{11} \neq T_{22} \neq T_{33}$	2-fold ‖ **y** $\begin{bmatrix} T_{11} & 0 & T_{13} \\ 0 & T_{22} & 0 \\ T_{13} & 0 & T_{33} \end{bmatrix}$ 2-fold ‖ **z** $\begin{bmatrix} T_{11} & T_{12} & 0 \\ T_{12} & T_{22} & 0 \\ 0 & 0 & T_{33} \end{bmatrix}$ 2-fold ‖ **x** $\begin{bmatrix} T_{11} & 0 & 0 \\ 0 & T_{22} & T_{23} \\ 0 & T_{23} & T_{33} \end{bmatrix}$
Triclinic (6)	**x**, **y** & **z** in arbitrary orientations 6 independent values $T_{11} \neq T_{22} \neq T_{33} \neq T_{12} \neq T_{13} \neq T_{23}$	$\begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{13} & T_{32} & T_{33} \end{bmatrix}$

x, **y** and **z** are the orthogonal reference axes for Cartesian tensors

Thermal expansion of calcite

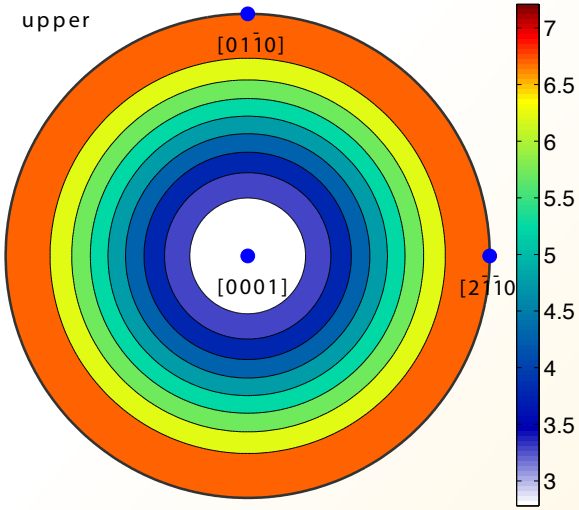


MTEX script

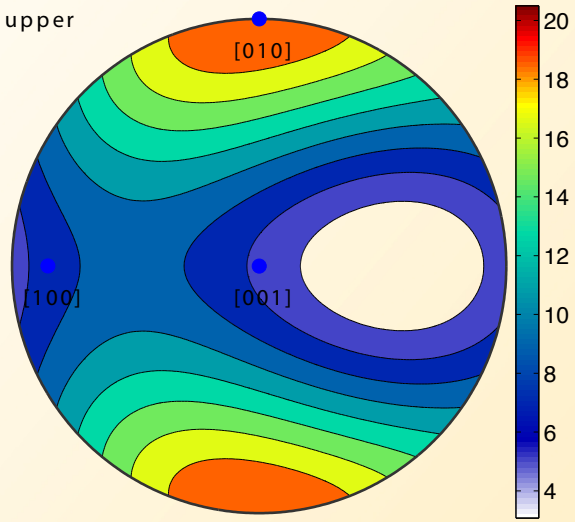
```
%************************************************************************
% Step 1 : Define the tensor reference frame for Calcite
%************************************************************************
cs_tensor = crystalSymmetry('-3m1',[4.9896, 4.9896, 17.0610],...
    [90, 90, 120]*degree,'mineral','calcite','x||a','z||c');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

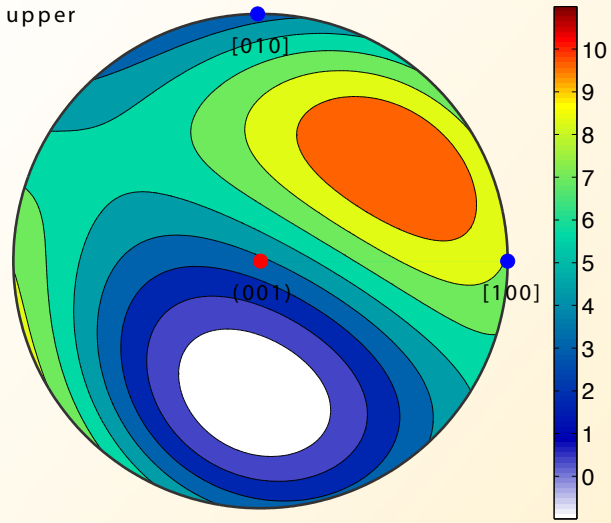
α-Quartz (trigonal -3m)



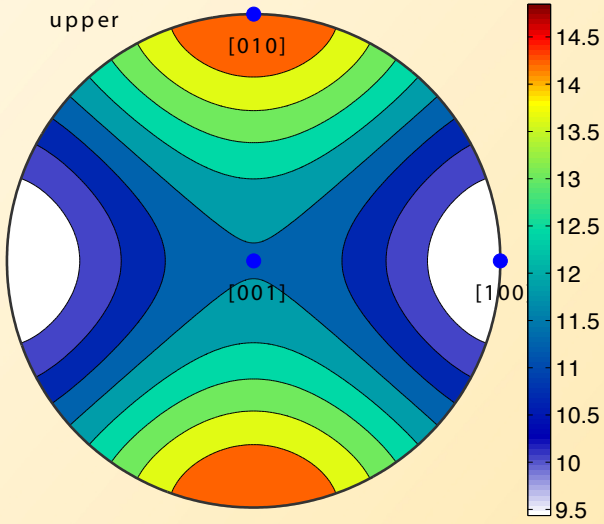
Diopside (monoclinic 12/m1)



Bytownite An76 (triclinic -1)



Forsterite (Orthorhombic mmm)



Optical properties - olivine

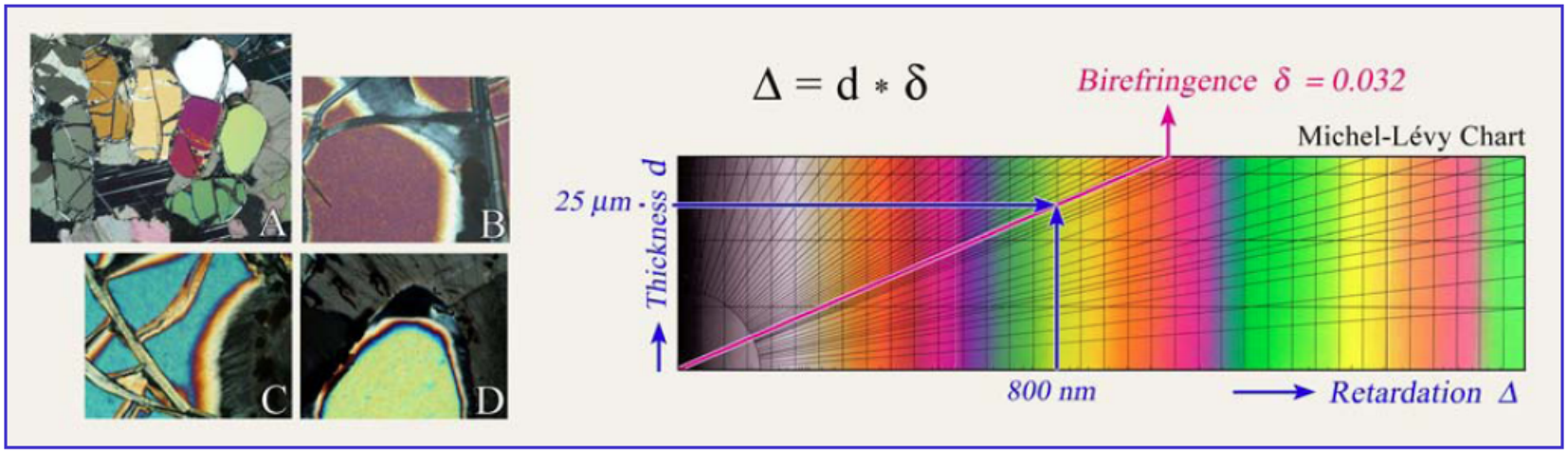
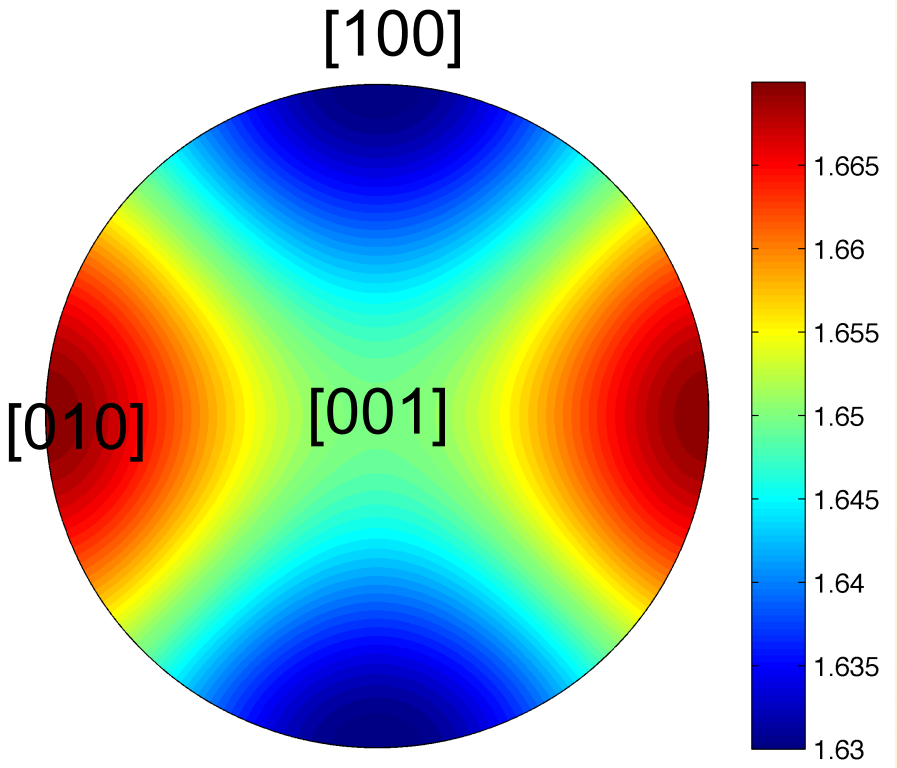
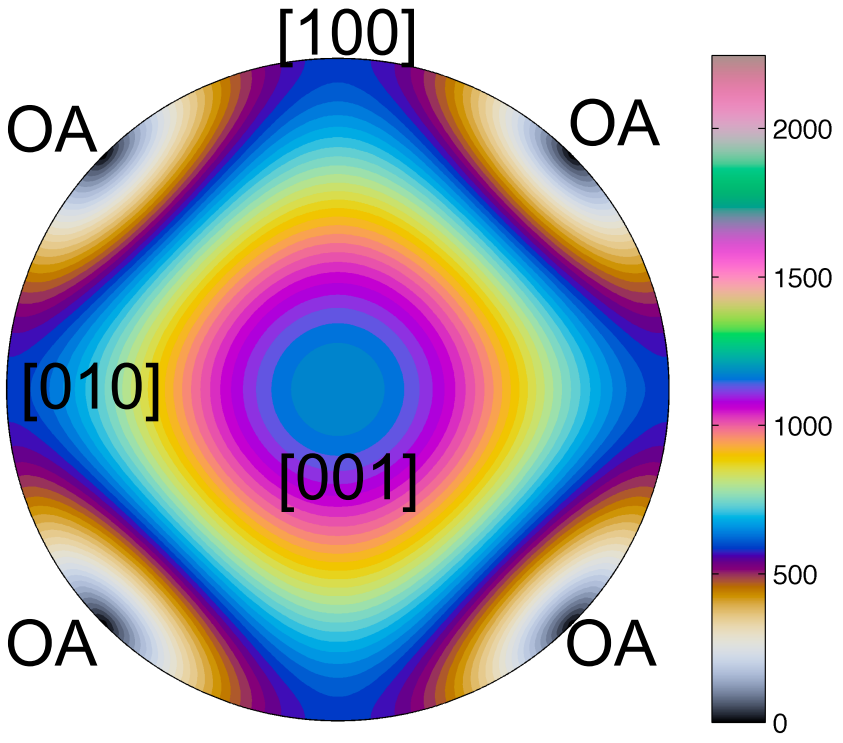


Figure 4.2.3-8: Left: (A) Variation of interference colour in differently oriented forsterite grains; (B) to (D) Decreasing interference colours at wedging-out edges of sections of forsterite grains that have different orientation in thin section. Right: Determination of birefringence using crystal thickness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

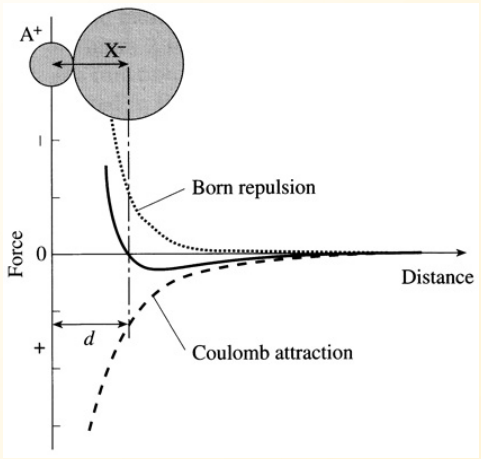
Retardation (nm): Michel Levy colours

Géosciences Montpellier

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

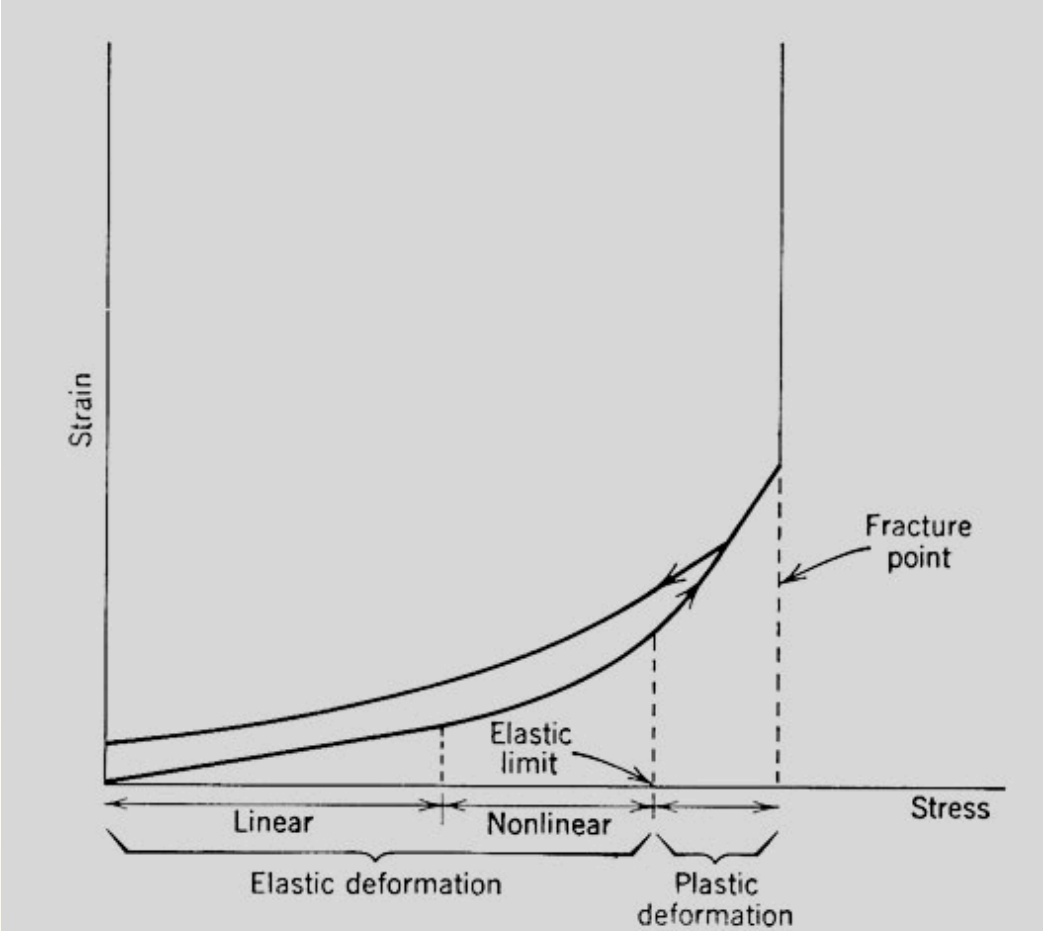
4th Rank Tensors - important for geophysics

- 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 $C_{ijkl} = C_{klij}$

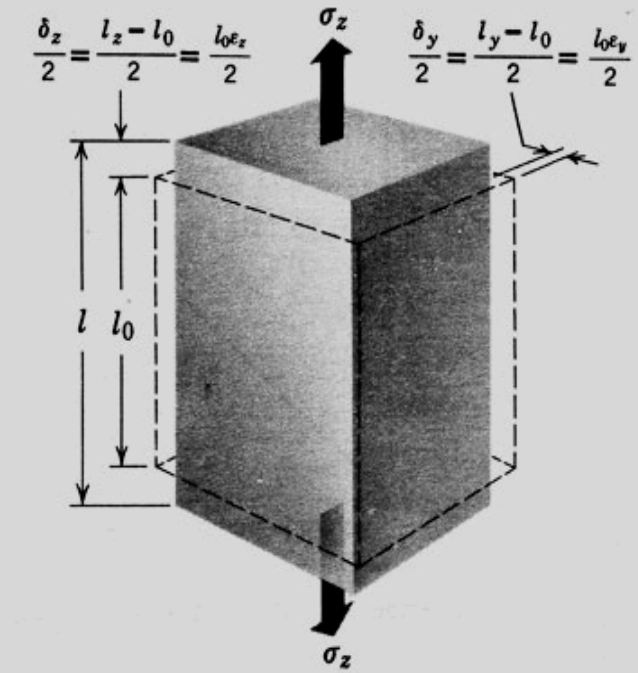
Life was not meant to be easy in elasticity !

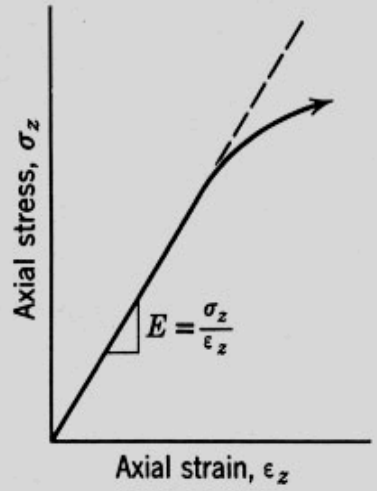
21 independant elastic constants 6 x 6 symmetric tensor

- 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.

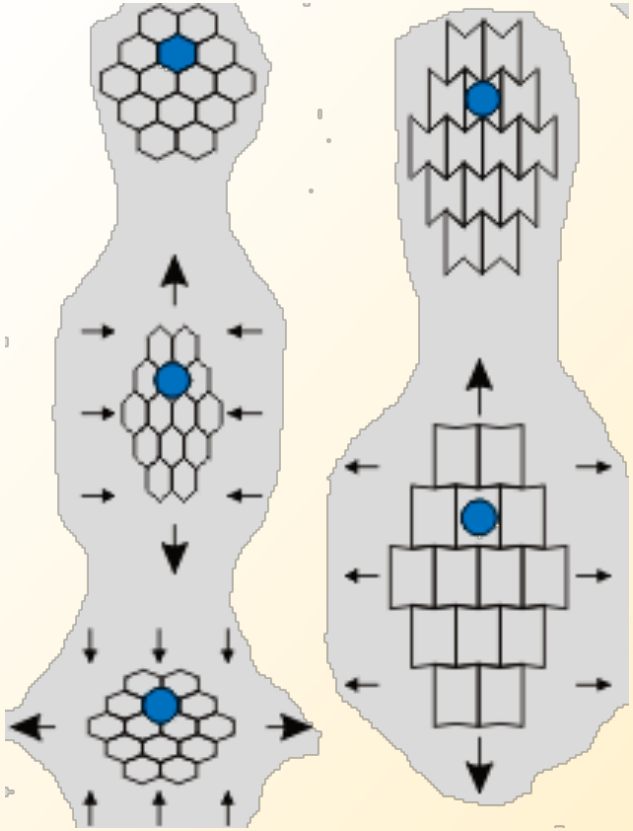
Poisson's ratio, ν, another elastic constant, is the ratio of transverse to axial strain

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

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
p,q = 1 to 6

Tensors
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

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

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

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 ε/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

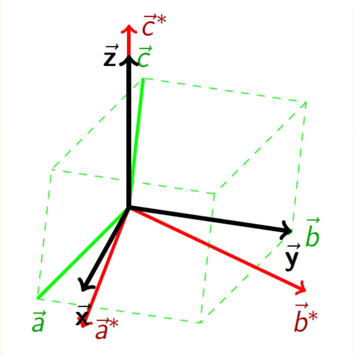
Material	ρ Mg/m^3	Subscript ij in modulus c_{ij} (GPa) 11	22	33	44	55	66	12	13	23	...s GPa	G GPa	Refer-ences
					Perovskites								
$MgSiO_3$	4.108	515	525	435	179	202	175	117	117	139	246.4	184.2	149
$NaMgF_3$	3.058	125.7	147.3	142.5	46.7	44.8	50.4	49.5	45.1	43.1	75.7	46.7	155
					Pyroxenes								
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

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…)



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

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')
%
```

