Contributions of Synchrotron X-Ray Powder Diffraction to Understanding High Pressure Rock Deformation

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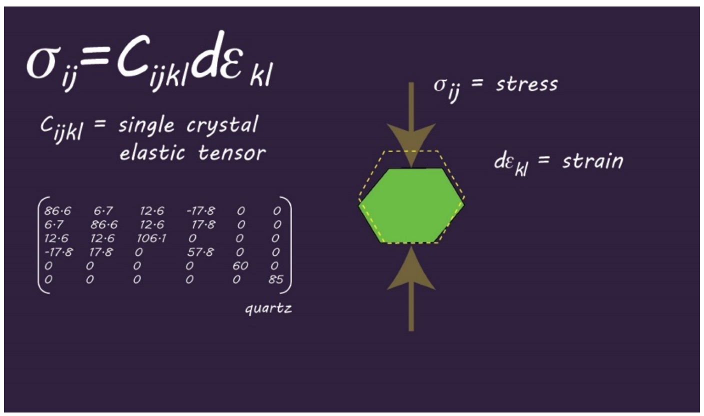
  - Beamline scientist: Haiyan Chen

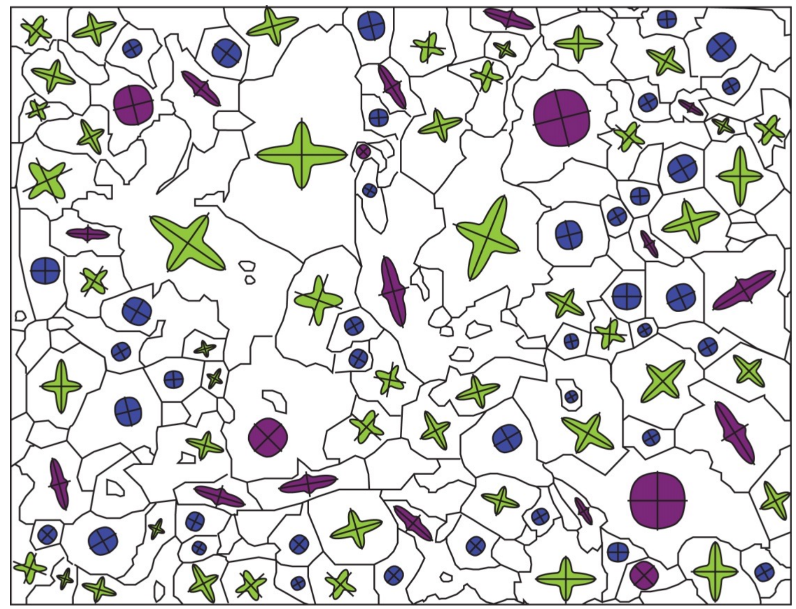
Outline

- Models for thinking about deforming rocks
- How x-rays look at polycrystalline materials
- Data interpretation with Elastic Plastic Self Consistent (EPSC) modeling
- Application of EPSC to diffraction data
  - Observing deformation mechanisms
  - Measuring strength and critical resolved shear stresses
  - Measuring the acoustoelastic effect

Deforming rocks are complicated!

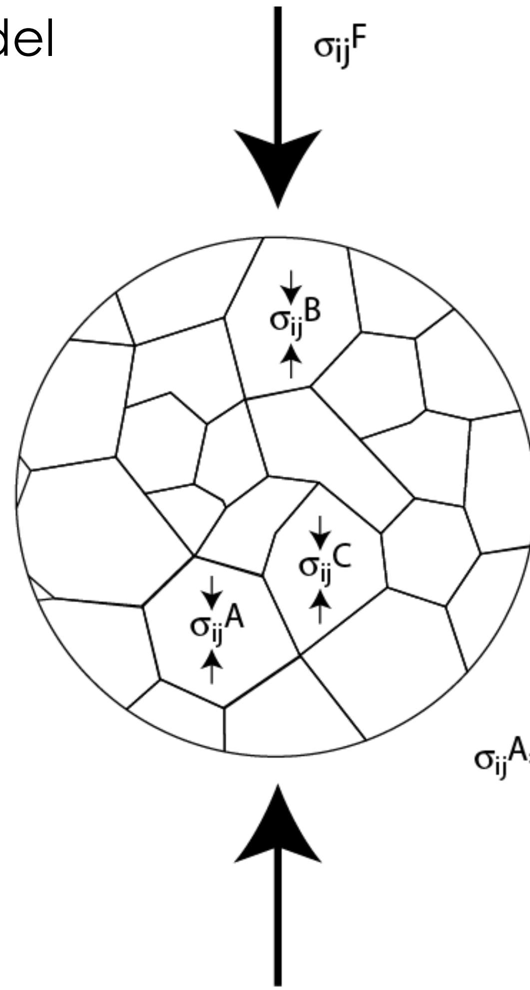
- Even for a single phase:
  - Elastic anisotropy
  - Plastic anisotropy





PS – there are also grain boundaries

Simplest model (scalar)

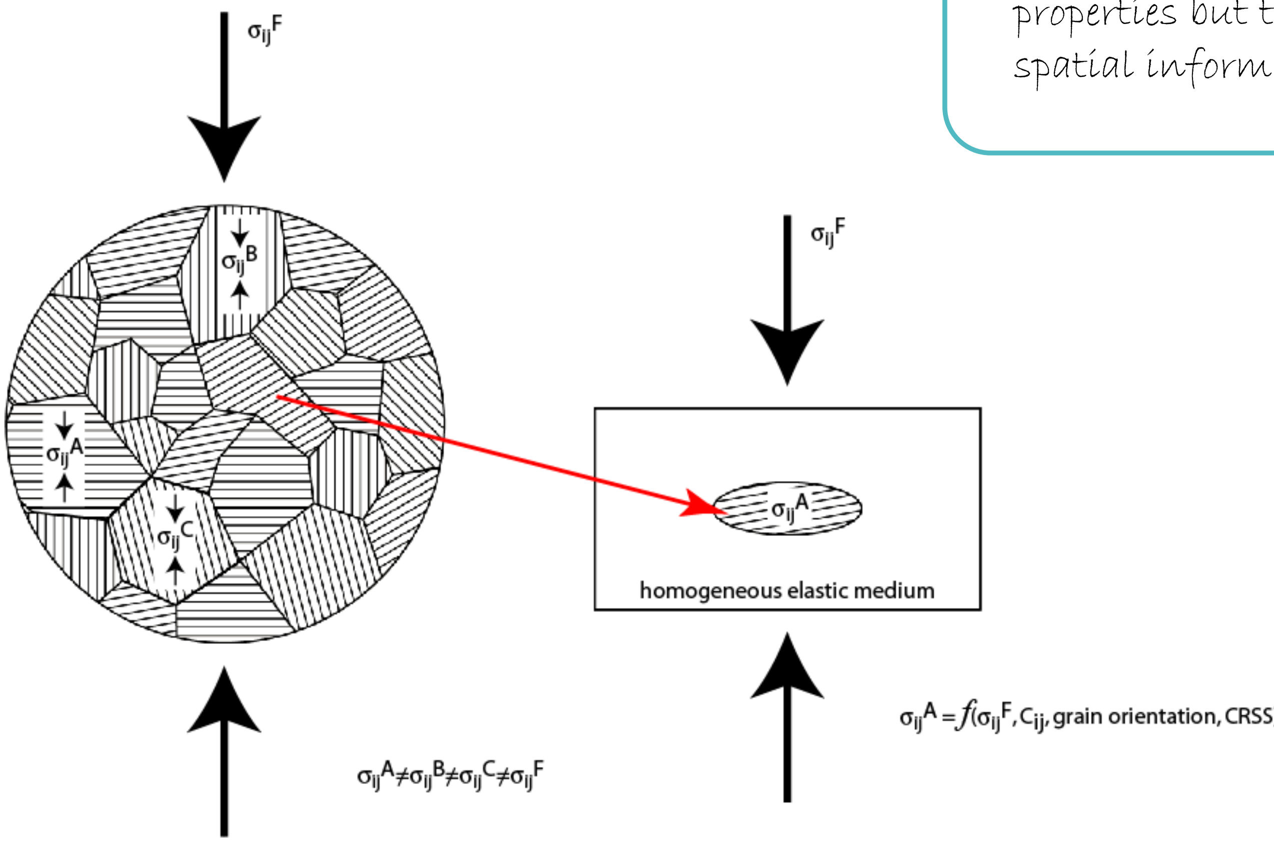


Everything is the same everywhere

$$\sigma_{ij}A=\sigma_{ij}B=\sigma_{ij}C=\sigma_{ij}F$$

Self-consistent models

Grains can have anisotropic properties but there is no spatial information

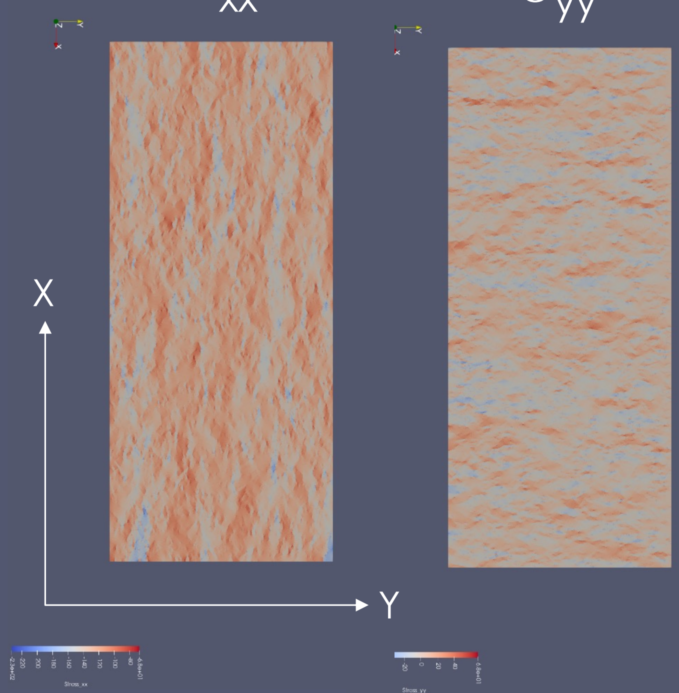


Self organized stress and strain

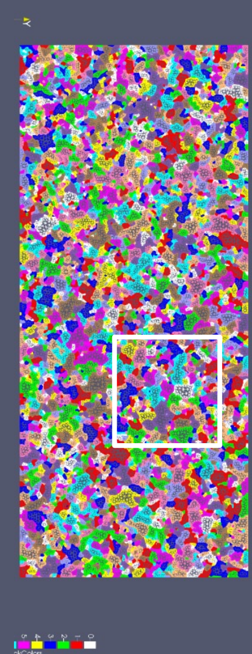
Model can be arbitrarily close to reality

Finite Element Model

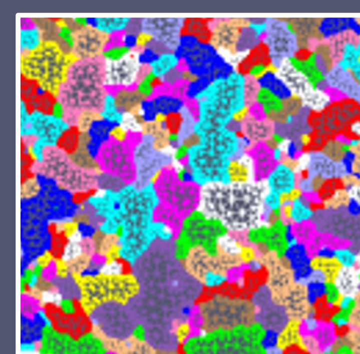
σ_{xx} σ_{yy}



Mesh of
Tigers eye sample



- Mtex2Gmsh
- Elastic only
- Moose Framework

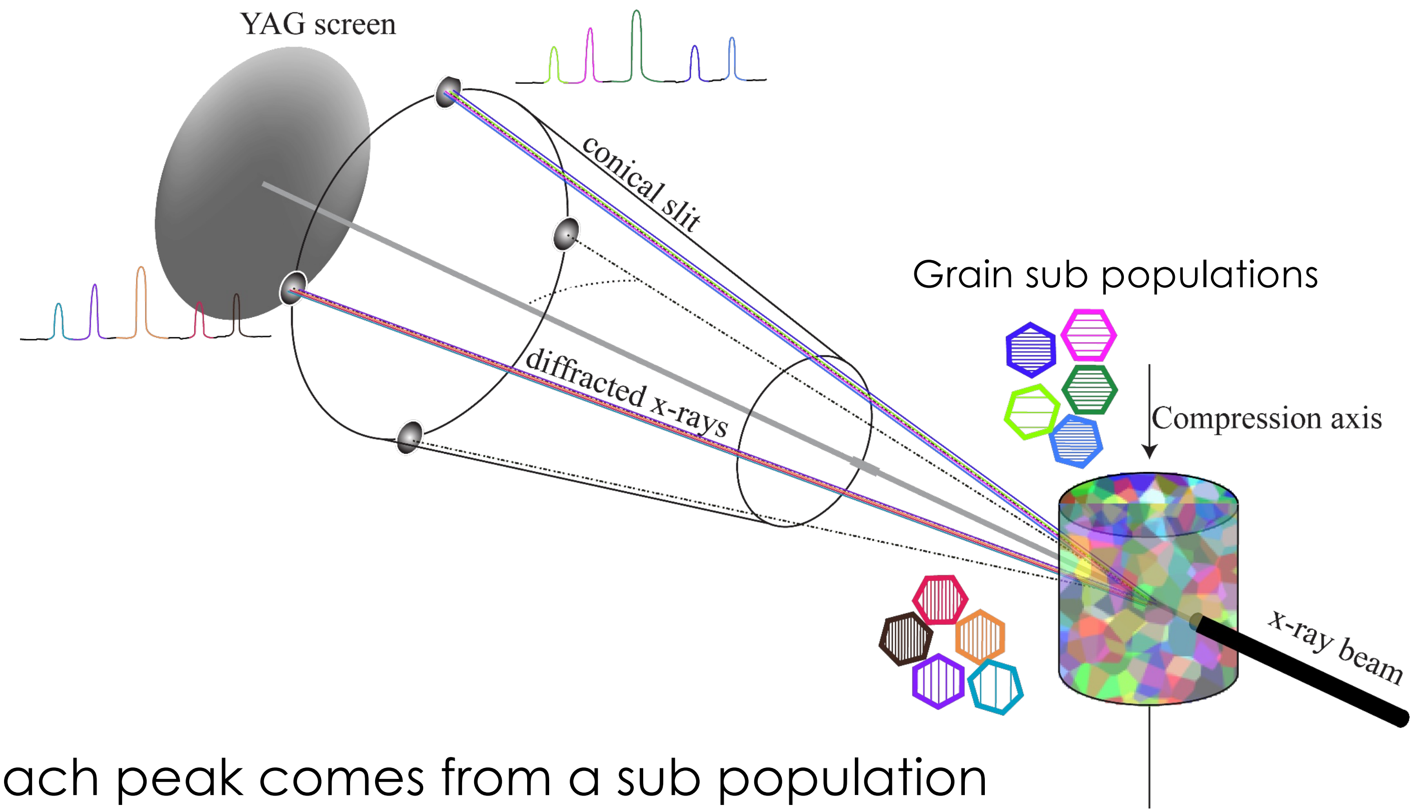


Kidman et al (in prep)