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

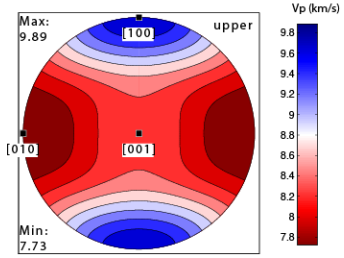
Solve Christoffel symmetric tensor (3 by 3)
at each grid point n

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

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

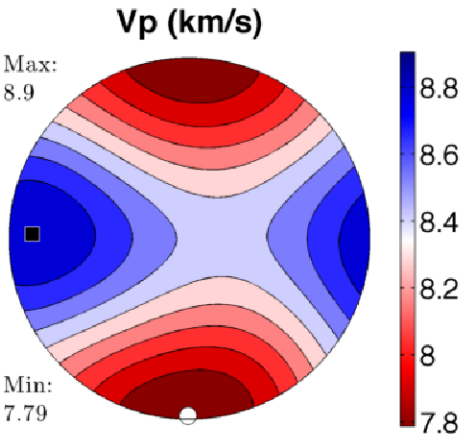
Single Crystal Cij for Olivine
(orthorhombic)

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



crystal coordinates

pcrystal coordinates



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

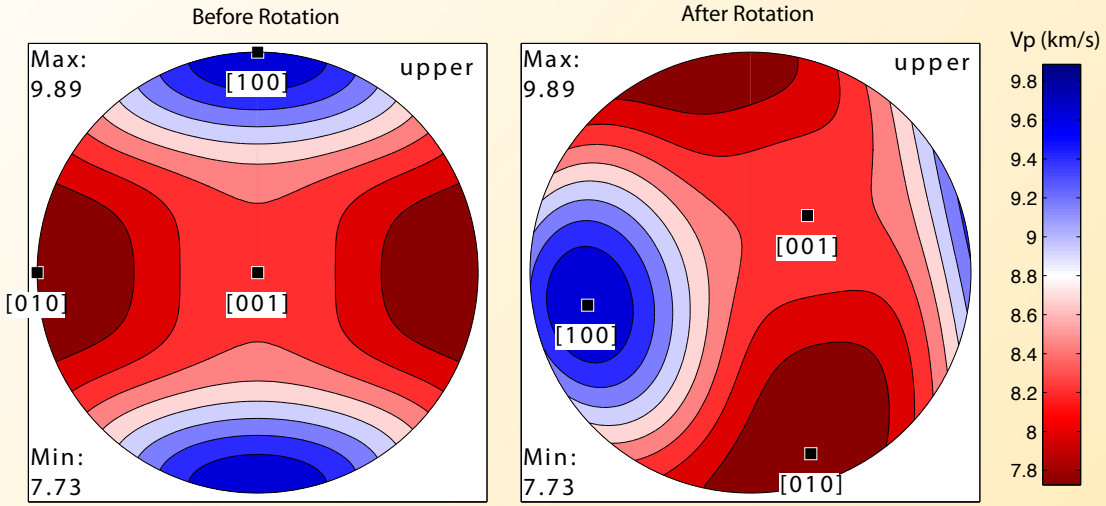
Plot and rotate a tensor of any rank

```
%% 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,'xIIa*','zIIc','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,'xIIa','zIIc*','mineral','Talc')
```

N.B. in **Euler frame** 'xIIa*','zIIc and in the **Tensor frame** 'xIIa','zIIc*'

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

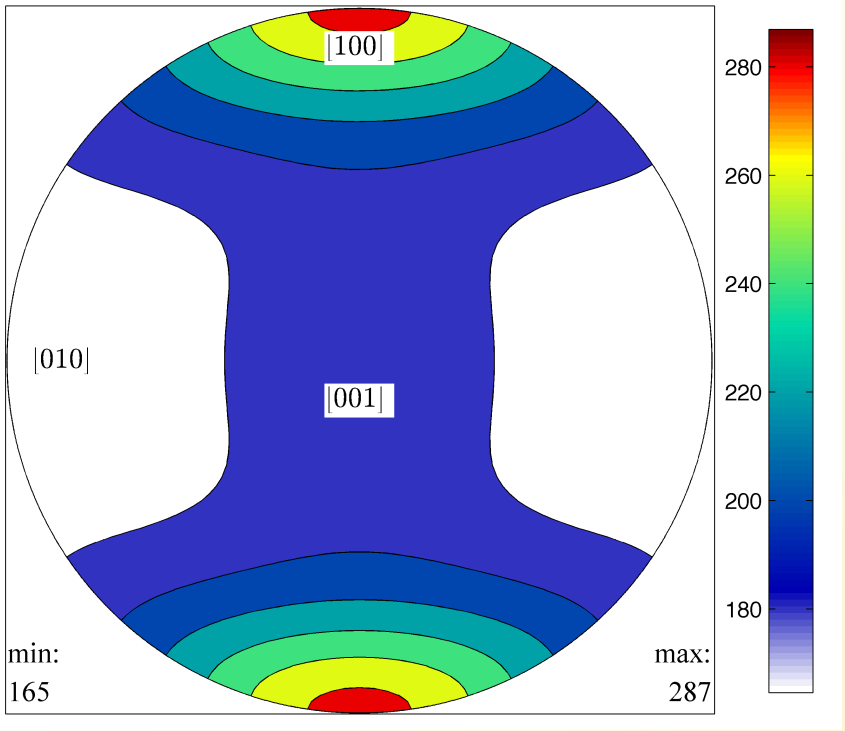
```
uvw_100 = Miller (show methods, plot)
  size: 1 x 1
  options: uvw
  mineral: Olivine (mmm)
  u 1
  v 0
  w 0

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
```

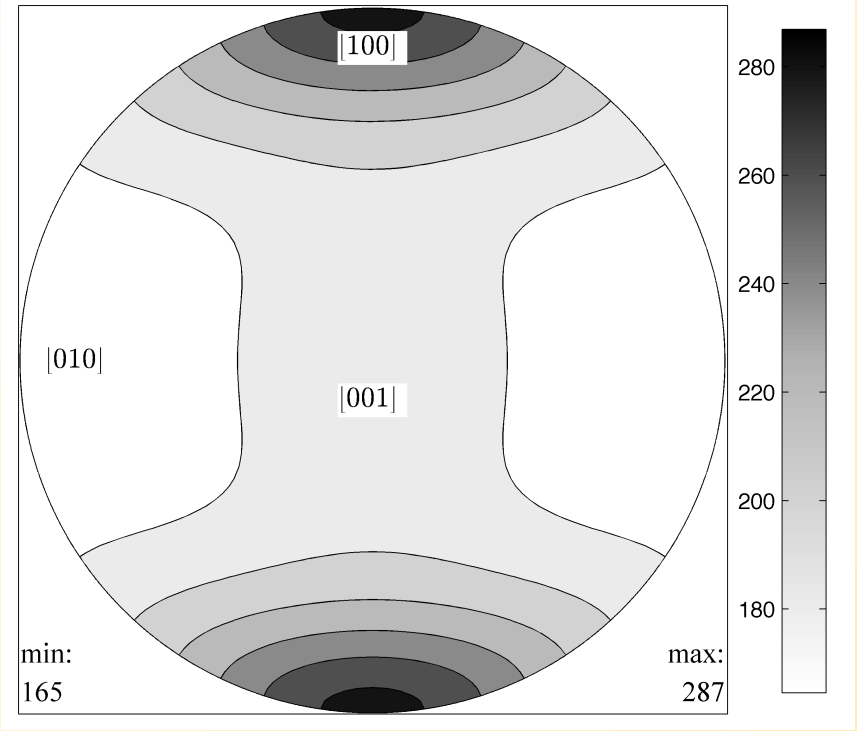
```
E_100 =

  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)

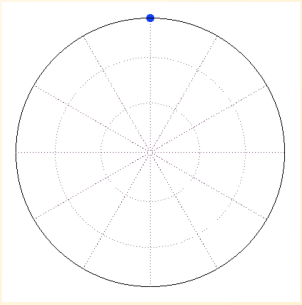
```
%%
%*************************************************************************
% Compute elastic wave velocities and polarizations in direction x = 1 0 0
%*************************************************************************
%
% compute Vp,Vs1,Vs2,particale motion for P,S1,S2 for direction
% xvector = 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