When to employ which model

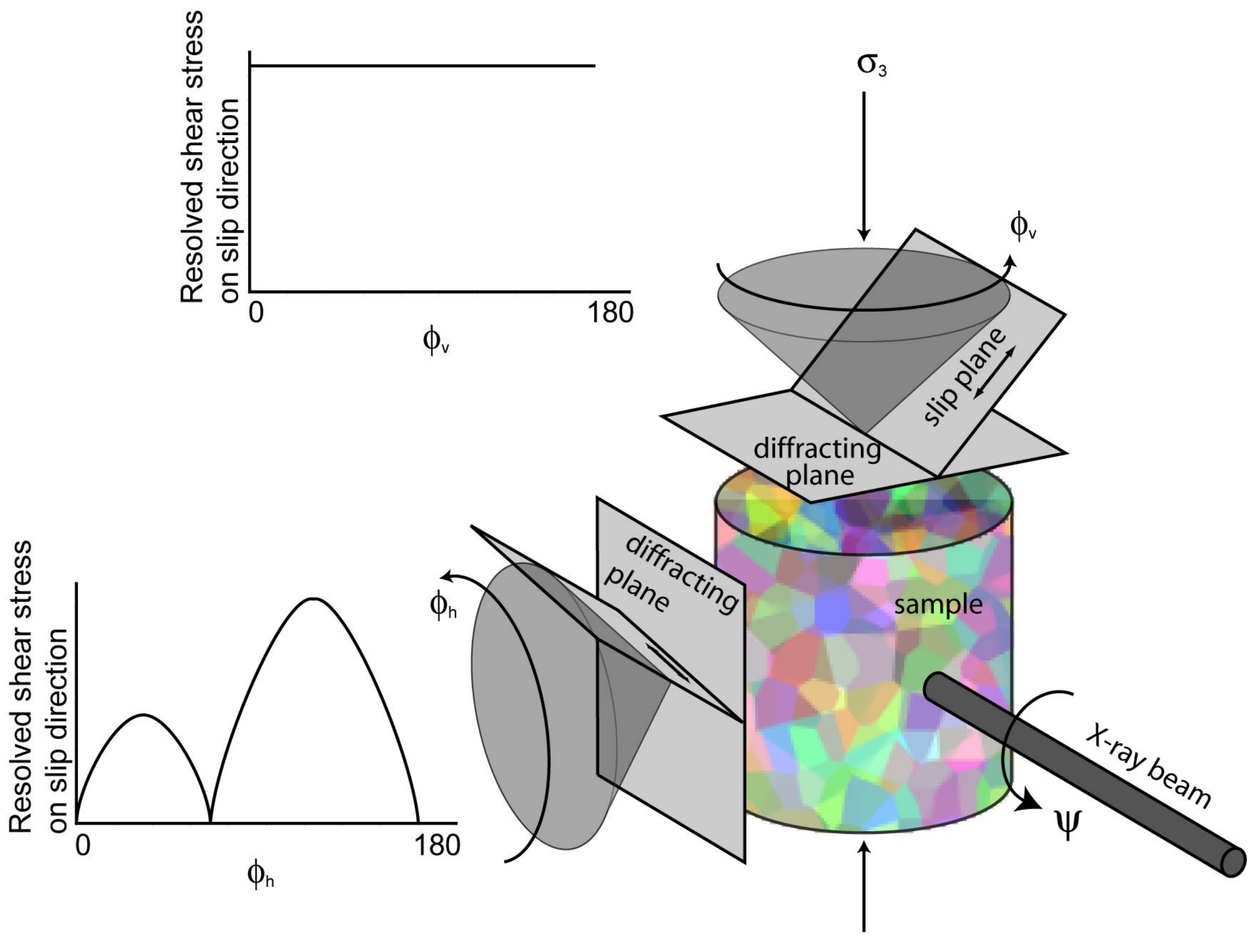
- Experiment produces a scalar result (e.g. flow strength)
  - Apply scalar model
- Experiment produces population averaged information (e.g. powder diffraction)
  - Apply EPSC, VPSC
- Experiment produces 2D or 3D spatial information
  - Apply FEM, DEM etc.

Information from powder diffraction



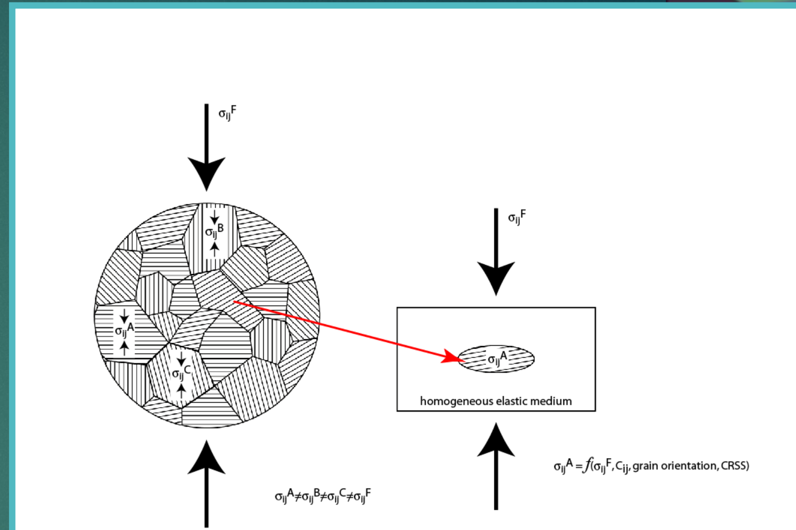
Each peak comes from a sub population

Each sub-population is doing its own thing



(Burnley & Zhang, 2008)

Elastic Plastic Self Consistent Models



- Input:
  - Stress and strain boundary conditions
  - Orientation information for each crystal in the system
  - Single crystal elastic constants
  - Slip systems with CRSS and hardening parameters

$$\tau = \tau_0 + (\tau_1 + \phi_1\Gamma)\left[1 - e^{-\left(\phi_0\Gamma/\tau_1\right)}\right]$$

Γ = shear strain
τ = CRSS

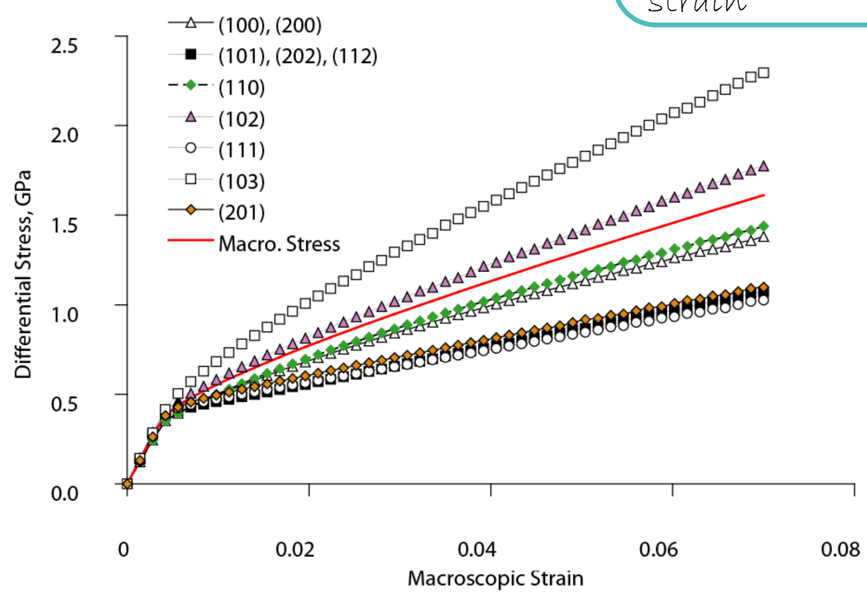
Elastic Plastic Self Consistent Models

- Increments the chosen boundary condition
- Calculates stress and strain for each crystal
- Homogeneous elastic medium is average of all crystals
- Iterates for each step
- Output for each step:
  - Macroscopic stress (or strain)
  - Elastic and plastic strain for each crystal
- EPSC code provided by Carlos Tome (LANL)

Advantages of self-consistent models for powder diffraction

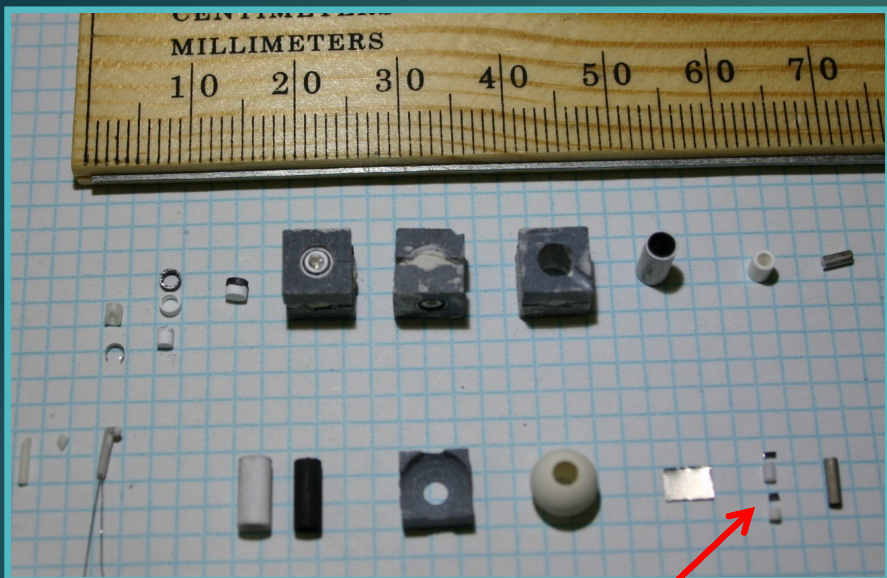
- Accounts for non-diffracting grains
- Uses anisotropic crystalline properties
- Forces experimentalist to 'listen' to what the sample is 'saying'
  - Not all grain sub populations are doing the same things
  - Can't rely on a small number of sub populations to get 'the answer'
  - Unanticipated deformation mechanisms are revealed

here lattice strain is recast as stress, usually we just plot differential lattice strain