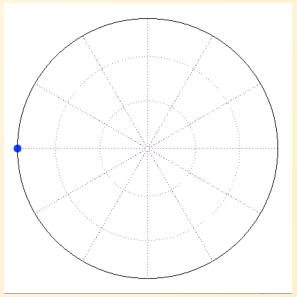
```
vp =

    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

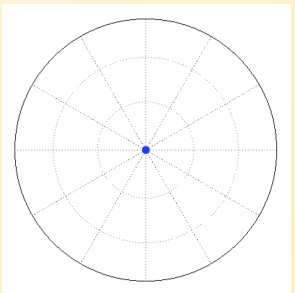
pp polarization vp



ps1 polarization vs1



ps2 polarization vs2



show methods

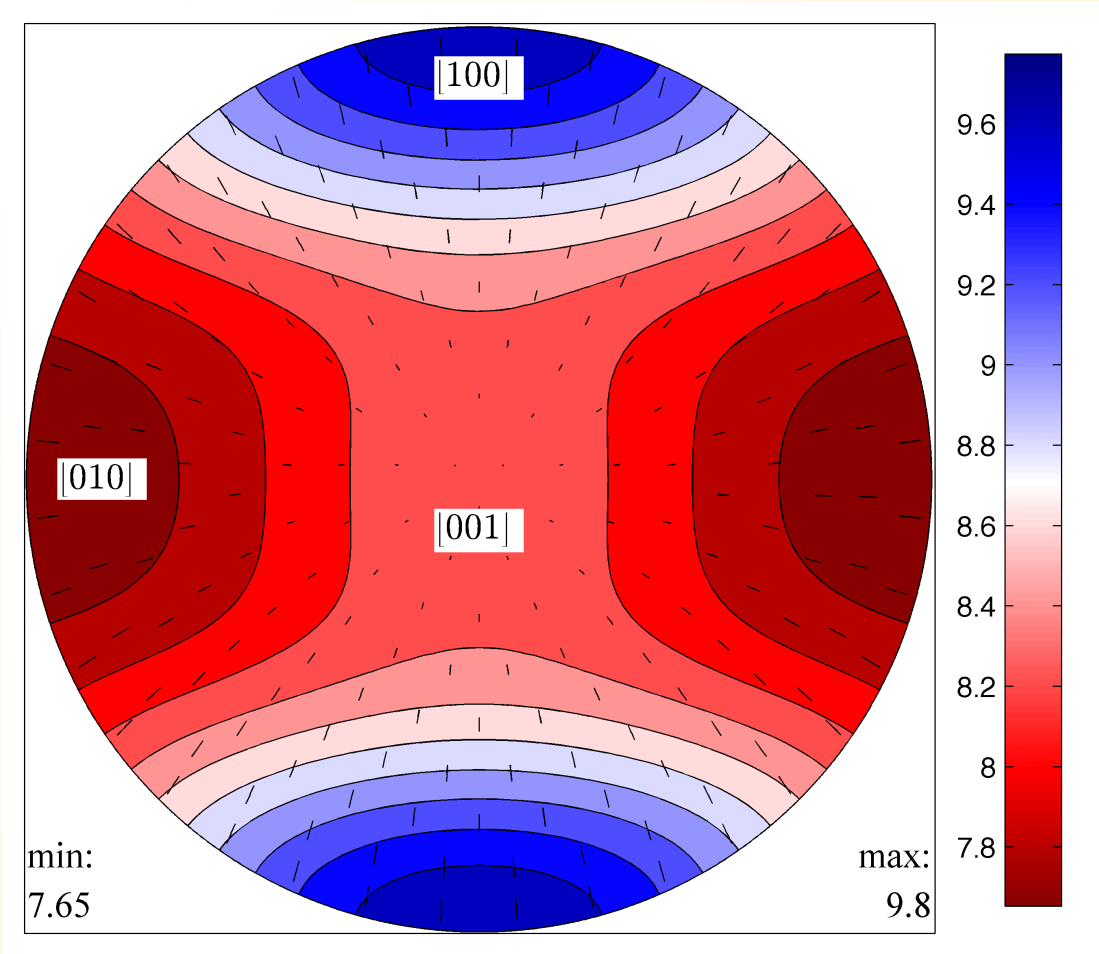
Methods for class vector3d:

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	

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)

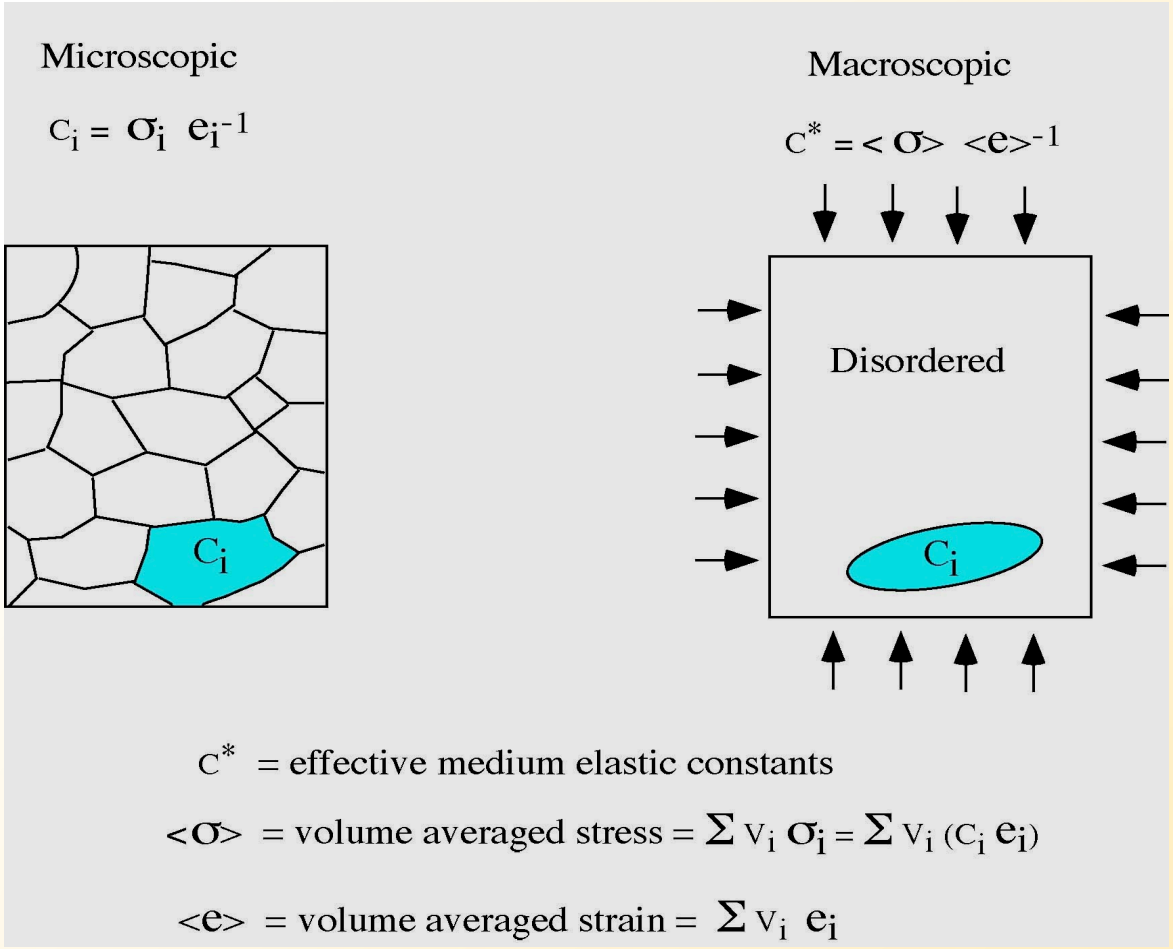
References – Tensors and Crystal Physics

- **Curie, P., Oeuvres , pp. 118, Paris, Société Français de Physique (1908)**
- **Voigt, W. 1928. Lehrbuch der Kristallphysik. Teubner-Verlag, Leipzig.**
- 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

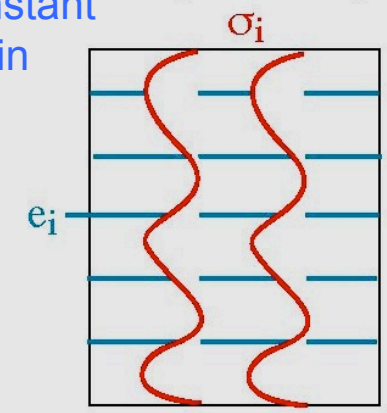


Homogeneous Effective Media (H.E.M.)

Simple volume averages

Voigt Average

Constant strain

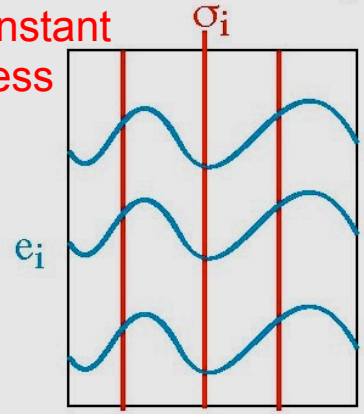


e_i = constant: $C^* \langle\sigma\rangle = \sum V_i (C_i\ e_i)$

$$C^* \approx C^{Voigt} = \sum V_i C_i$$

Reuss Average

Constant stress

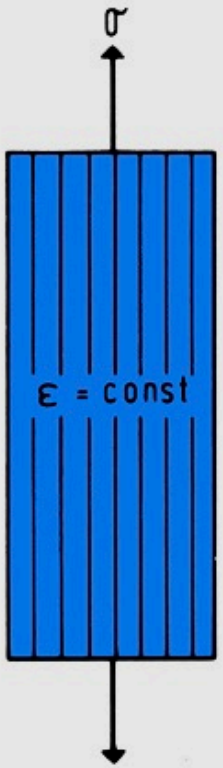


σ_i = constant: $C^* \langle e\rangle^{-1} = (\sum V_i\ e_i)^{-1} = (\sum V_i\ (S_i\ \sigma_i))^{-1}$

$$C^* \approx C^{Reuss} = (\sum V_i\ S_i)^{-1}$$

- 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

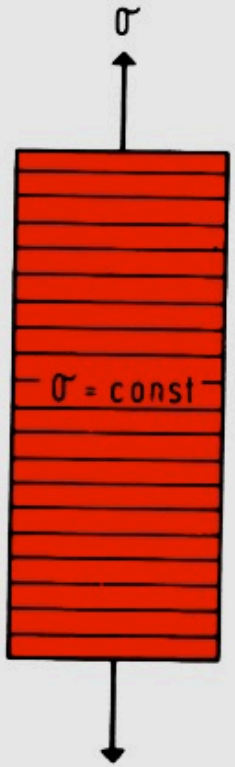
Voigt & Reuss micro-structural models



Voigt (a)

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

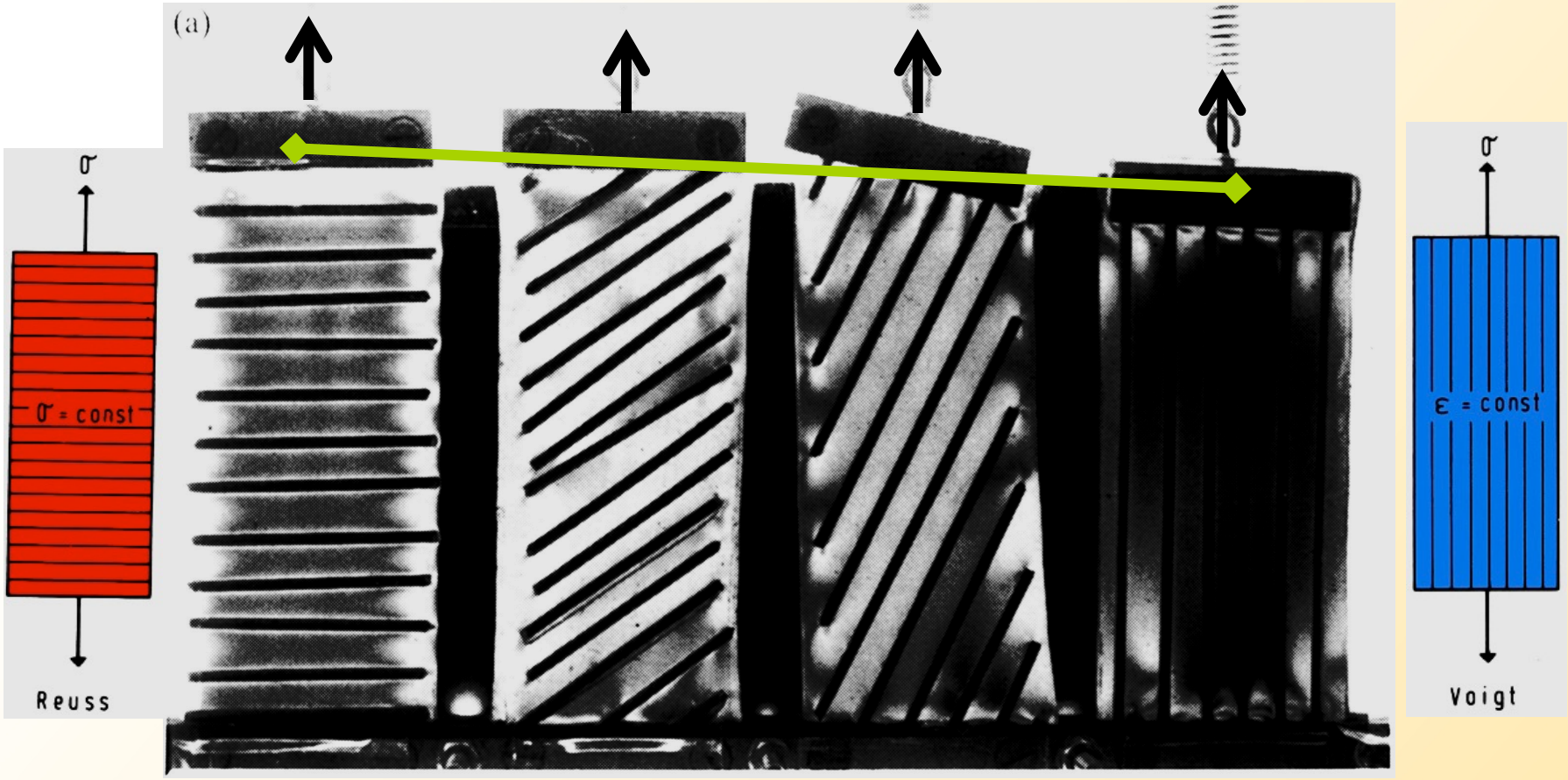
No microstructural or theoretical basis, but in practice it is close to the experimentally measued values



Reuss (b)

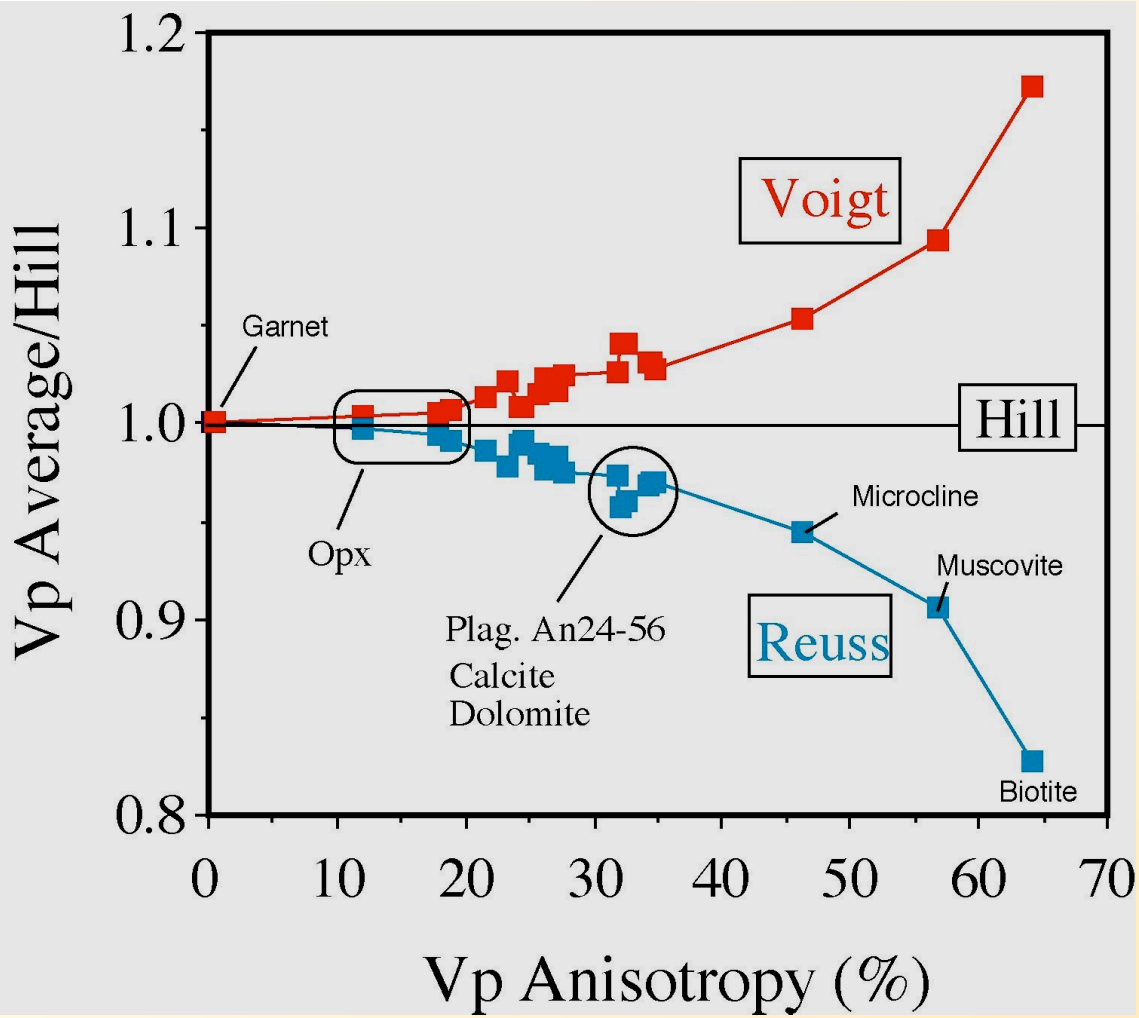
(a) Grain structure of a polycrystal for which Voigt's assumption is valid. (b) Grain structure of a polycrystal for which Reuss's assumption is valid.

Macromodel composite laminates



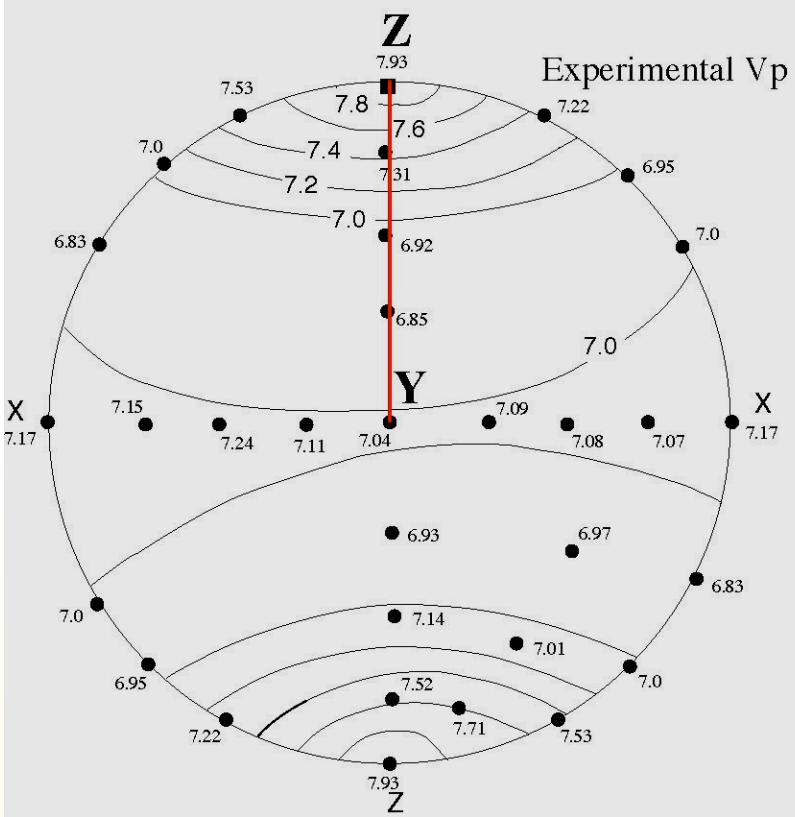
Aligned metal rods(black) in polyurethane matrix grey where lighter greys - larger shear strains

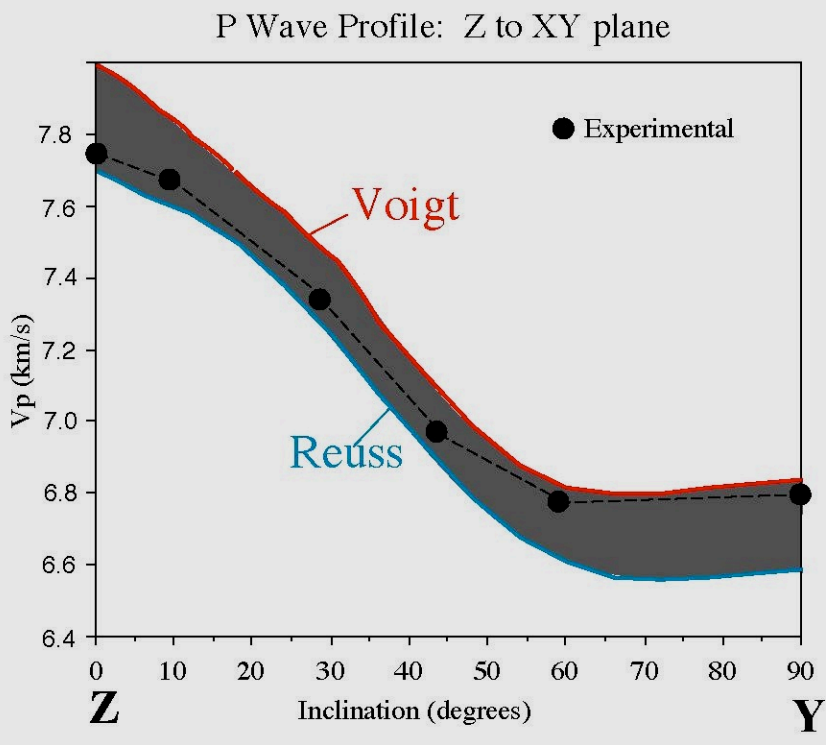
Vp Polycrystal Averages



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

Oklahoma Gabbro
Stereo & Vp YZ profile

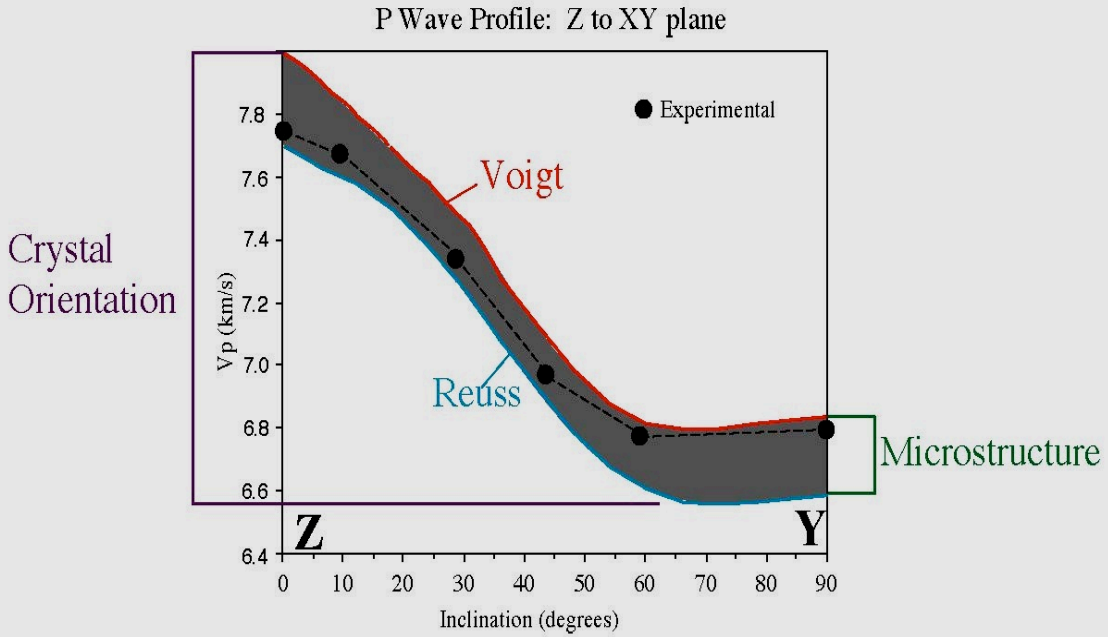




Confining pressure = 800 MPa

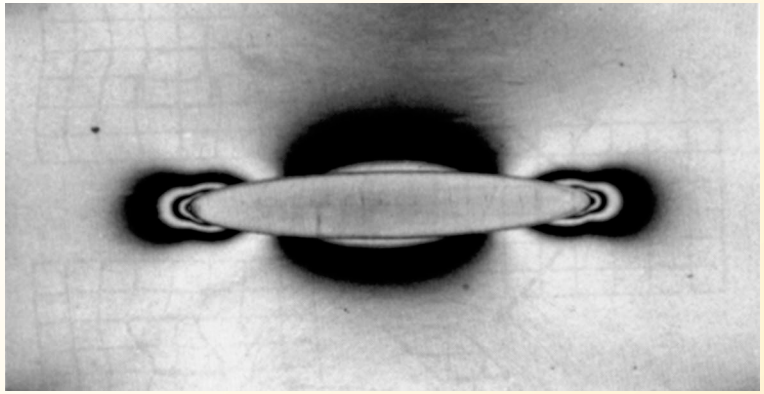
SERONT, B., MAINPRICE, D. AND CHRISTENSEN, N.I. (1993)
J. Geophy. Res. 98: 2209-2221.

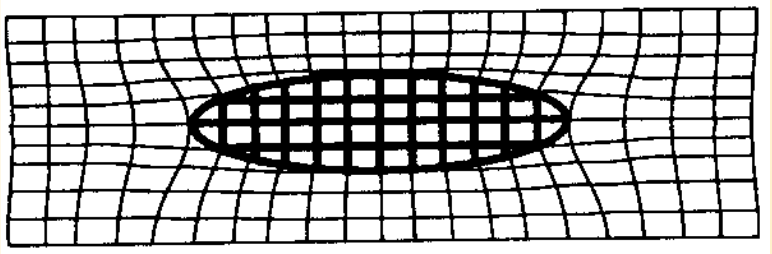
Physical Properties & Microstructure - Composite materials approach



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

Ellipsoidal inclusion - special properties



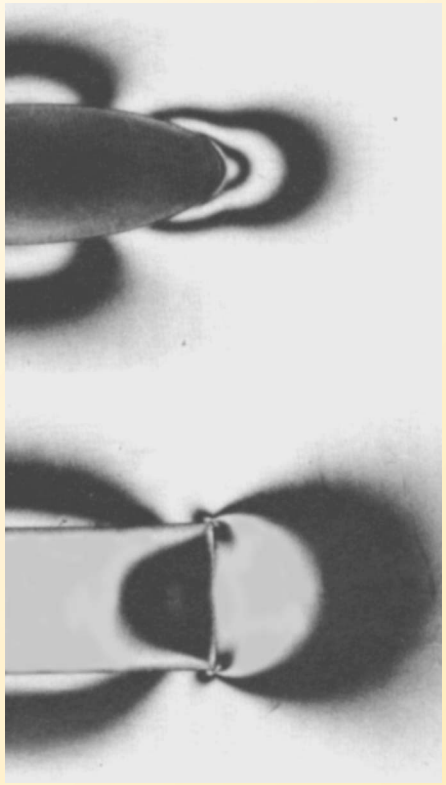


Uniform stress and strain field within the inclusion

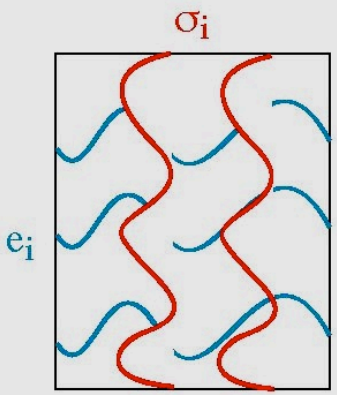
Ellipsoid and Cylinder

homogeneous stress & strain fields

heterogeneous stress & strain fields



Self Consistent (SC) Method

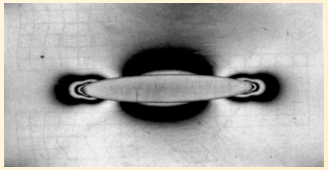


$e_i \neq$ constant $\sigma_i \neq$ constant : $C^* = \langle \sigma \rangle \langle e \rangle^{-1}$

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

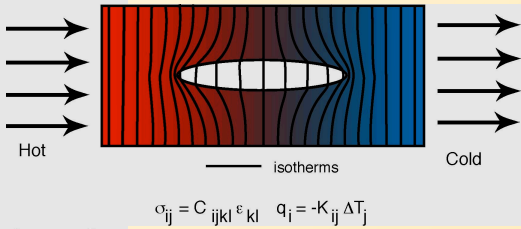
$$\langle \sigma \rangle = \Sigma V_i (C_i e_i) \qquad \langle e \rangle = \Sigma V_i e_i$$

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



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

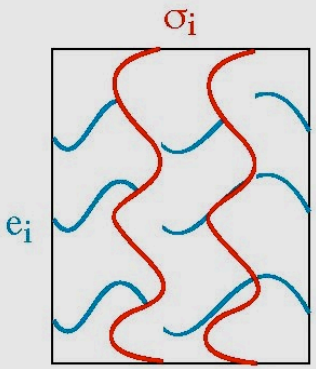
$$e_i = [\mathbf{I} + \mathbf{G} (C_i - C^*)]^{-1}$$



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

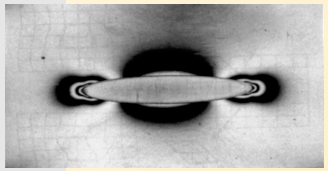


$e_i \neq$ constant $\sigma_i \neq$ constant : $C^* = <\sigma> <e>^{-1}$

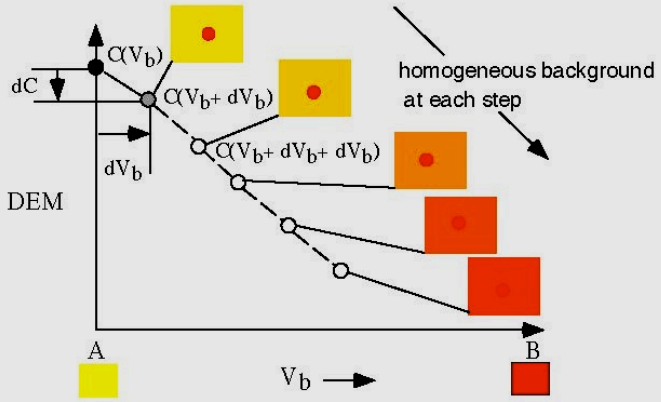
$$C^* = <\sigma> <e>^{-1}$$

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

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

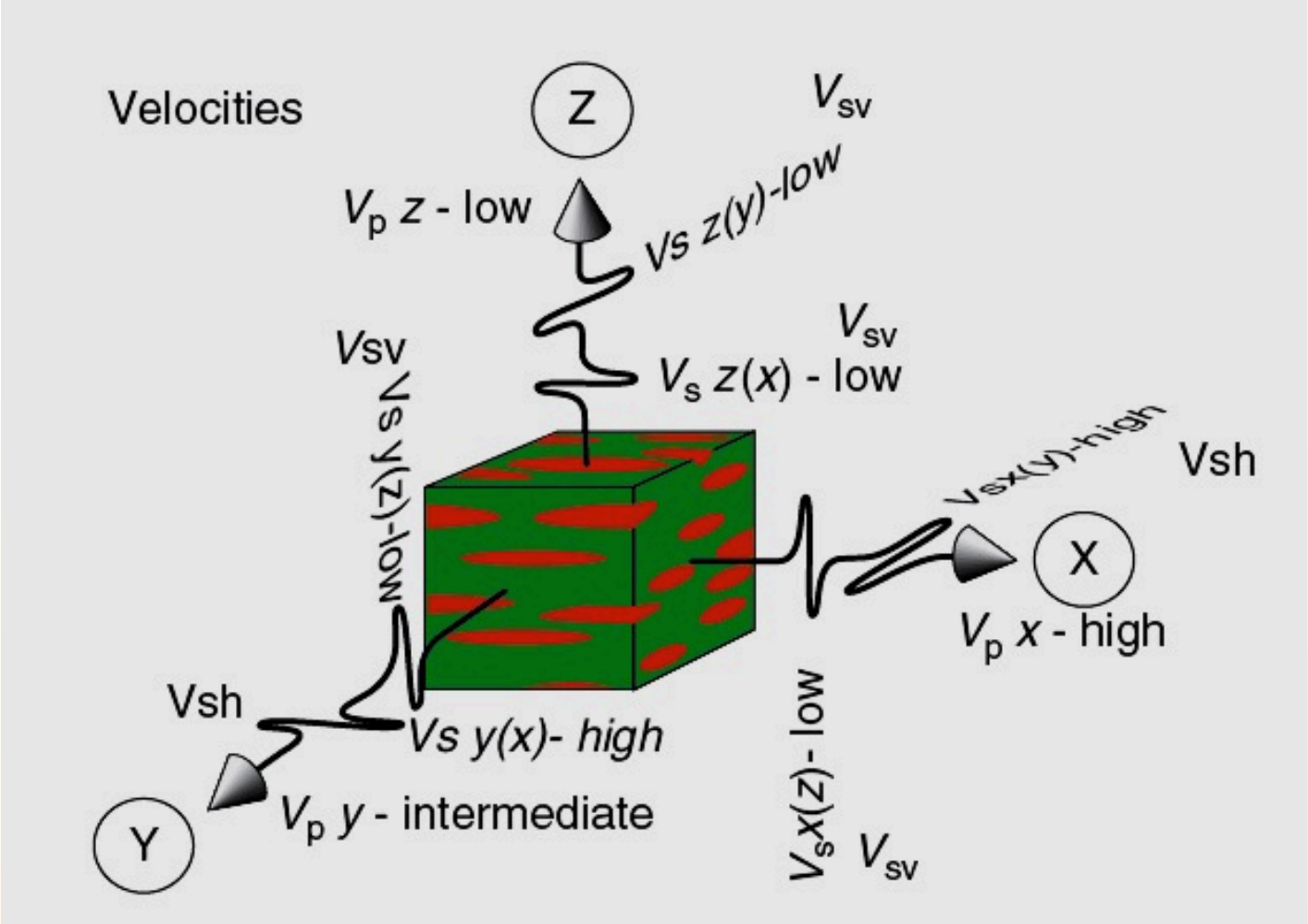


Developed for two phase aggregates type AB (McLaughlin,1977) where Vb = 1-Va. The phase B is the included phase and phase A is the host phase. Requires some inital value of C* at a compostion Vb - this may be a pure end member.The incremental nature of the differential approch preserves the percolating (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