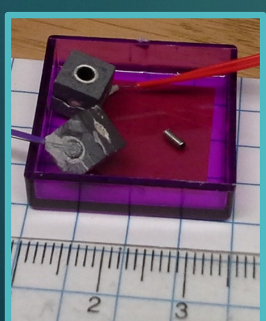


EPSC model for quartz

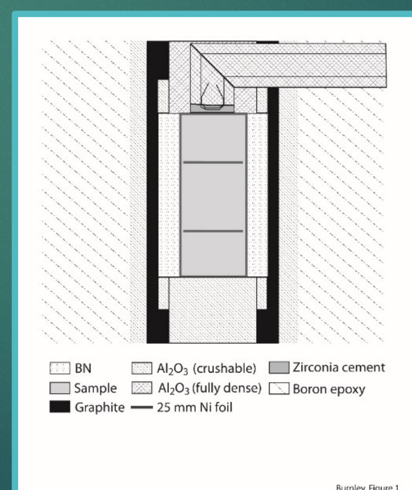
D-DIA experiments

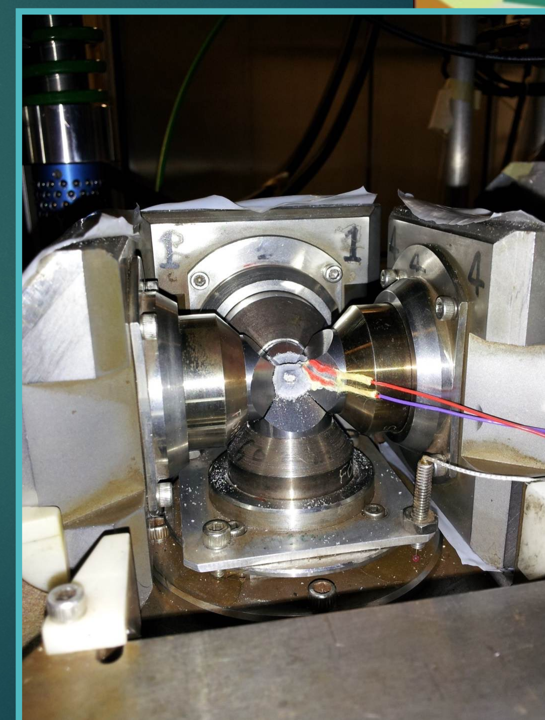


1 x 2 mm

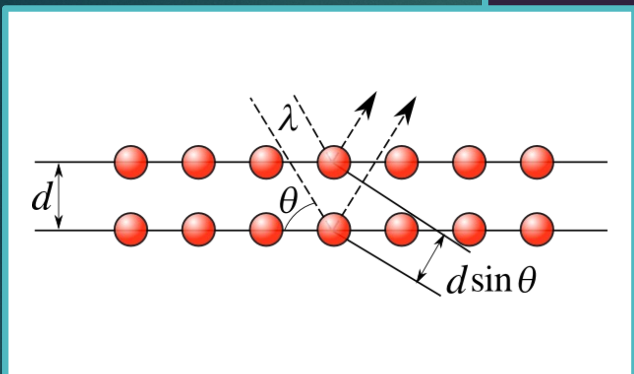


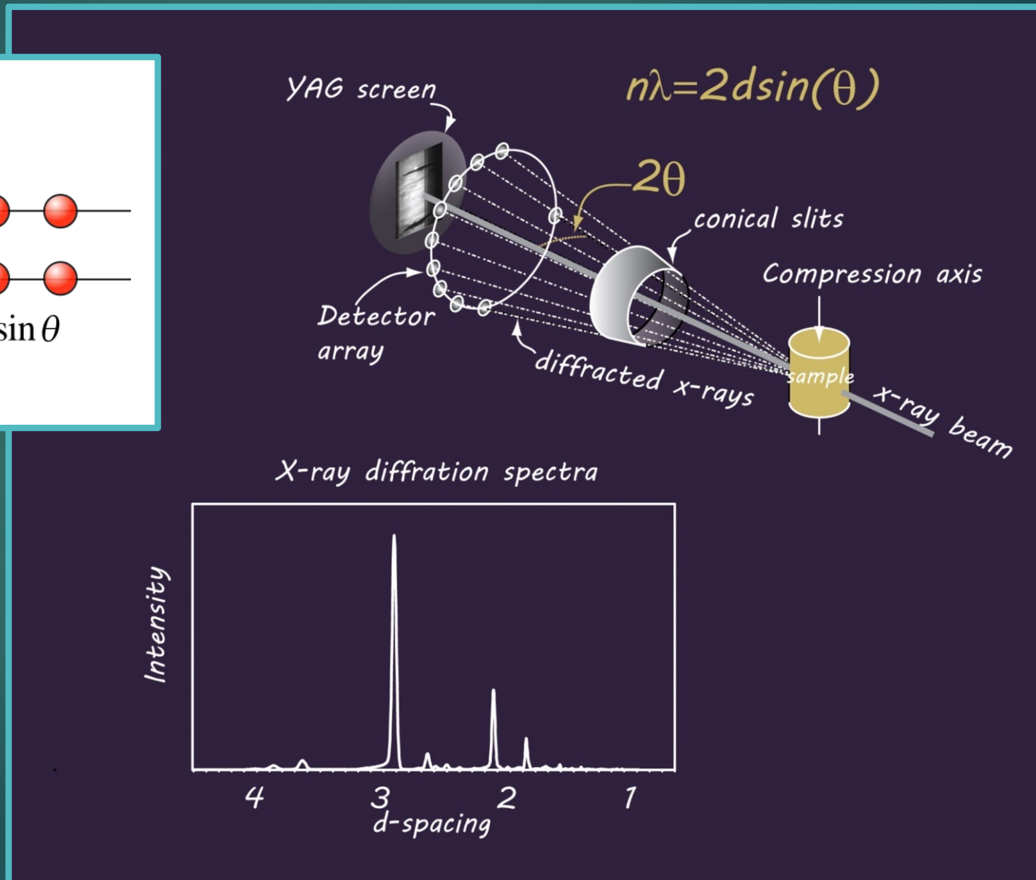
(Wang et. al. 2004)