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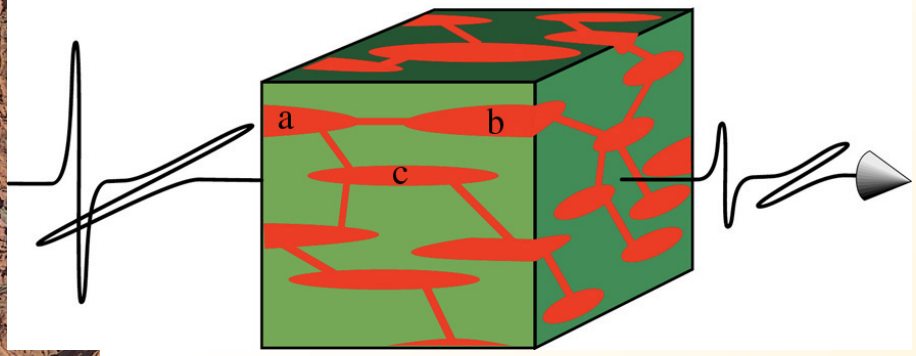
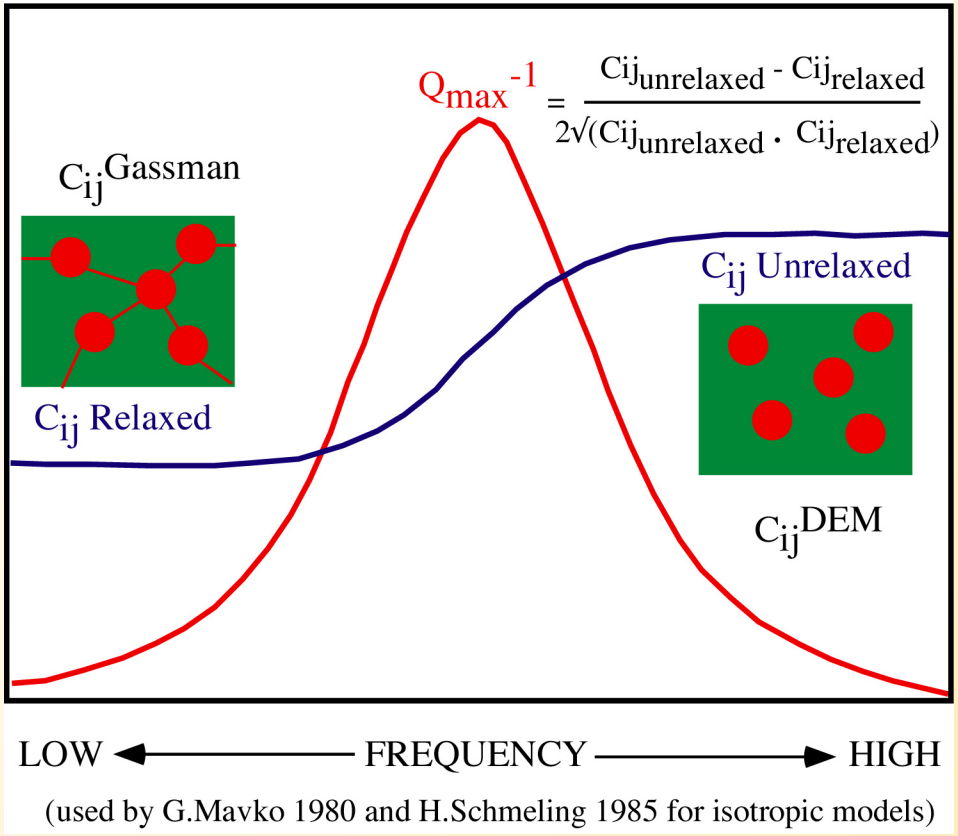
squirt flow attenuation



Standard Linear Solid (Zener, 1948)

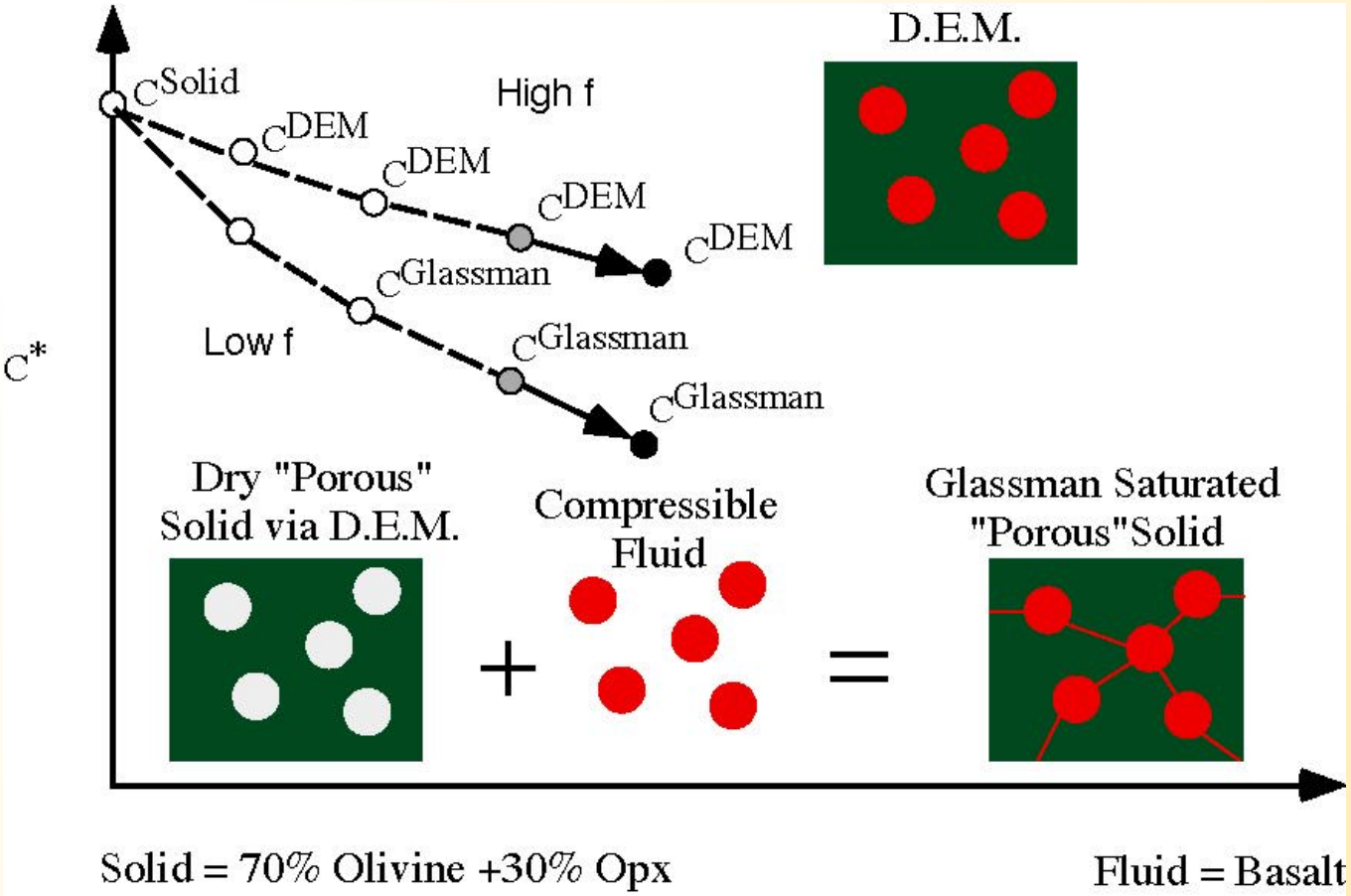


(used by G.Mavko 1980 and H.Schmeling 1985 for isotropic models)

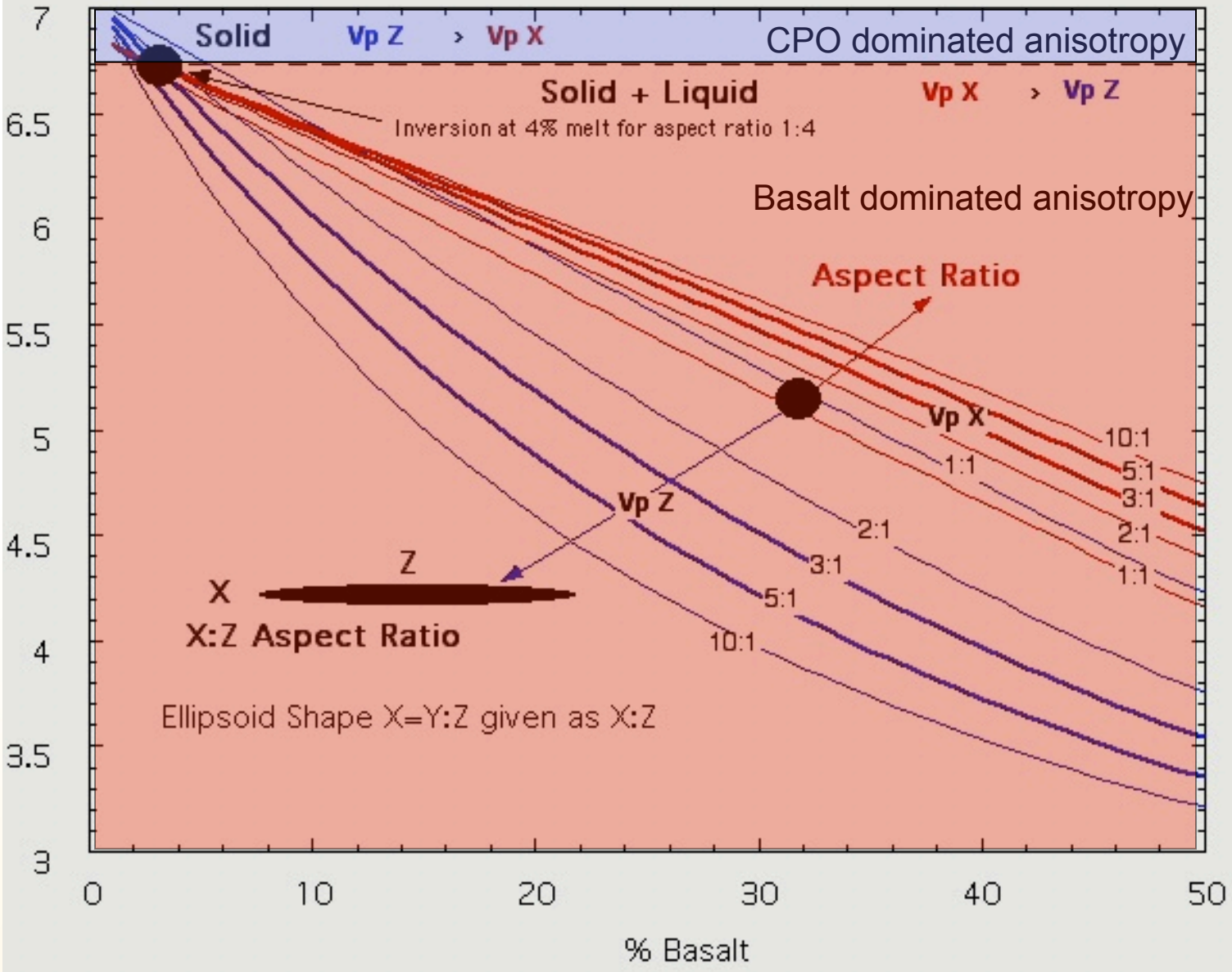
Unrelaxed Modulus - High Frequency : Pa ≠ Pb ≠ Pc...0% connectivity
--> given by Self Consistent (S.C.) or Differential Effective Medium (D.E.M.).

Relaxed Modulus - Low Frequency : Pa = Pb = Pc...100% connectivity
--> given by Gassmann (1951) relationship extended to anisotropic media (Brown & Korringa, 1975).

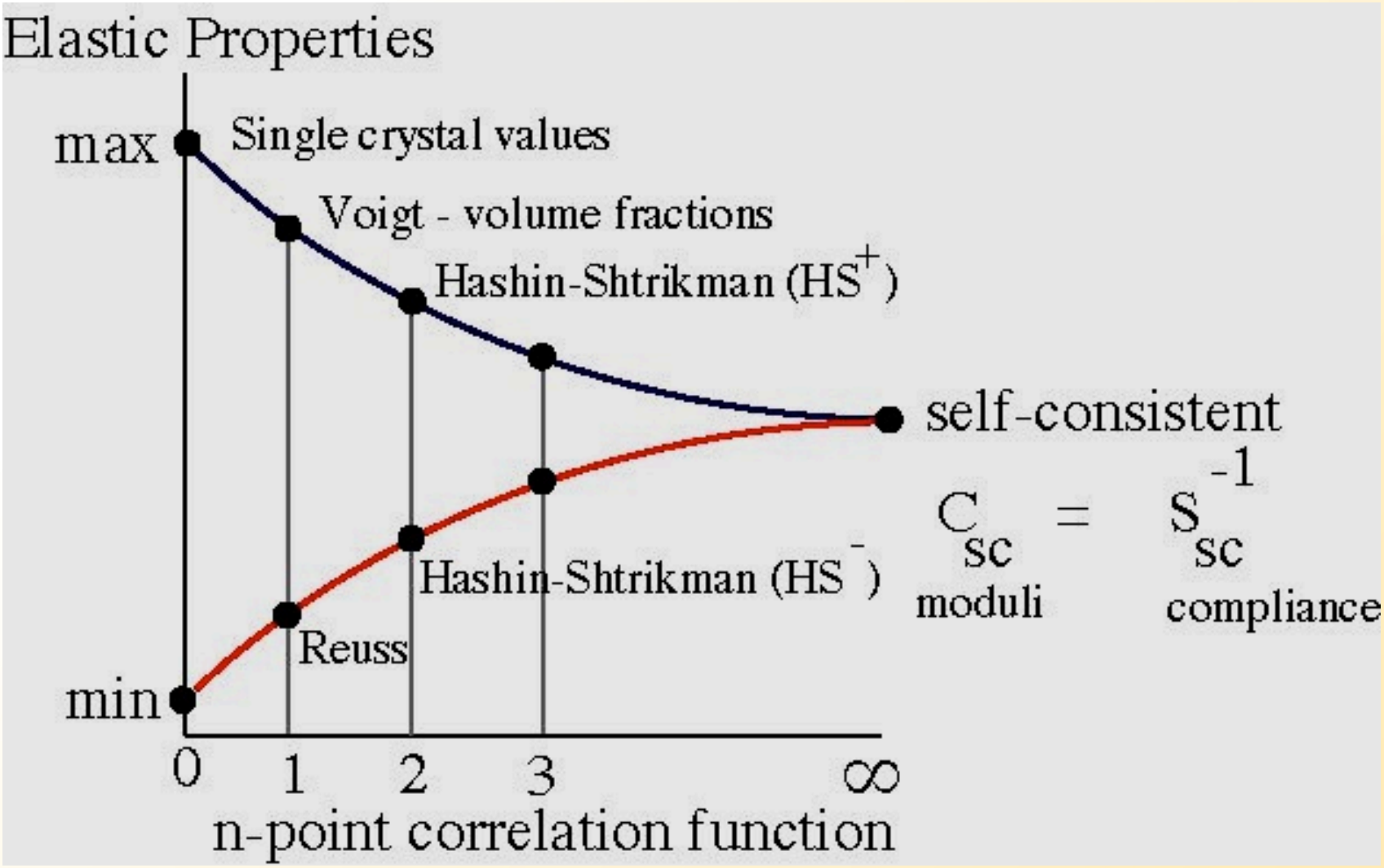
Combining DEM and Poroelasticity theory



VpX and VpZ Gabbro - Basalt : Effect of Aspect Ratio



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


Elastic Properties
max
Single crystal values
Voigt - volume fractions
Hashin-Shtrikman (HS+)
self-consistent
Hashin-Shtrikman (HS-)
Reuss
min
0
1
2
3
∞
n-point correlation function
C sc = S sc -1
moduli
compliance

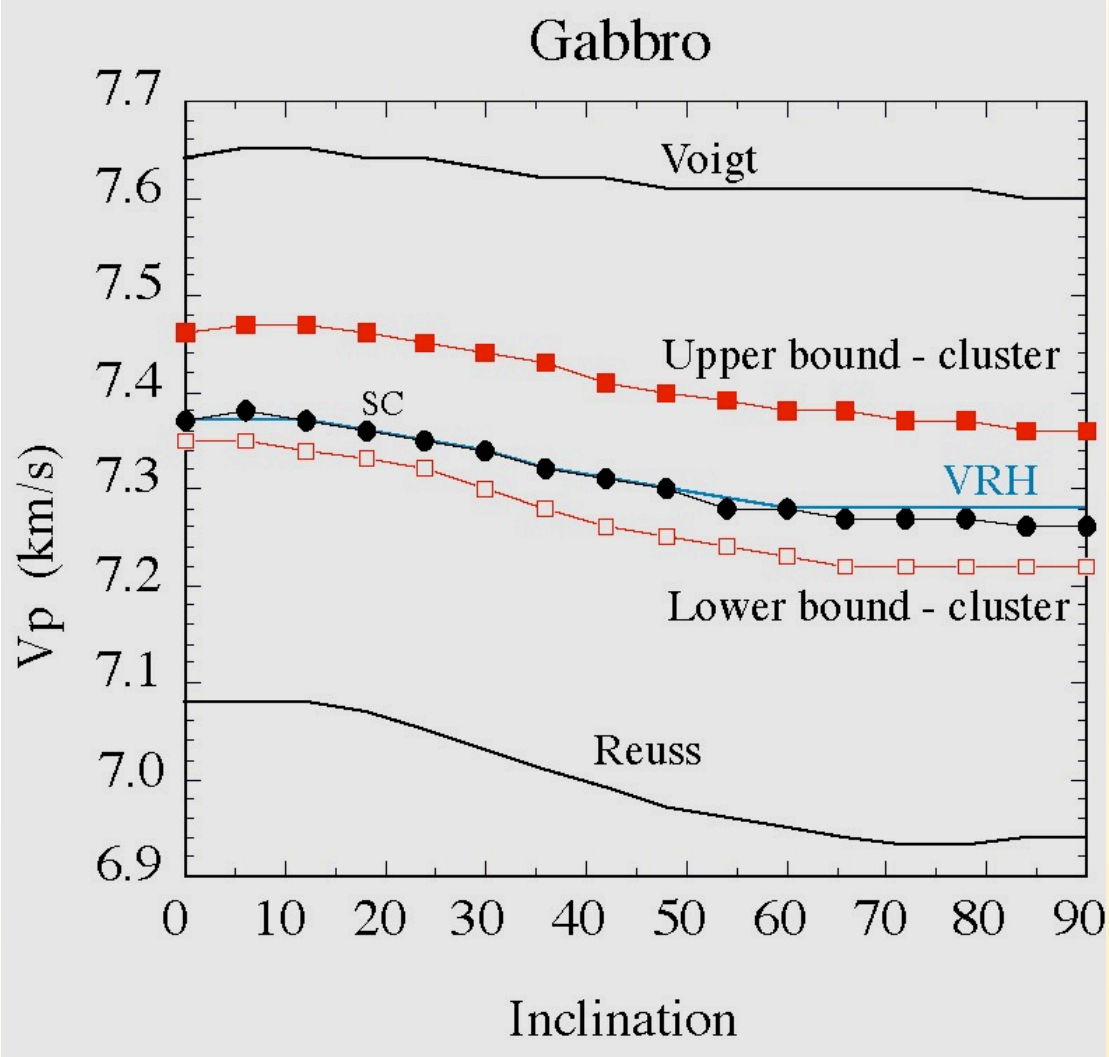
The Hill Series

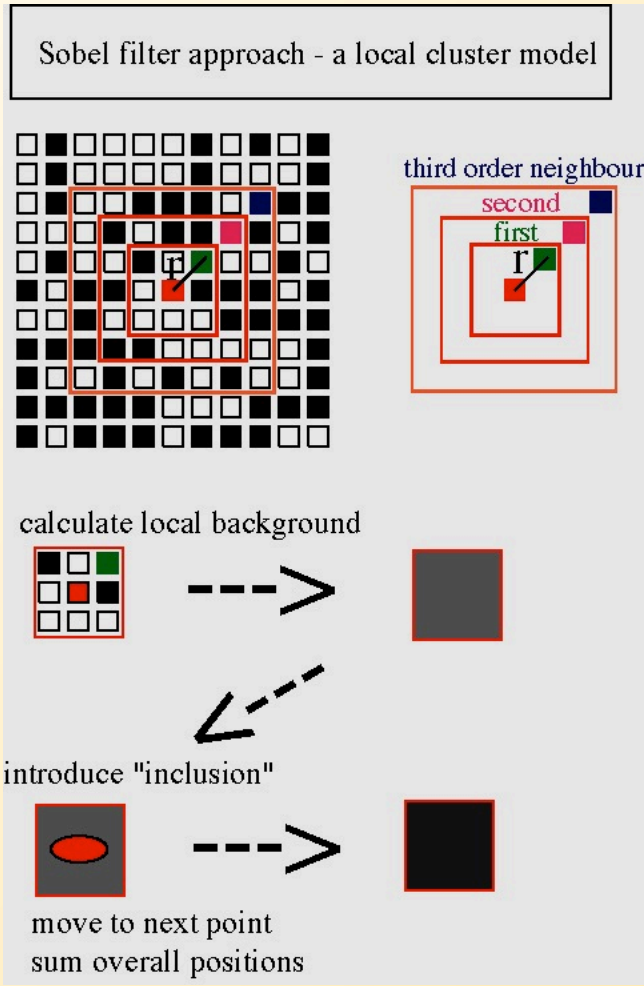
The ideal of Hill series originally suggested by Adam Morawiec

Using the Hill average it iterates untill the Cij =inv(Sij) considered to be of physical importance

I have tested this 3 iterates gives result, it is very close to the Hill average.

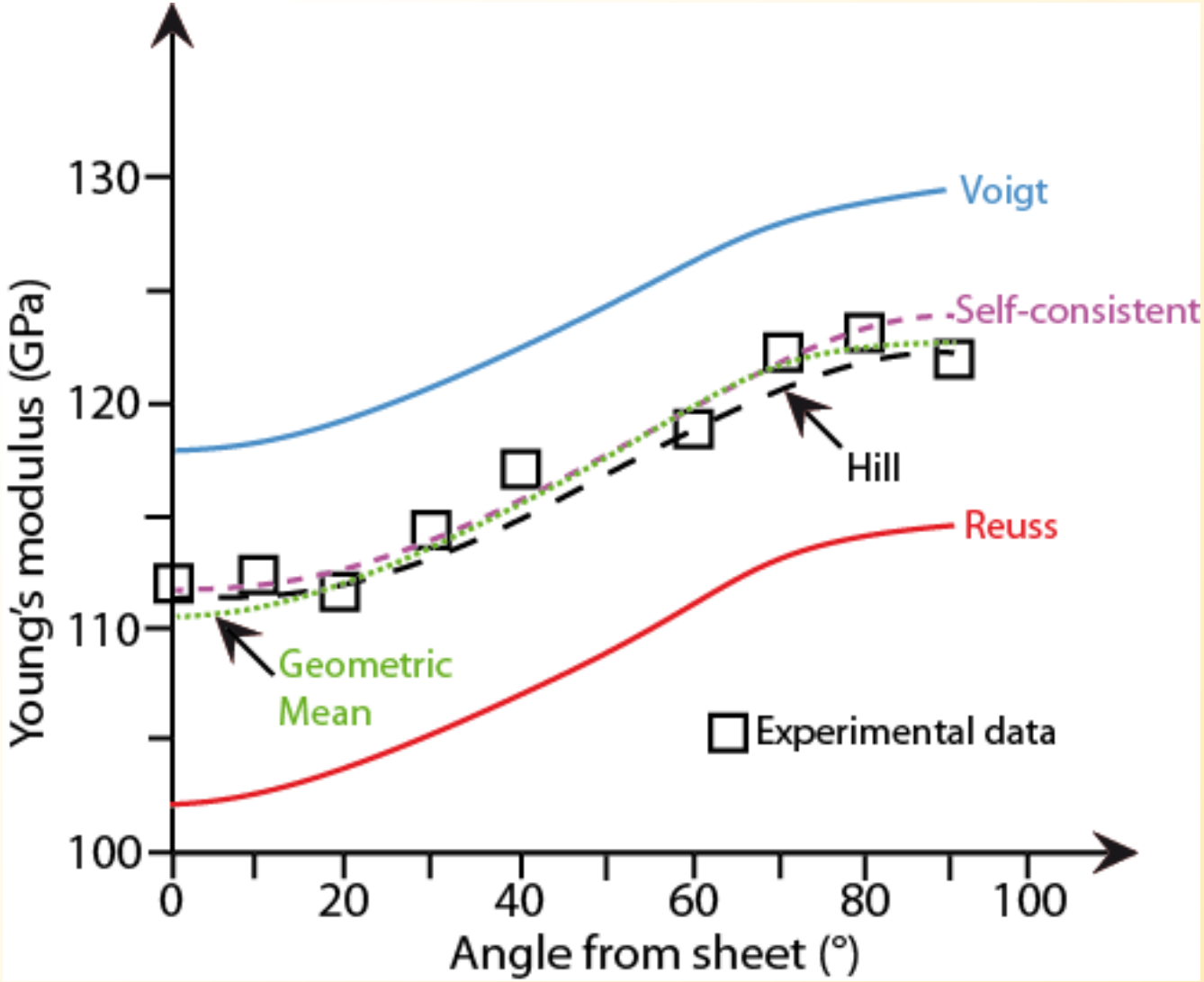
Cluster method





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

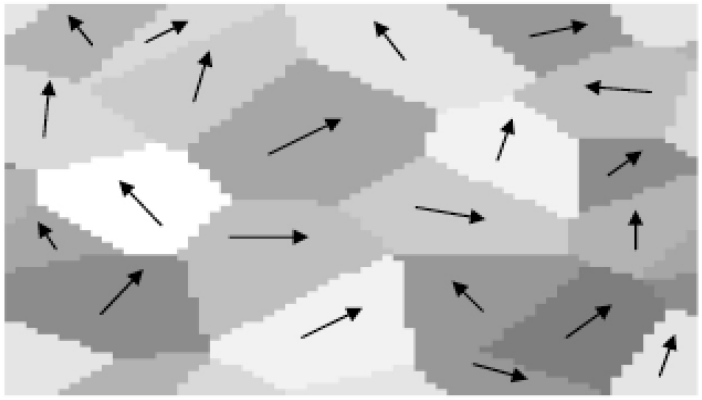
Upper Voigt SC(shape) GM Lower Reuss



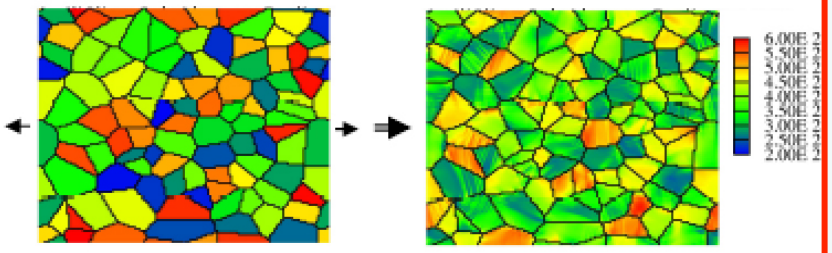
Polycrystal models: full-field vs. mean-field (statistical) approaches

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

Full-field solution



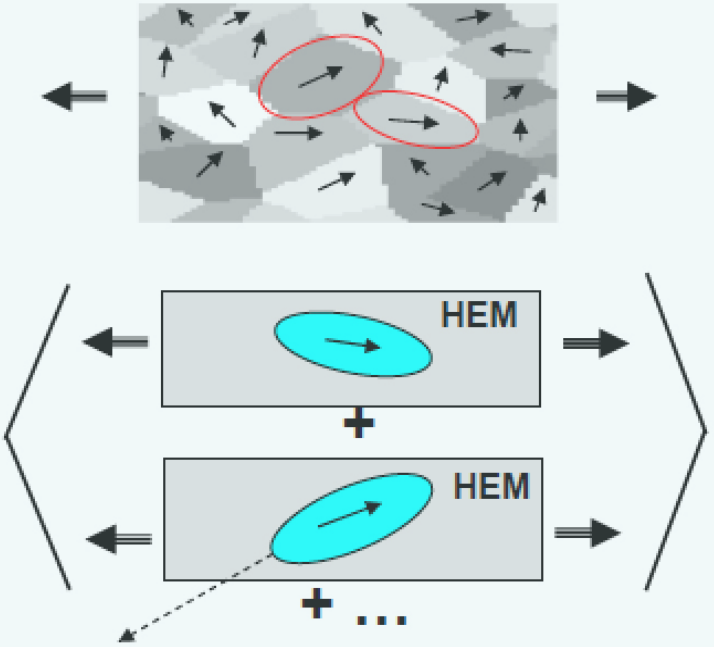
Solving equilibrium + compatibility:



grain structure stress field

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

Mean-field statistical solution



Solving Eshelby inclusion problem

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

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

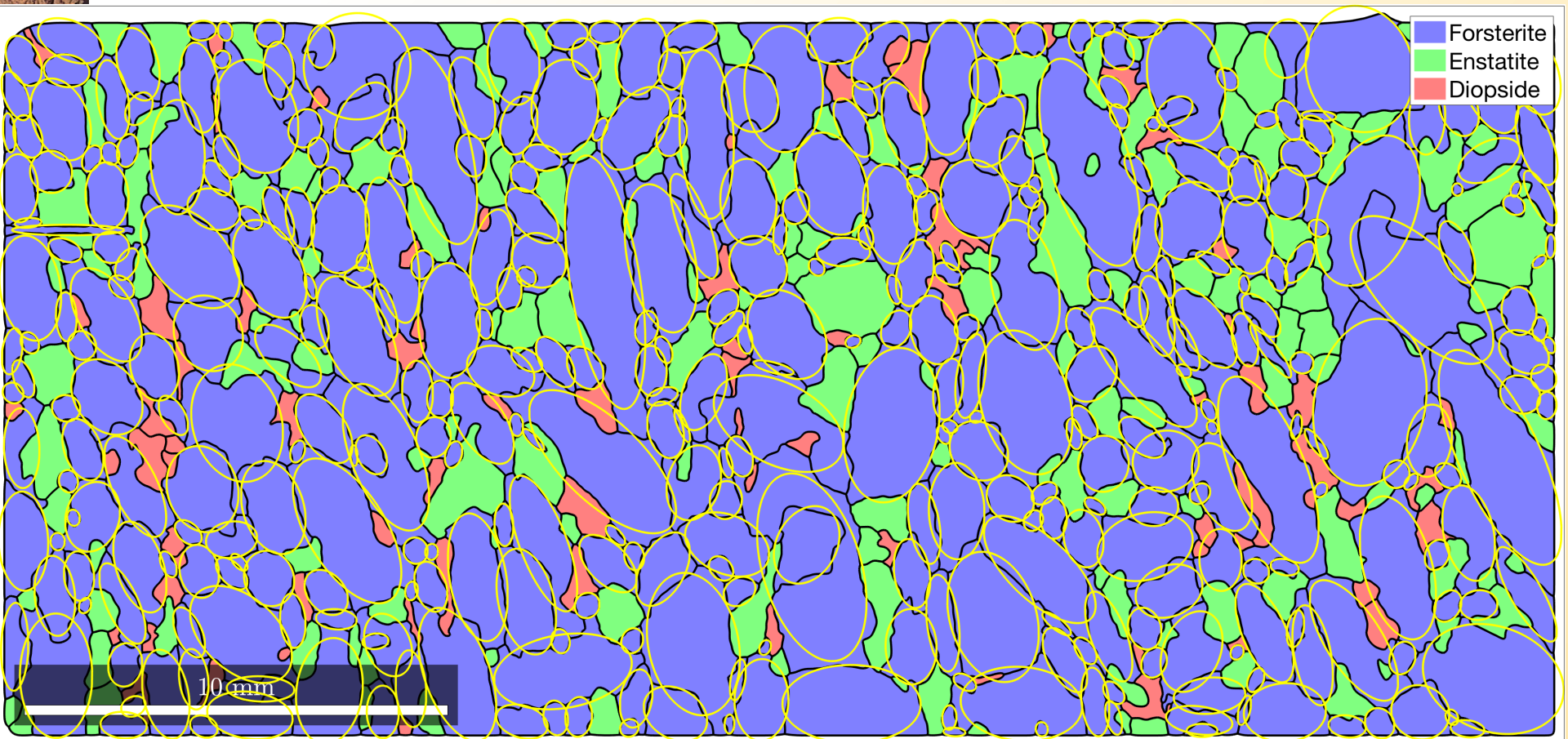
- DEM scheme as translated into MatLab scripted with GUI interface. Published in Computers & Geosciences
- You can download the script and manual from ; https://github.com/ekim1419/GassDem
- The SC scheme has translated into MatLab scripted, we use MTEX function to export EBSD 2D data into the SC scheme. Demo_SC_Data_export.m

phi1	Phi	phi2	area	omega	a	b
39.91	131.882	337.894	85356	177.047	263.951	102.935
Mean grain orientation			**area for weighting**		**omega angle of long & short axes**	

Self-consistent

For each mineral

1. Fit ellipses – get long and short axis & orientation (omega)
2. Grain mean orientation, not ebsd pixels !
3. Grain Area for weighting



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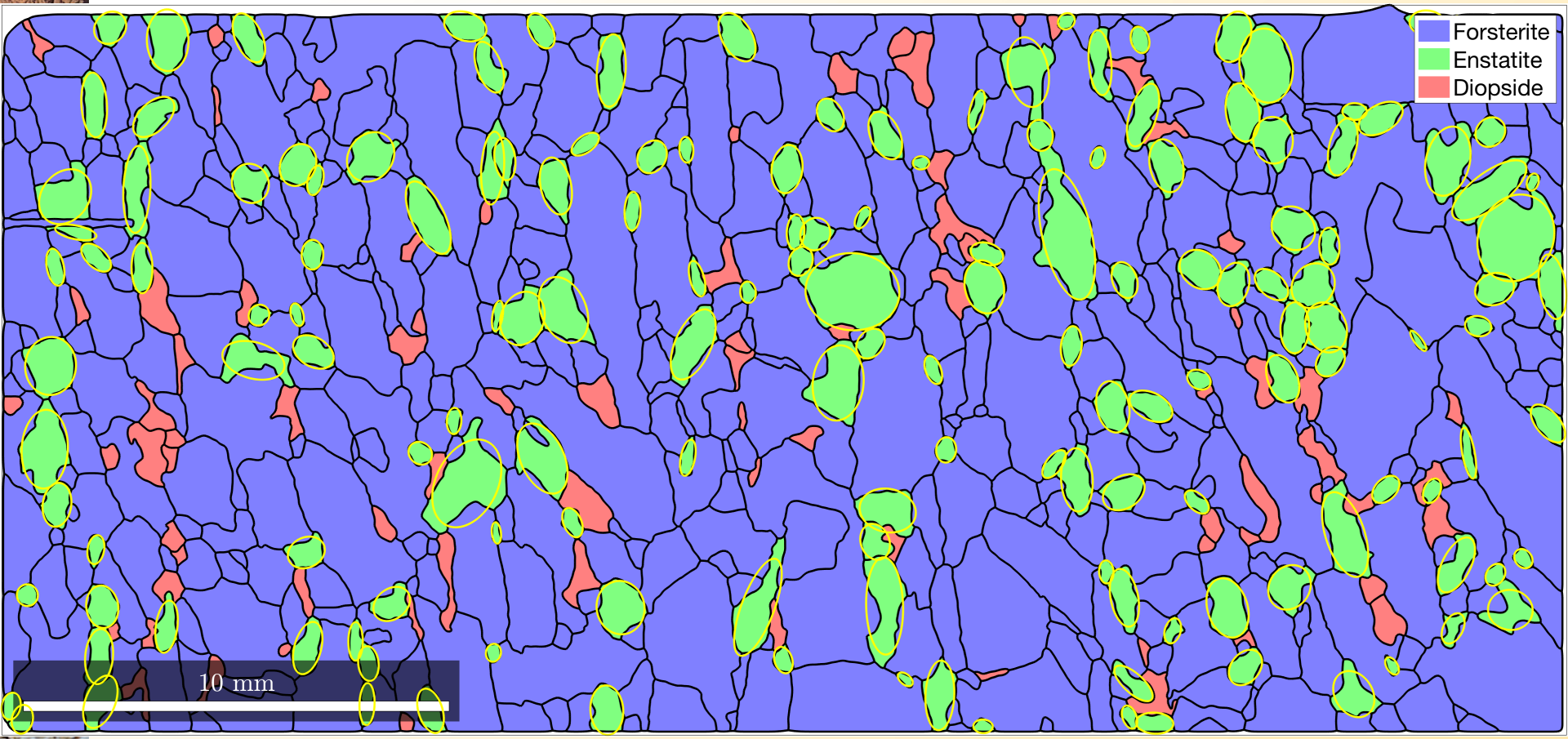
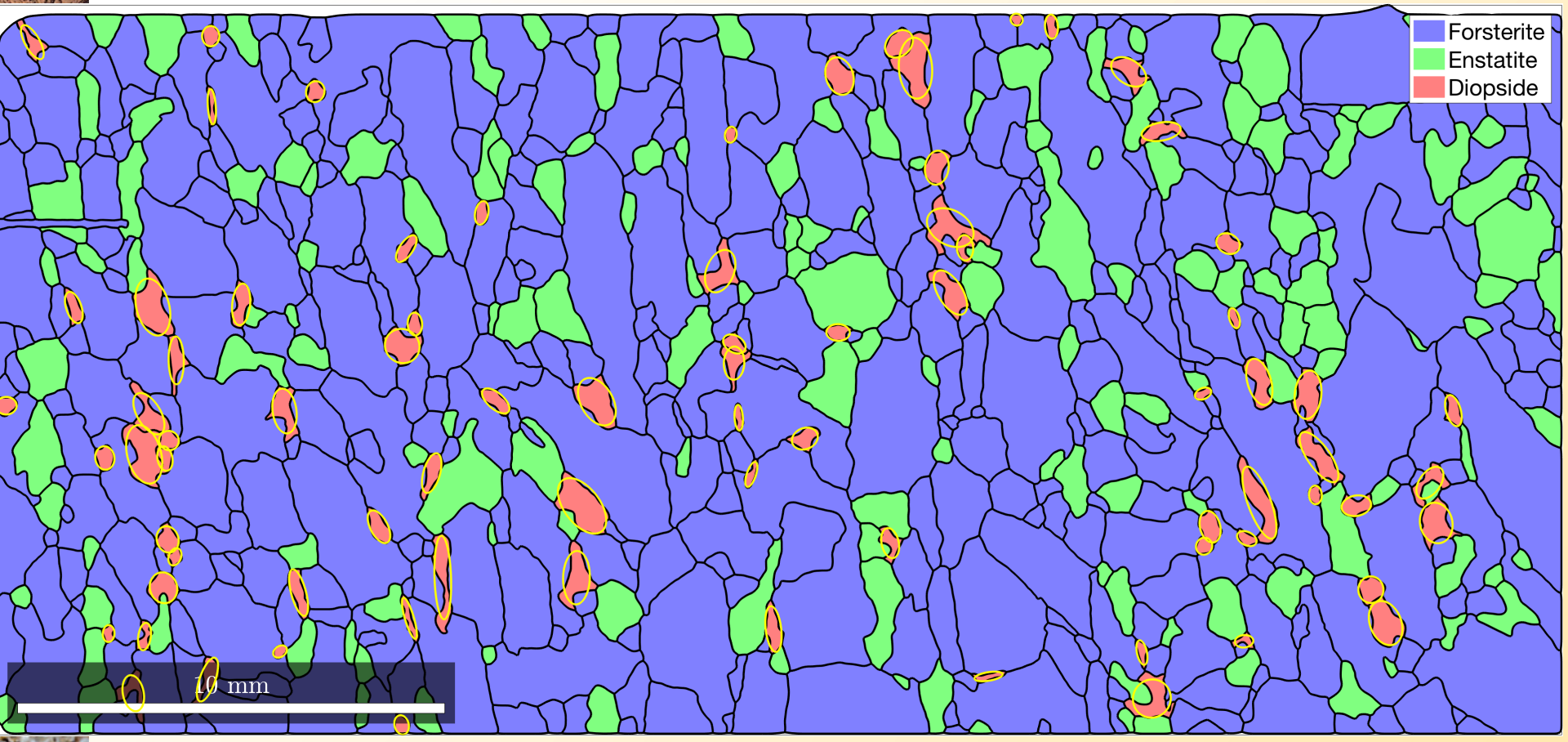
Enstatite Orthopyroxene green



Diopside Clinopyroxene red



Future developments; Importing single crystal tensors from a database

- 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.

Anisotropy of for stiffness elastic tensors

- First example for Cubic symmetries Zener(1948)
- $$\mathbf{AZ} = \frac{2C_{44}}{C_{11} - C_{12}}$$
- Used in geophysics
- $$\mathbf{A} = \frac{2C_{44} + C_{12}}{C_{11}} - 1$$
- Chung and Buessem (1967) Voigt and Reuss bounds are identical for isotropic case and far apart for anisotropic case.

$$\mathbf{AC} = \frac{G^{Voigt} - G^{Reuss}}{G^{Voigt} + G^{Reuss}}$$

- Ranganathan and Ostoja-Starzewski (2008)
- Universal − requires to subtract to get zero

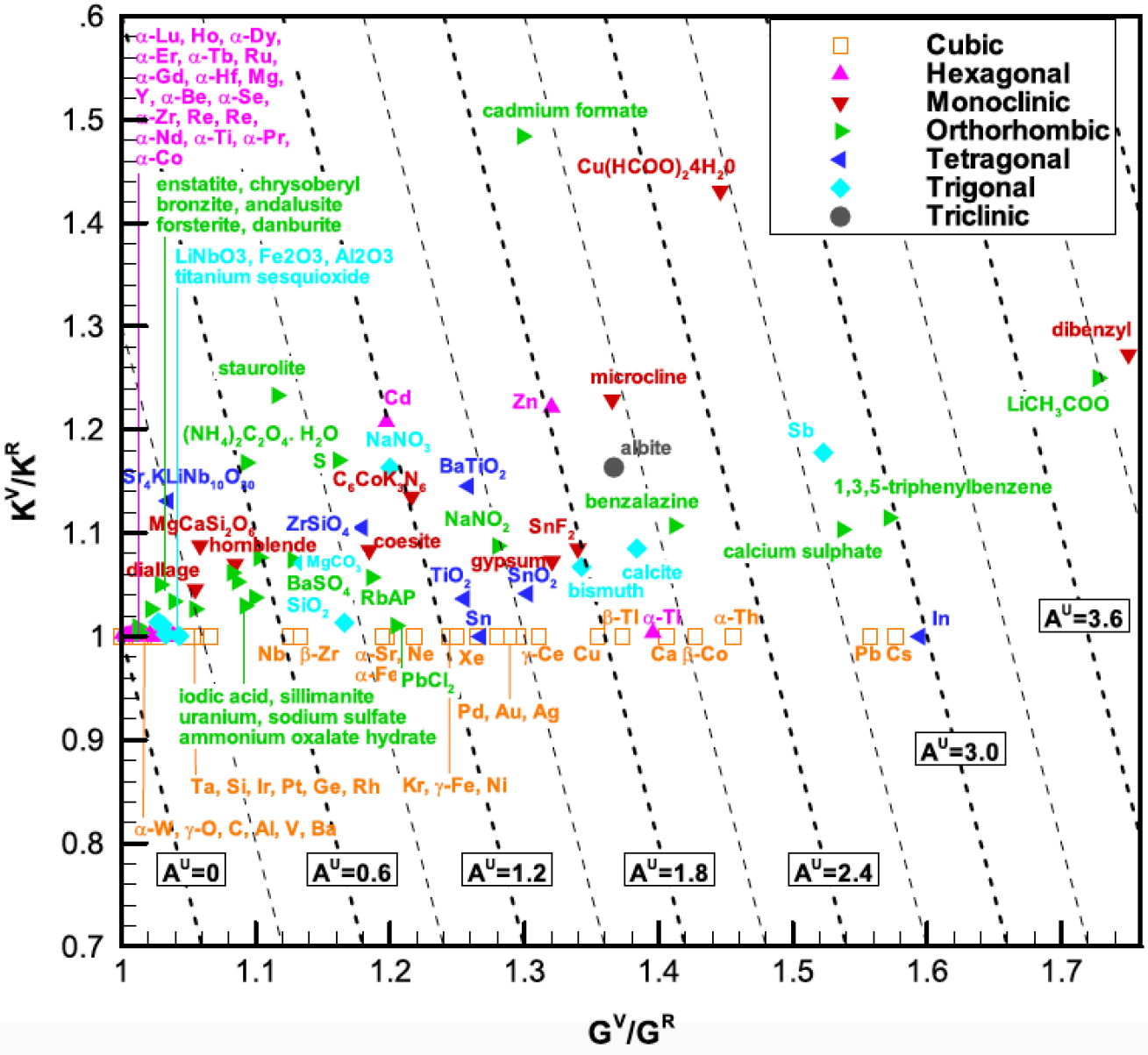
$$\mathbf{AU} = \frac{K^{Voigt}}{K^{Reuss}} + 5\frac{G^{Voigt}}{G^{Ruess}} - 6 > 0$$