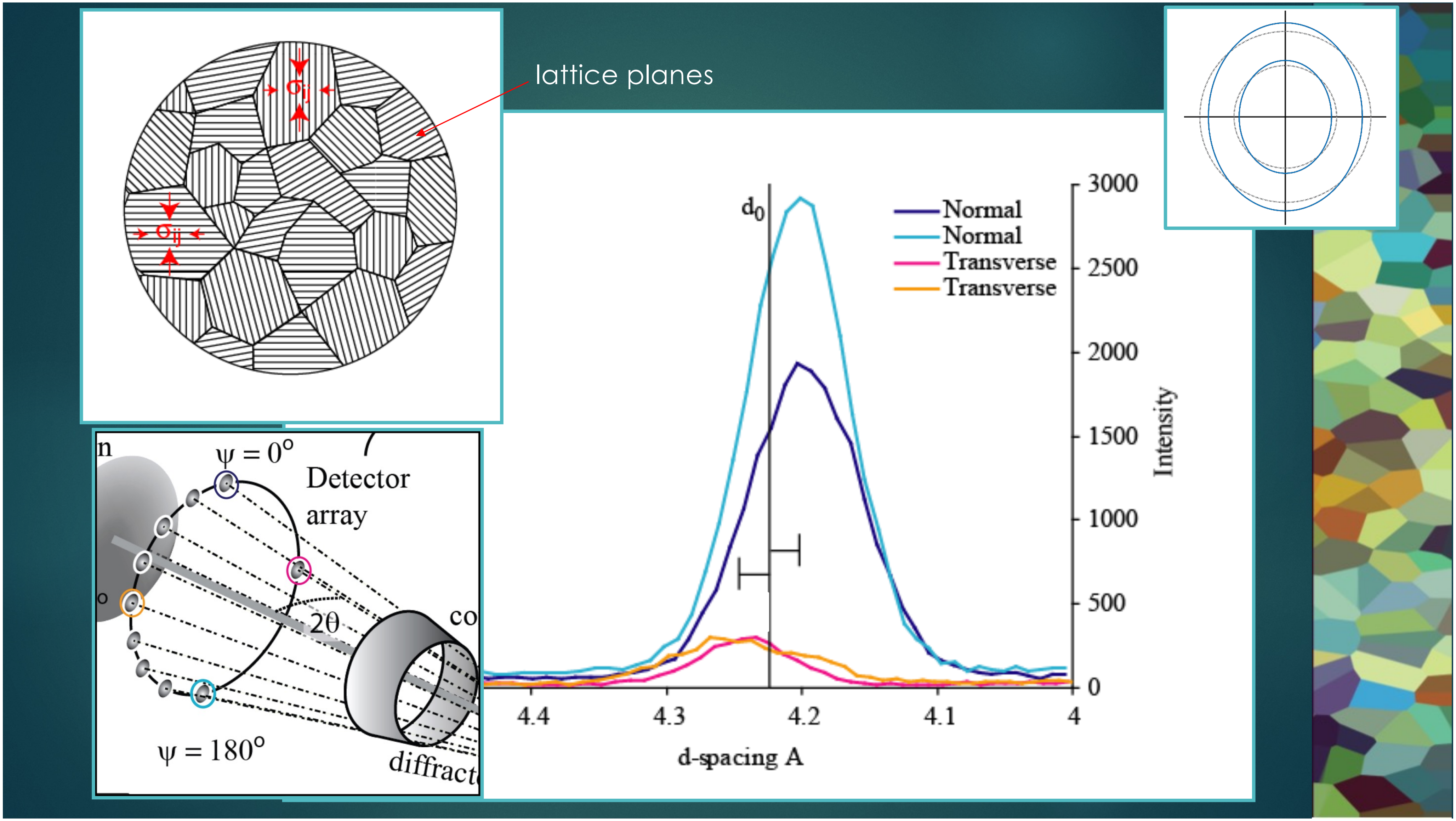




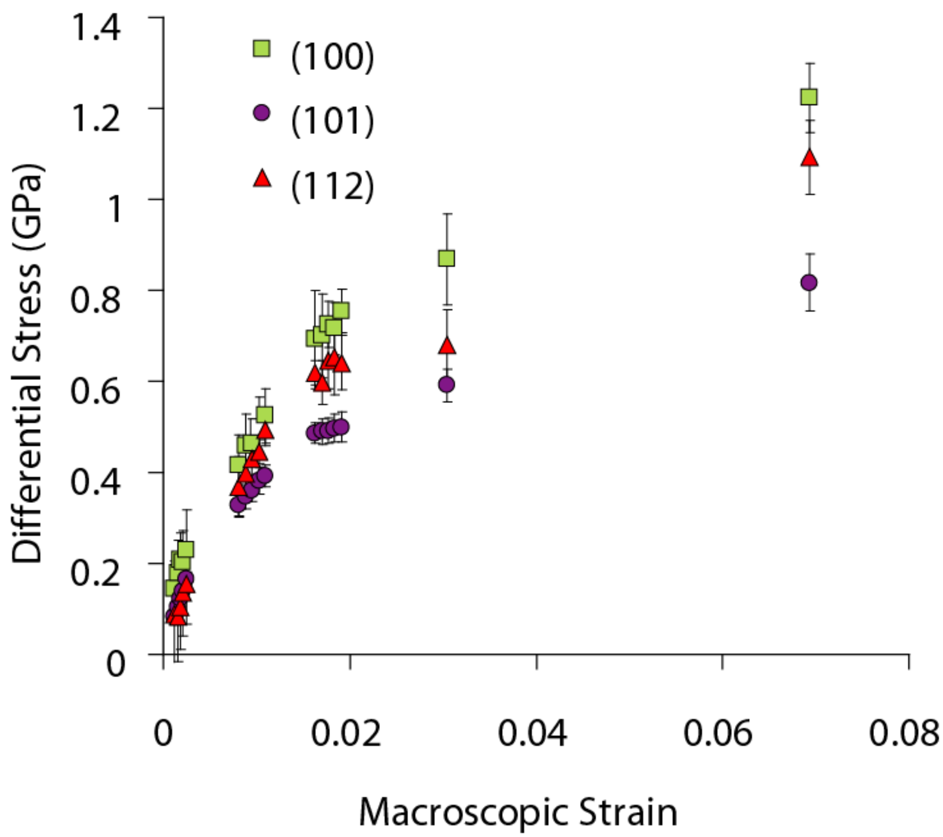
In-situ Powder Diffraction





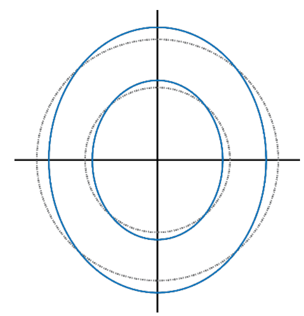

lattice planes
σij
σij
ψ = 0°
Detector
array
2θ
ψ = 180°
d0
Normal
Normal
Transverse
Transverse
3000
2500
2000
1500
1000
500
0
Intensity
4.4
4.3
4.2
4.1
4
d-spacing A

(SiO_2 (α-quartz), 800 C, 2 GPa, 2 x 10^{-5}/sec)



Stresses calculated using Singh et al. (1998) diffraction elastic constants

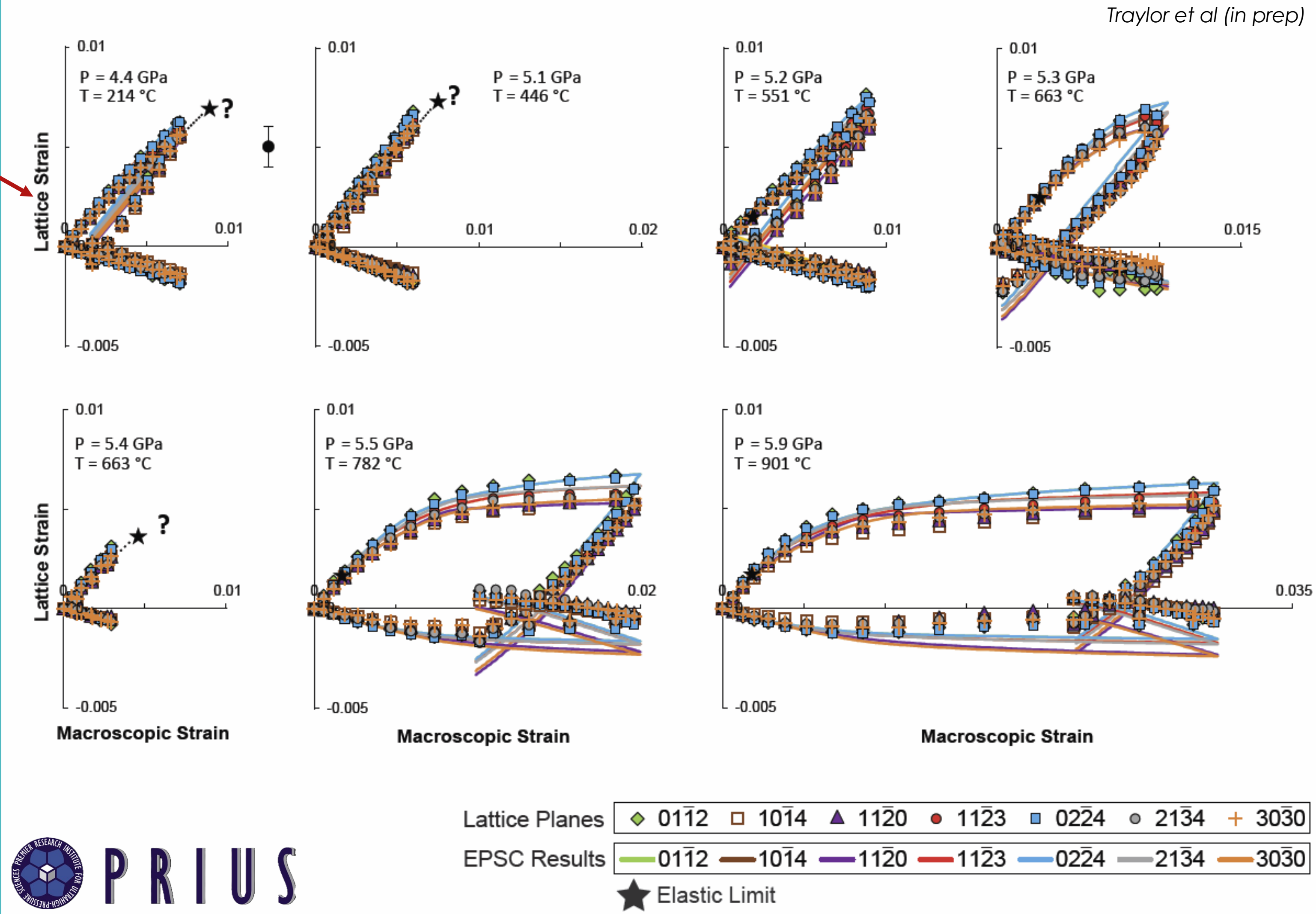
$$\frac{d(hkl) - d_p(hkl)}{d_p(hkl)} = Q(hkl)(1 - 3cos^2\varphi)$$



(Burnley and Zhang, 2008)

$$\varepsilon^{hkl} = \frac{\left(d^{hkl} - d_0^{hkl}\right)}{d_0^{hkl}}$$

- Polycrystalline alumina sample
- Nano-polycrystalline diamond piston



Applications

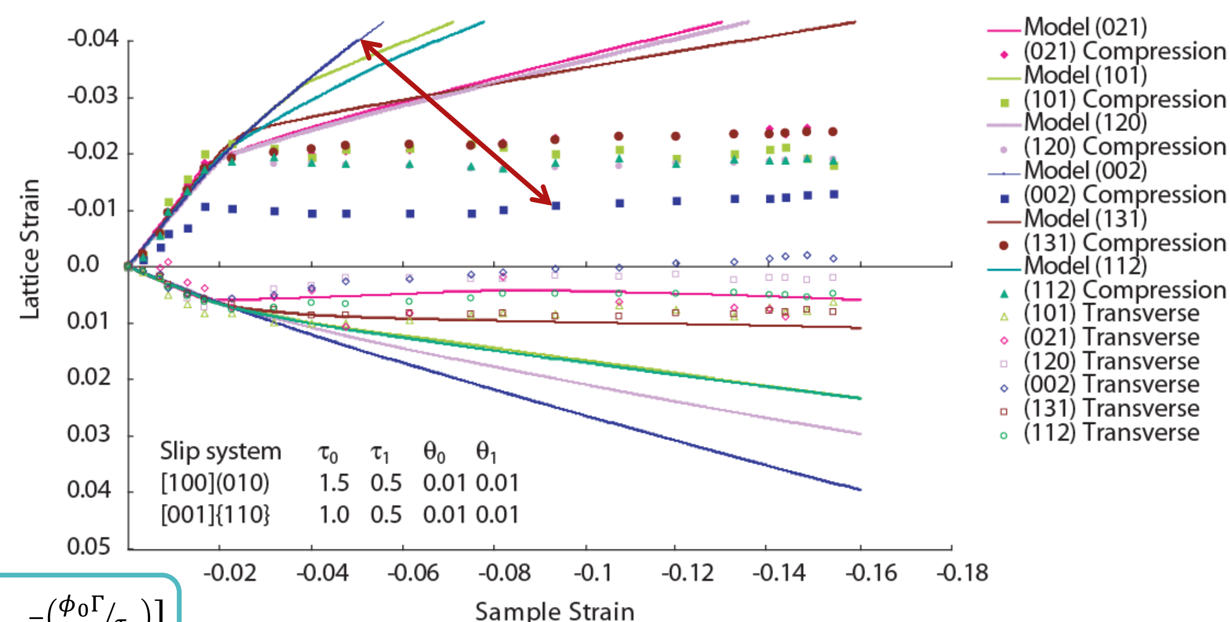
- Investigate deformation mechanisms
  - Identify missing mechanisms
    - Kink bands in olivine
    - Dauphine twinning in quartz
    - Anelastic deformation at low strain
  - Determine critical resolved shear stress for slip systems
- Determine sample strength
- Measure acoustoelastic effect

- Applications
  - Investigate deformation mechanisms

Olivine slips systems do not have a closed yield surface

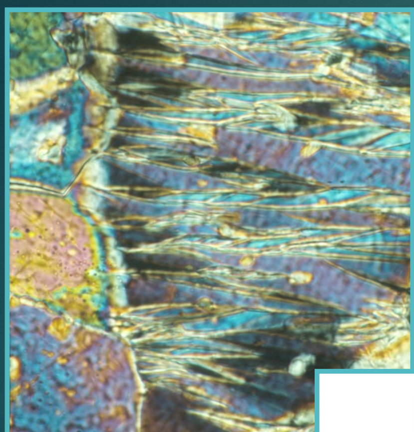
- Models work harden
- (002) reflection cannot be matched

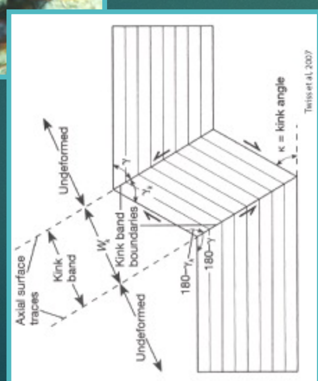
Fayalite, 25 C, 2.5 GPa



$$\tau = \tau_0 + (\tau_1 + \phi_1 \Gamma)\left[1 - e^{-\left(\phi_0 \Gamma / \tau_1\right)}\right]$$

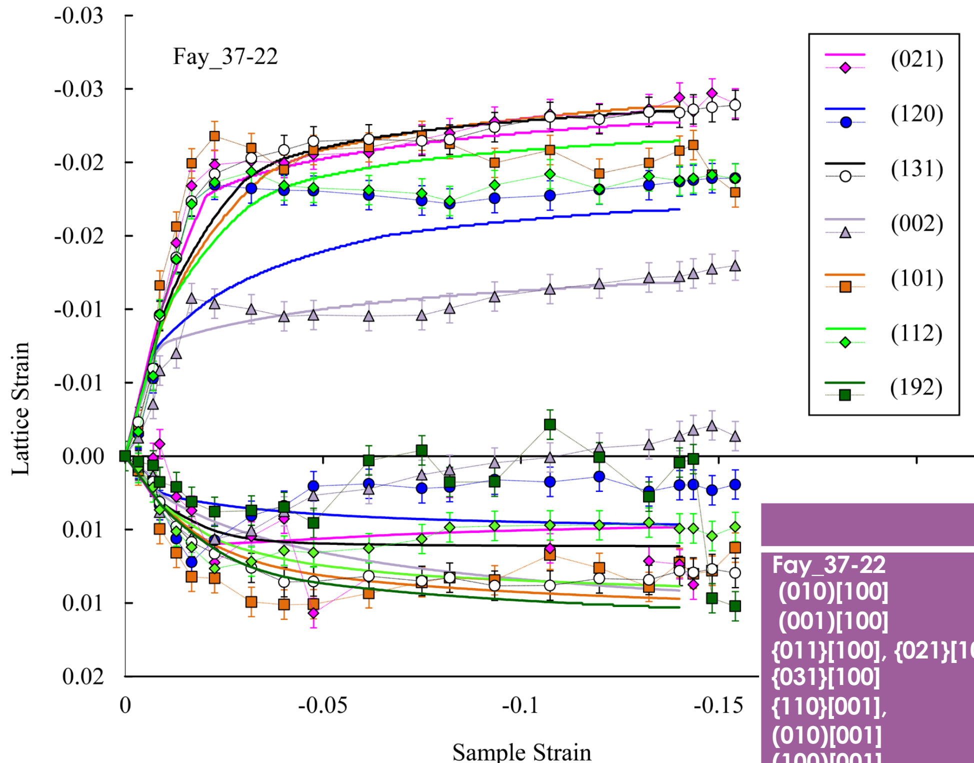
- Applications
  - Investigate deformation mechanisms
    - Olivine kink bands