- Kube (2016) Log-Euclidean natrually has zero for isotropic

$$\mathbf{AL} = \sqrt{\left[ln\left(\frac{K^{Voigt}}{K^{Reuss}}\right)\right]^2 + 5\left[ln\left(\frac{G^{Voigt}}{G^{Reuss}}\right)\right]^2}$$

Ranganathan and Ostoja-Starzewski (2008) Universal

$$\mathrm{AU} = \frac{K^{Voigt}}{K^{Reuss}} + 5\frac{G^{Voigt}}{G^{Ruess}} - 6 > 0$$



Ranganathan and Ostoja-Starzewski (2008)

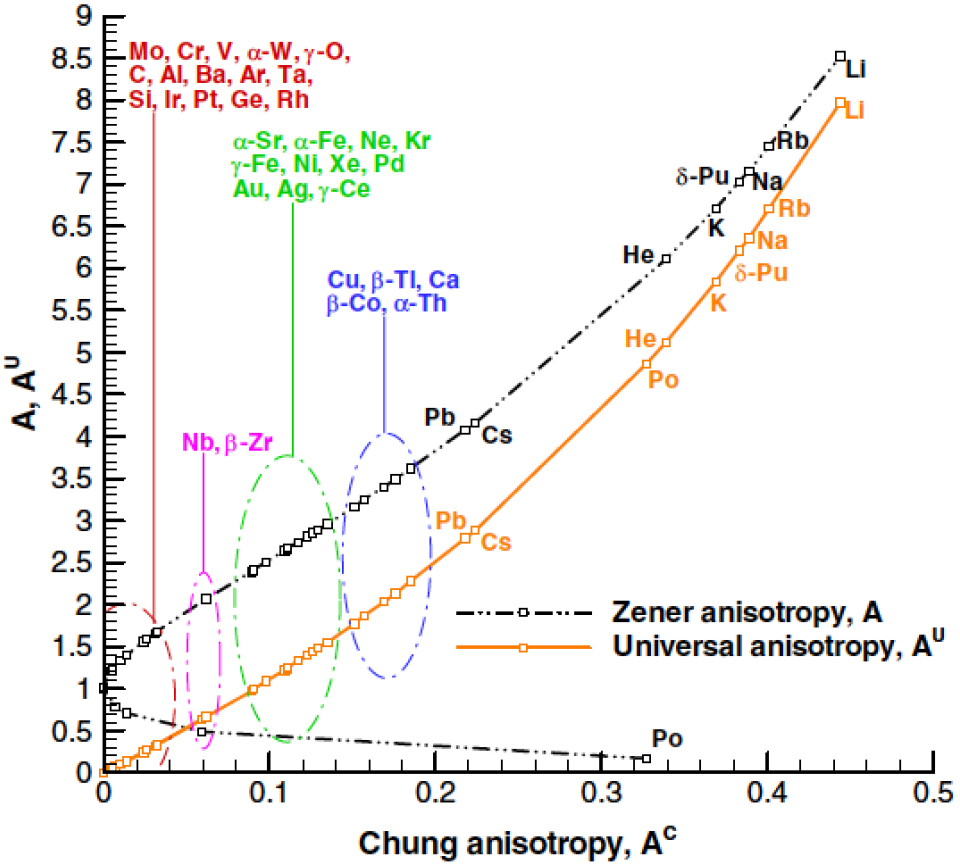
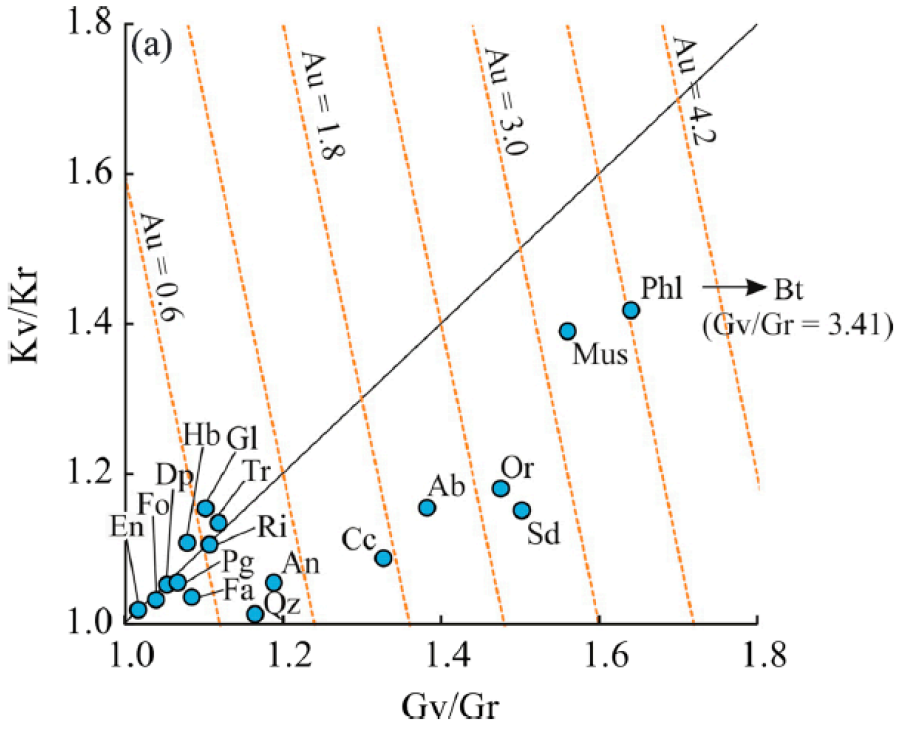
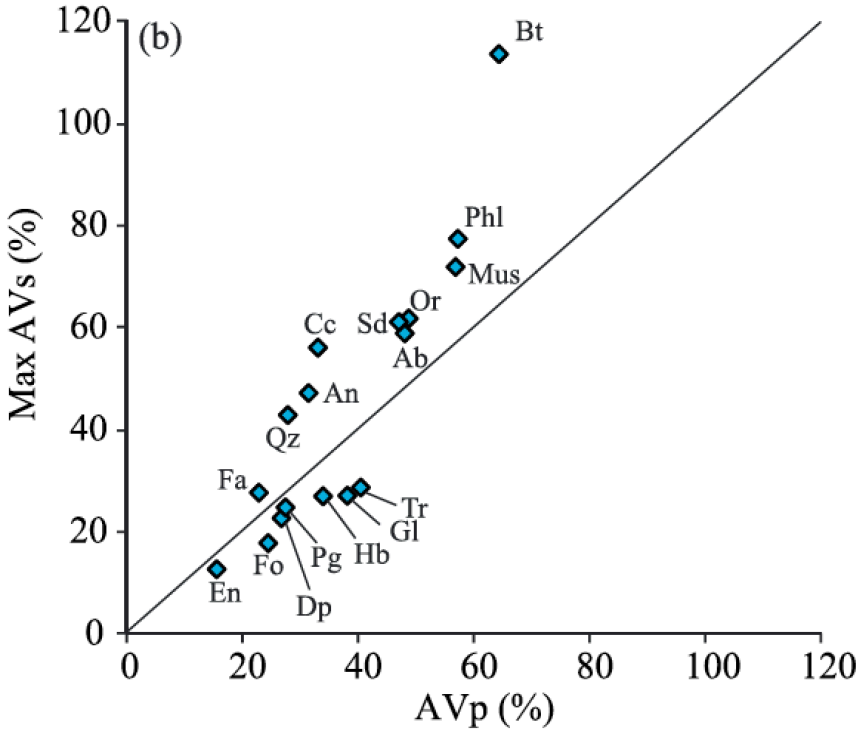


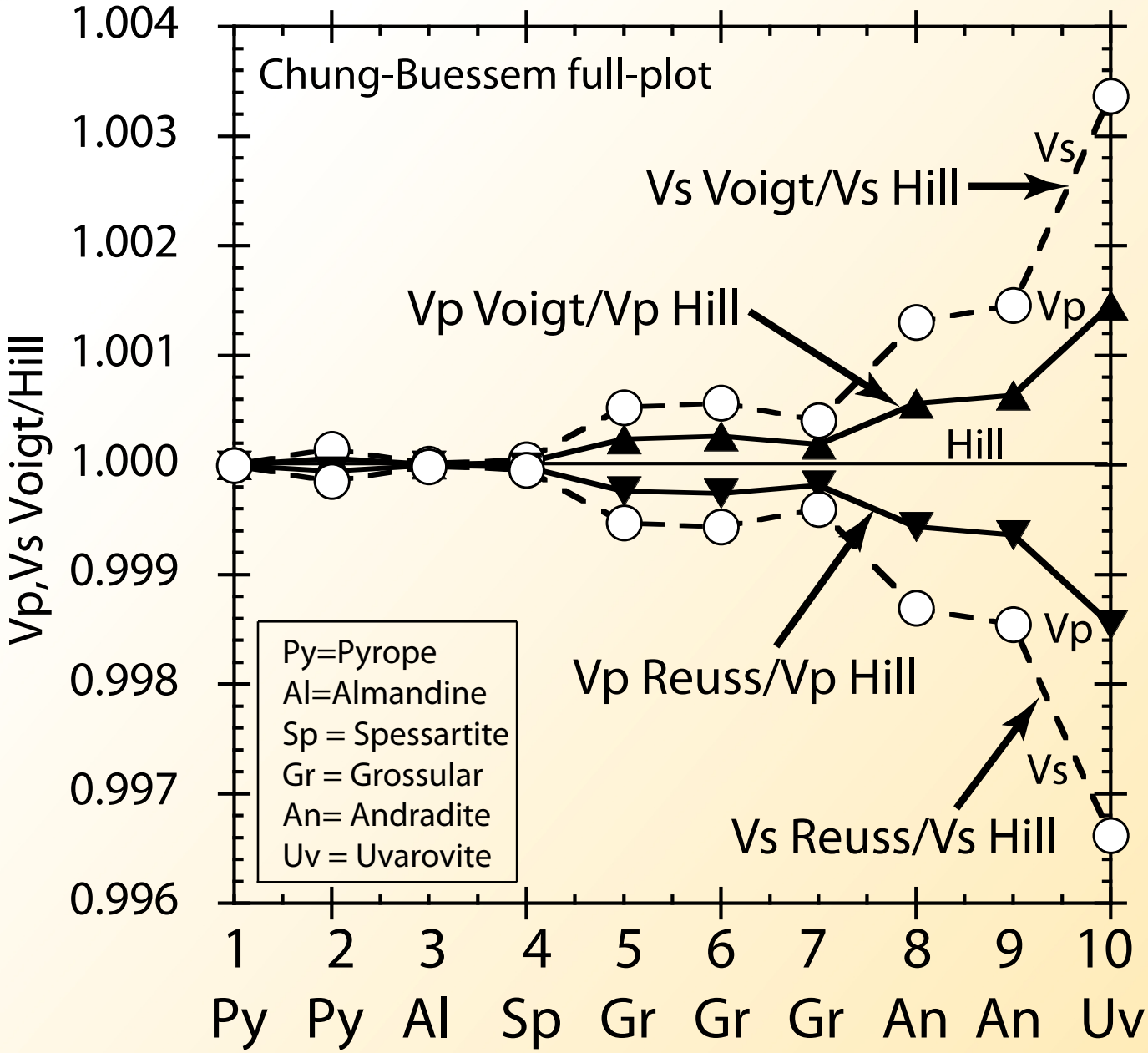
FIG. 1 (color online). Anisotropy measures for cubic crystals (Zener and Ledbetter-Migliori anisotropy measures coincide for cubic crystals). Single crystal data obtained from [3,11].

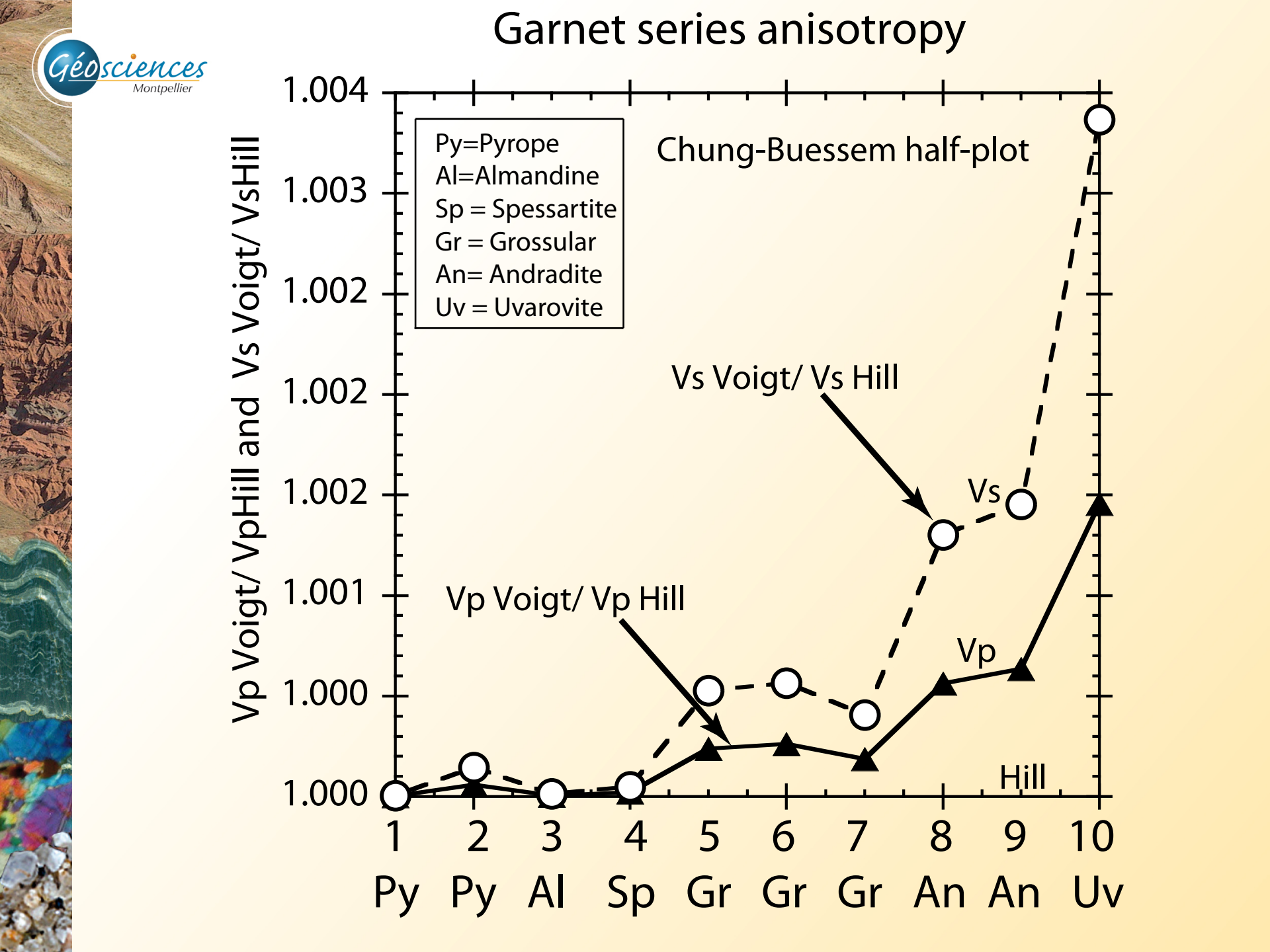
Layered minerals always largest anisotropy





Garnet series anisotropy




Garnet series anisotropy
Chung-Buessem half-plot
Py=Pyrope
Al=Almandine
Sp = Spessartite
Gr = Grossular
An= Andradite
Uv = Uvarovite
Vp Voigt/ VpHill and Vs Voigt/ VsHill
Vs Voigt/ Vs Hill
Vp Voigt/ Vp Hill
Vs
Vp
Hill
1.004
1.003
1.002
1.002
1.002
1.001
1.000
1.000
1 2 3 4 5 6 7 8 9 10
Py Py Al Sp Gr Gr Gr An An Uv

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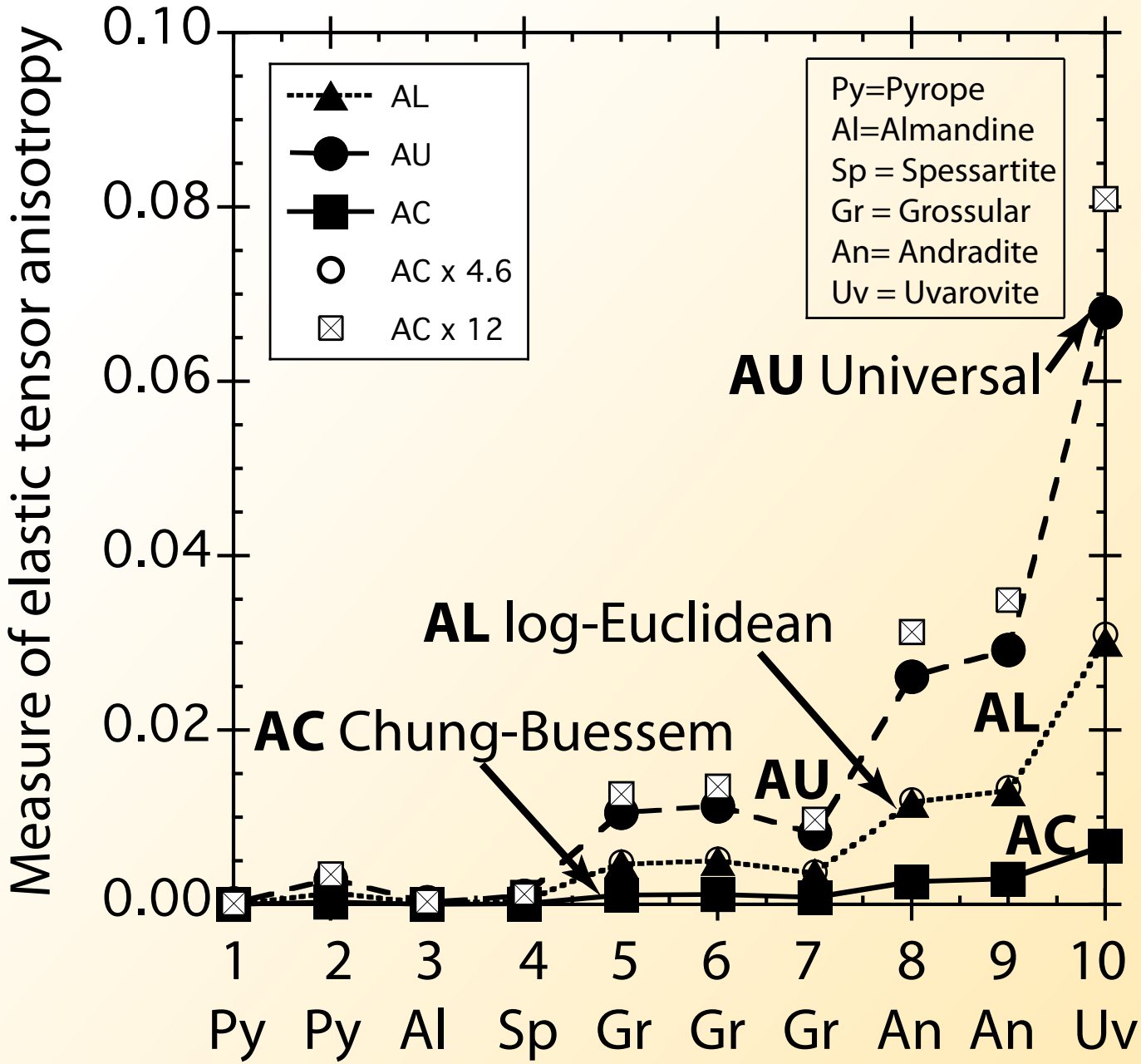
Garnet series anisotropy



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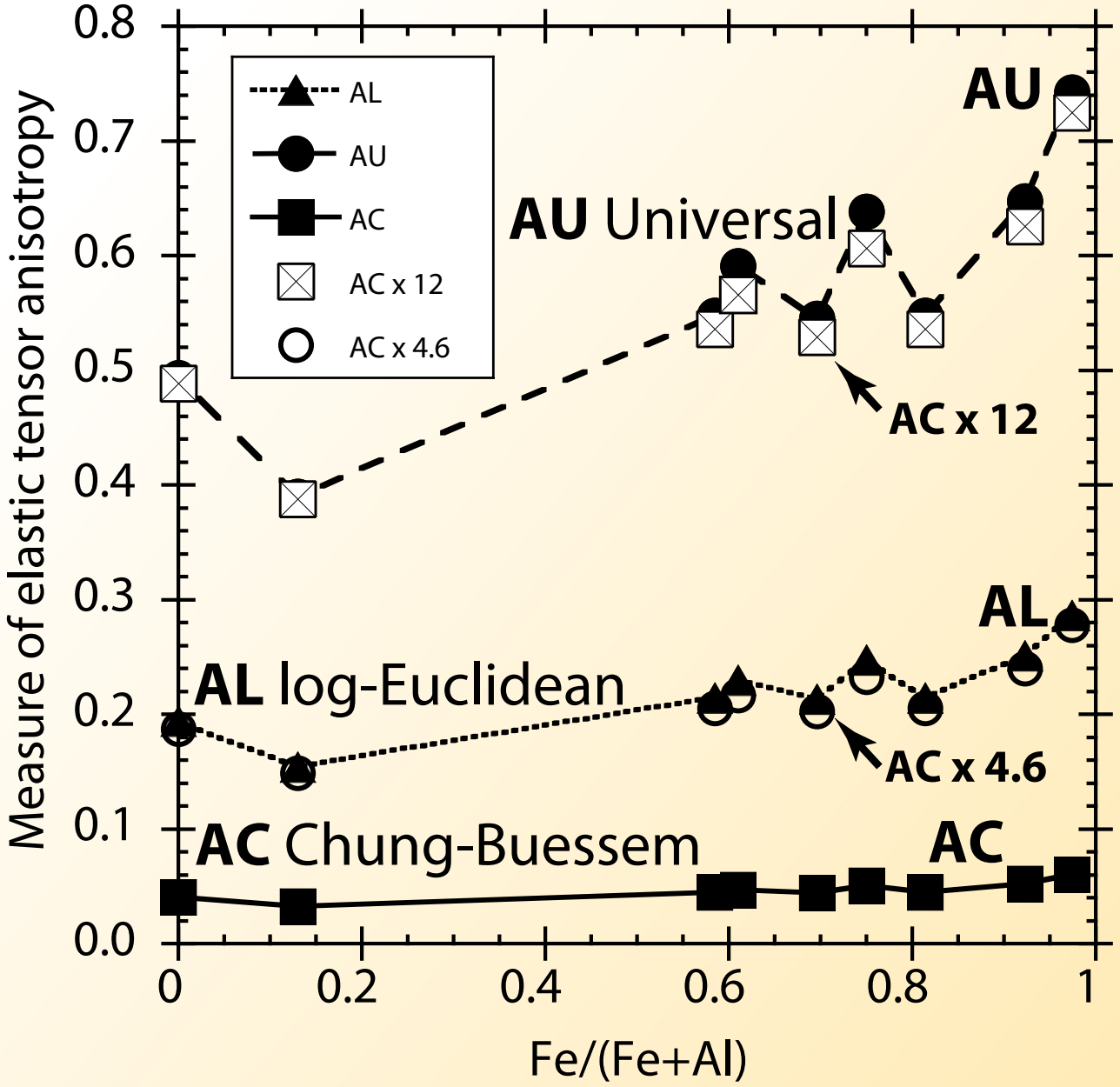
Amphibole series anisotropy



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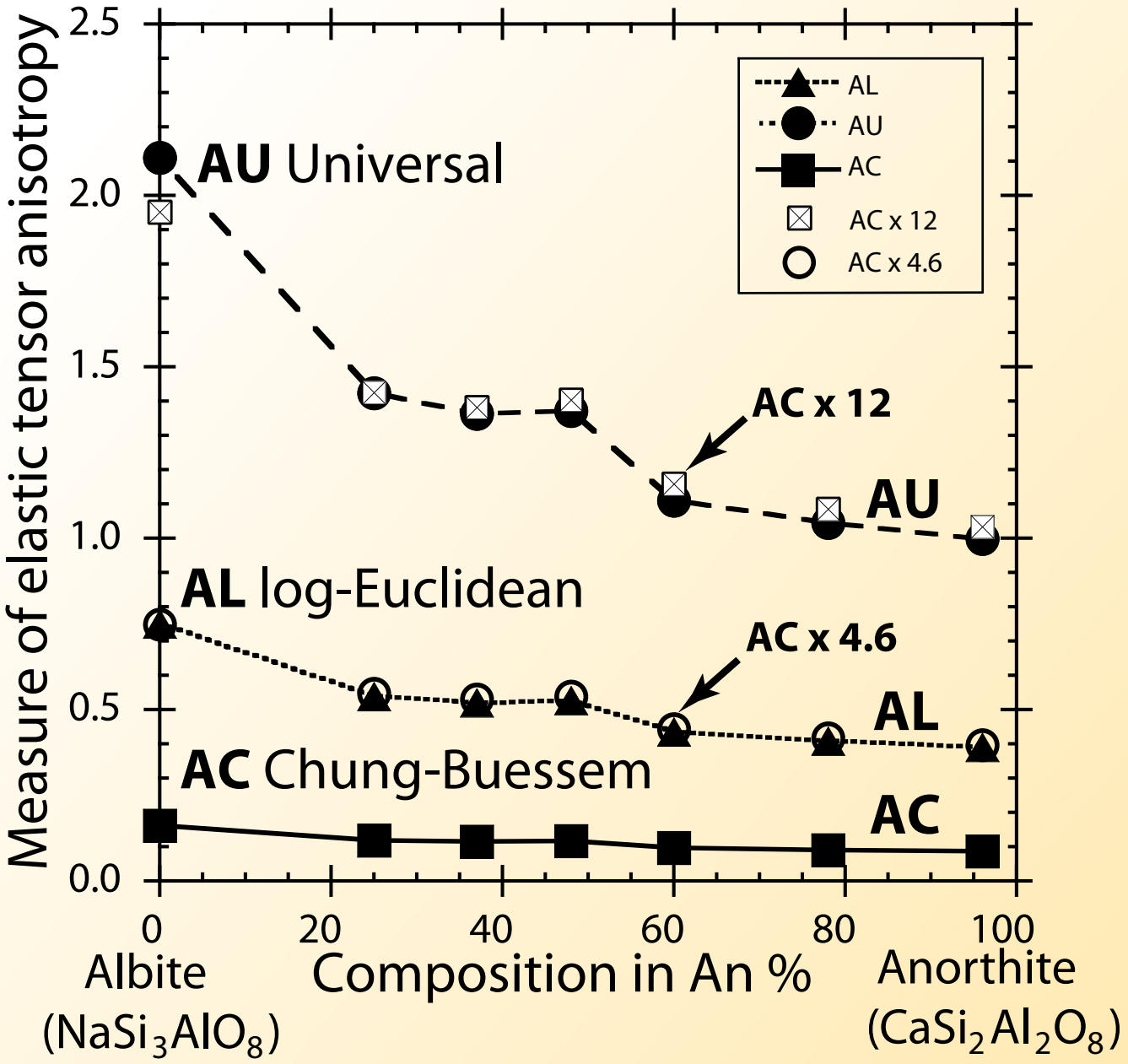
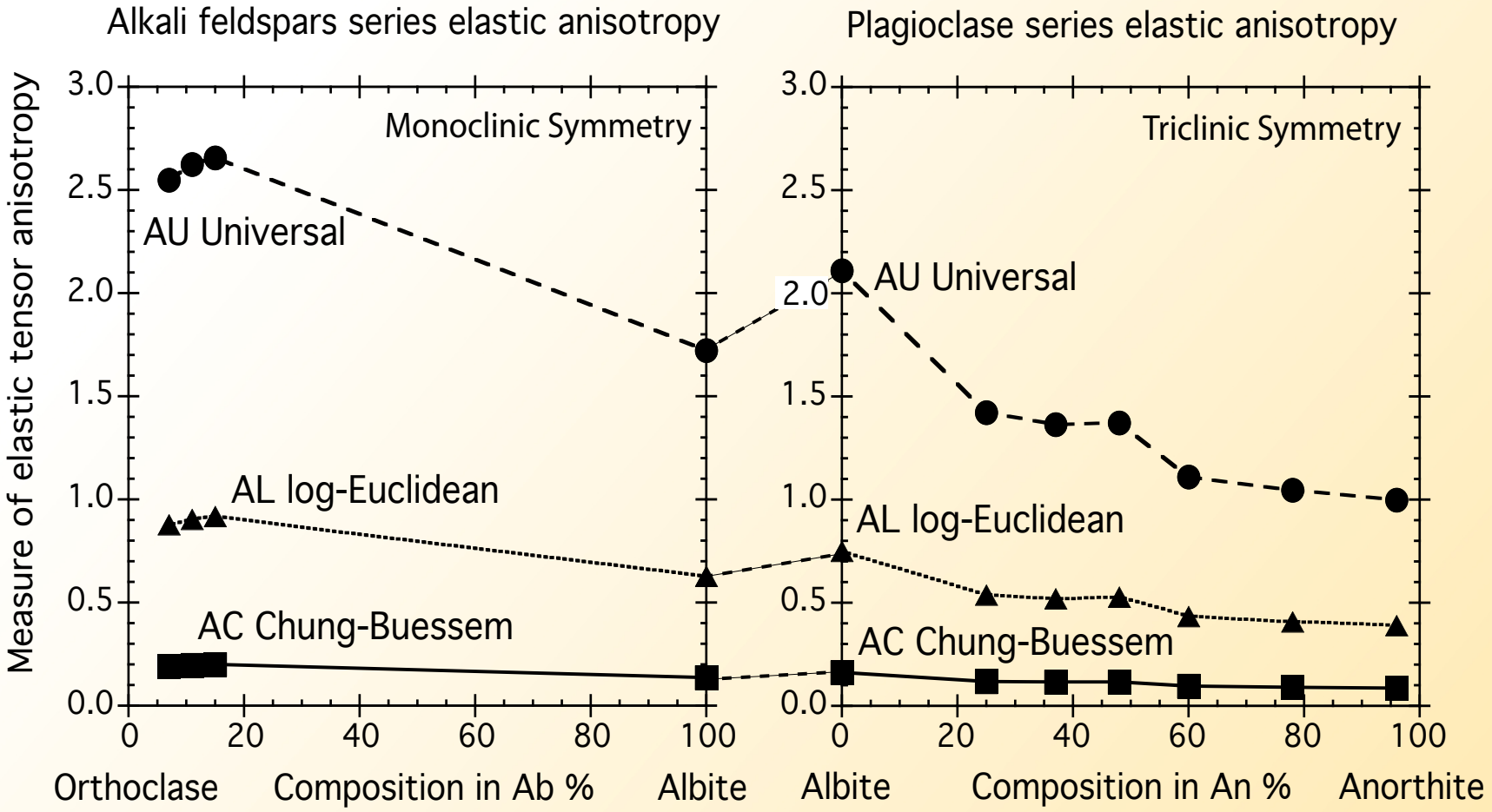
Plagioclase series elastic anisotropy





Albite – monoclinic 13 Albite – triclinic 21

Differential effective medium modeling with Matlab

Eunyoung Kim

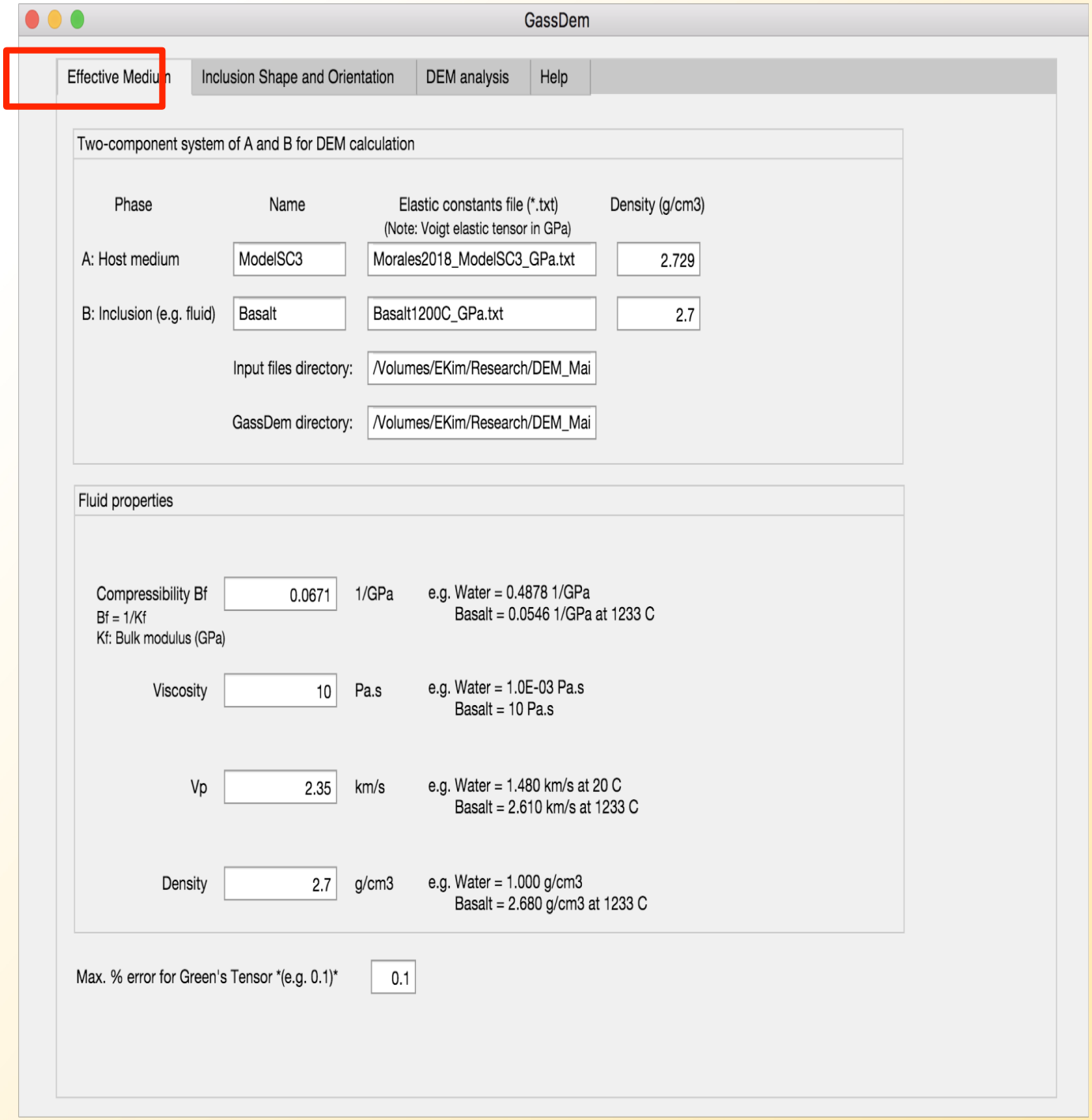
Ph.D. candidate
School of Earth and Environmental Sciences
Seoul National University

Géosciences Montpellier

Contents

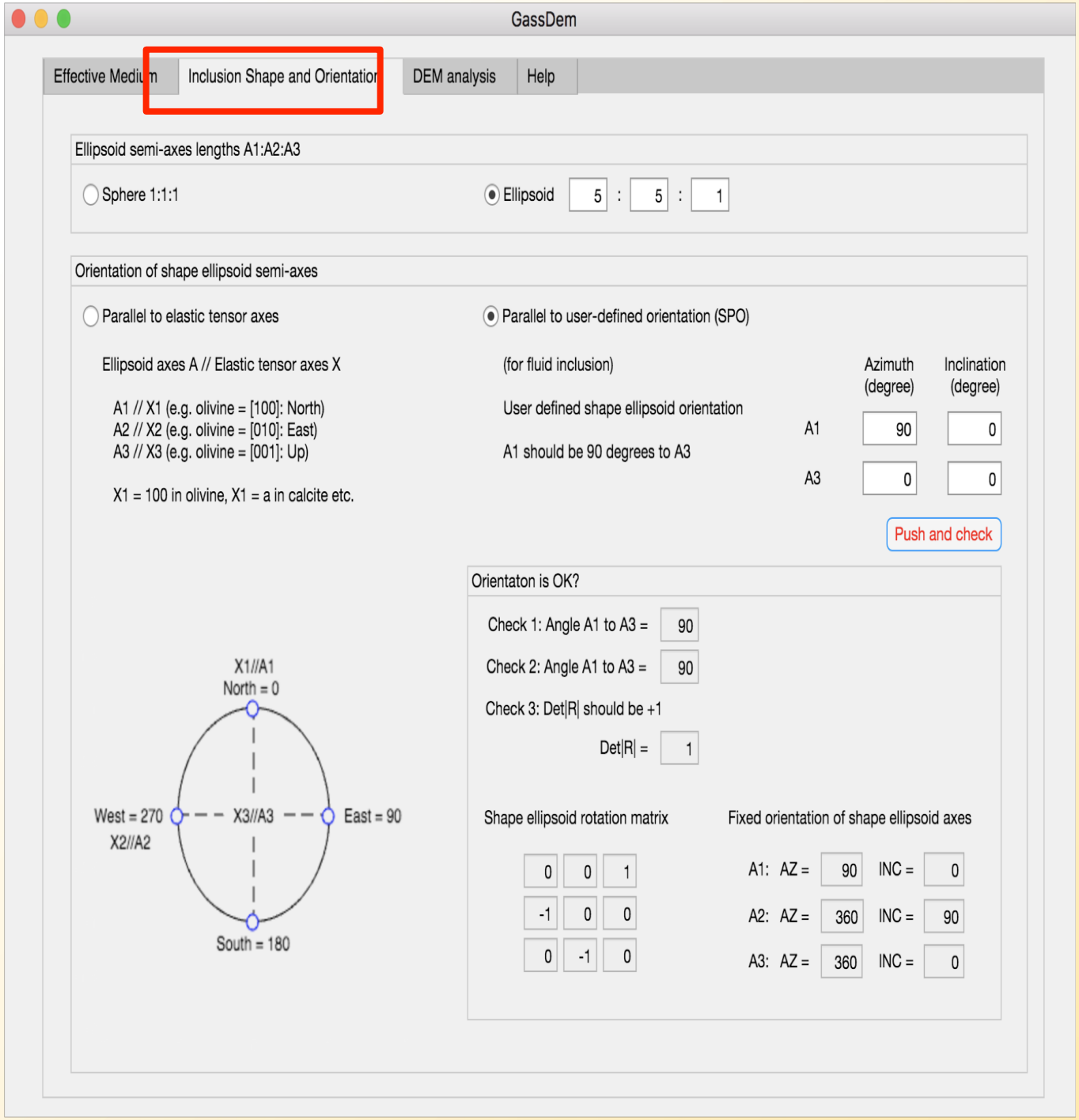
1. GassDem

- A MATLAB program for modeling the anisotropic seismic properties of porous medium using differential effective medium theory and Gassmann's poroelastic relationship.



1. GassDem

- A MATLAB program for modeling the anisotropic seismic properties of porous medium using differential effective medium theory and Gassmann's poroelastic relationship.



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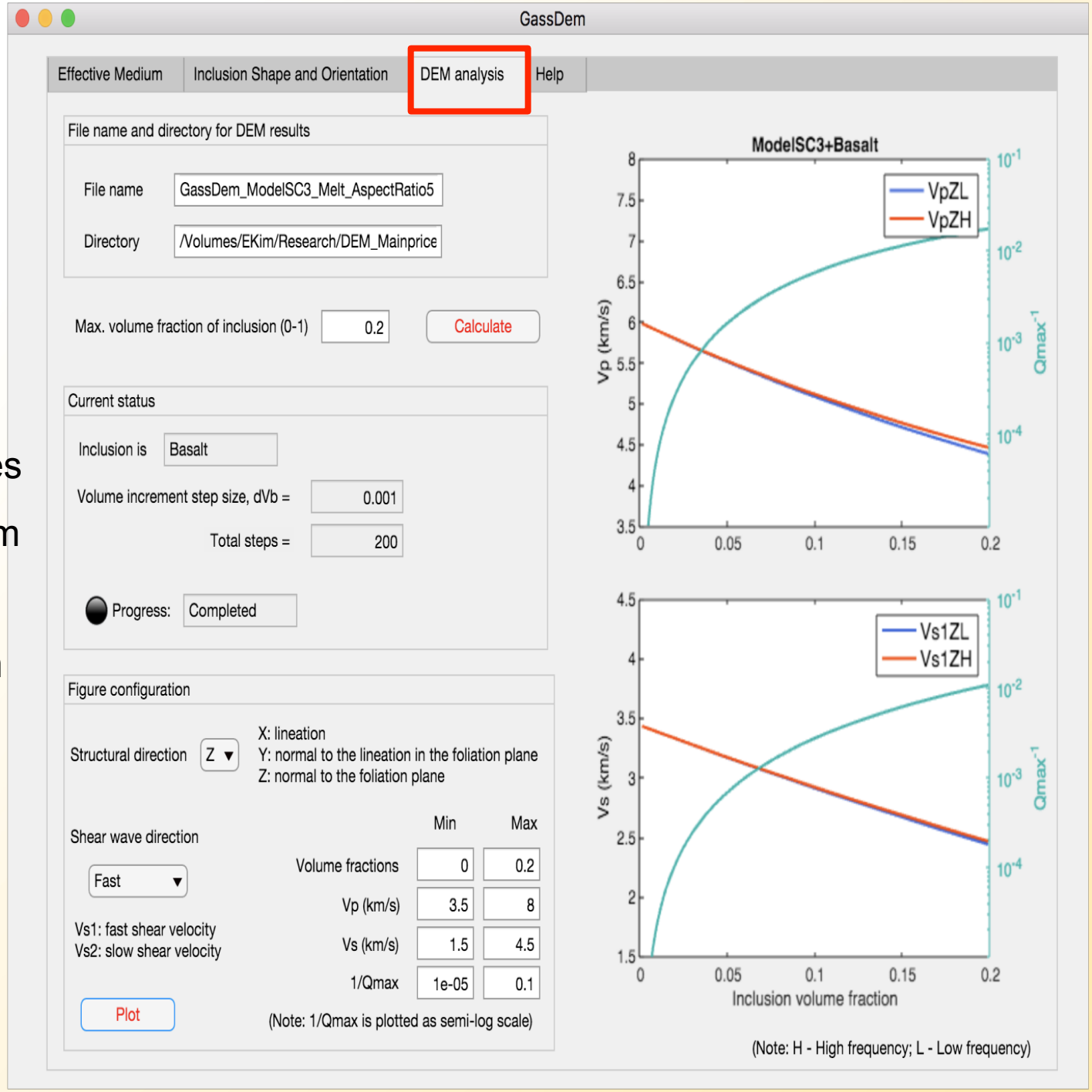

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Table of elastic stiffness constants for cubic minerals.

Mineral	Structure	Density (g/cm ^{3})	C_{11}(GPa)	C_{12}(GPa)	C_{44}(GPa)
Pyrope	Garnet	3.839	301.4	110.0	94.3
Ringwoodite	Spinel	3.559	327.0	114.0	131.0
Ferropericlase	Halite	4.323	499.0	137.0	160.0

H

Table of results cubic symmetry ($m\bar{3}m$) pure modes for propagation along [100],[110] and [111] with polarizations, equations and velocities (km/s) for each mineral.

Propagation	Polarization	Equation	Pyrope	Ringwood	Periclase
[100]	[100]	$Vp = \sqrt{\frac{C_{11}}{\rho}}$	8.86	9.58	10.74
[100]	[010]	$Vs = \sqrt{\frac{C_{44}}{\rho}}$	4.96	6.07	6.08
[110]	[110]	$Vp = \sqrt{\frac{C_{11}+C_{12}+2C_{44}}{2\rho}}$	8.84	9.94	10.52
[110]	[$\bar{1}$10]	$Vs = \sqrt{\frac{C_{11}-C_{12}}{2\rho}}$	4.99	5.47	6.47
[110]	[010]	$Vs = \sqrt{\frac{C_{44}}{\rho}}$	4.96	6.07	6.08
[111]	[111]	$Vp = \sqrt{\frac{C_{11}+2C_{12}+4C_{44}}{3\rho}}$	8.83	10.05	10.44
[111]	in plane(111)	$Vs = \sqrt{\frac{C_{11}-C_{12}+C_{44}}{3\rho}}$	5.68	5.67	6.34

To determine the elastic constants C_{11} and C_{44}; $\rho(Vp^{[100]})^2 = C_{11}$ and $\rho(Vs^{[100]})^2 = C_{44}$ From the equations above determine C_{12}.

Hint : generic velocity $V = \sqrt{M/\rho}$ units km/s and ρ units g/cm3 and generic modulus is $M = \rho * V^2$ (units GPa) use either

$$\rho(Vp^{[110]})^2 = \sqrt{\frac{C_{11} + C_{12} + 2C_{44}}{2\rho}}$$

or

$$\rho(Vp^{[111]})^2 = \sqrt{\frac{C_{11} + 2C_{12} + 4C_{44}}{3\rho}}$$

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