Olivine slips systems do not have a closed yield surface

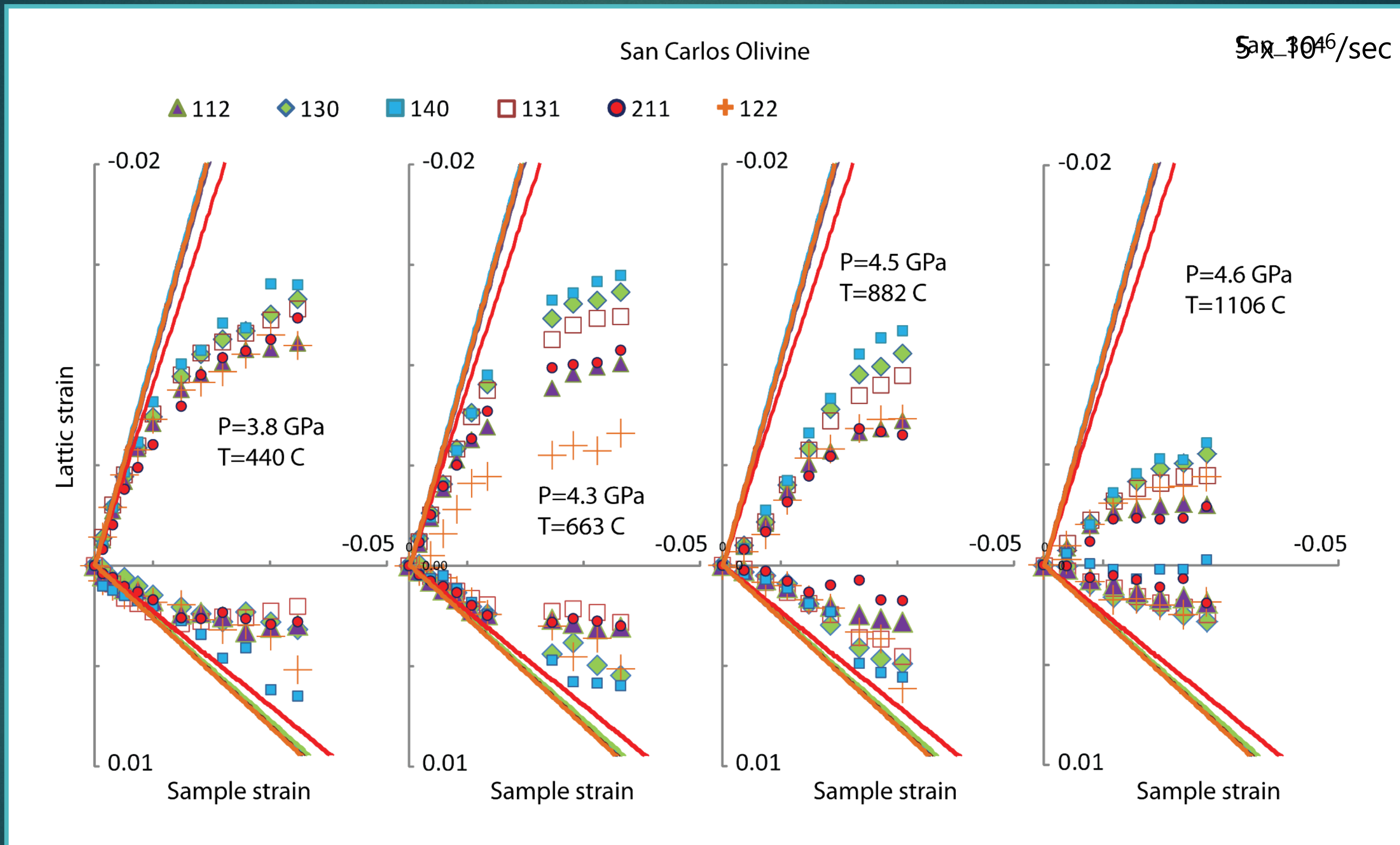
- Models work harden
- (002) reflection cannot be matched



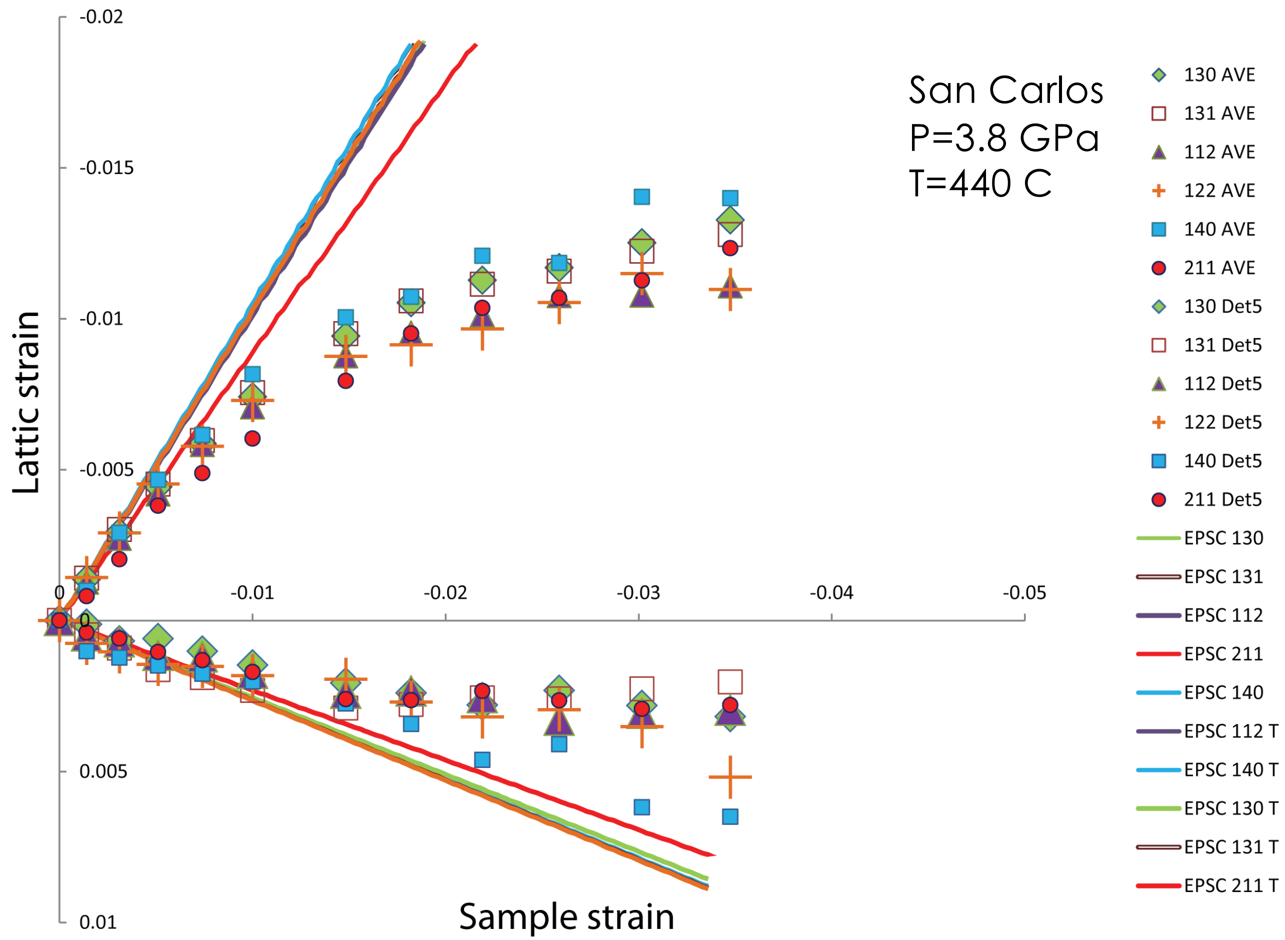
	T_0	T_1	Φ_0	Φ_1
Fay_37-22				
(010)[100]	1.0	0.01	0.2	0.01
(001)[100]	1.7	0.01	0.2	0.01
{011}[100], {021}[100]	1.7	0.01	0.2	0.01
{031}[100]	1.7	0.01	0.2	0.01
{110}[001],	1.0	0.01	0.2	0.01
(010)[001]	∞			
(100)[001]	0.62	0.01	0.5	0.01
Kink systems*				

Fayalite, 25 C, 2.5 GPa

The trouble with Young's modulus in polycrystalline materials



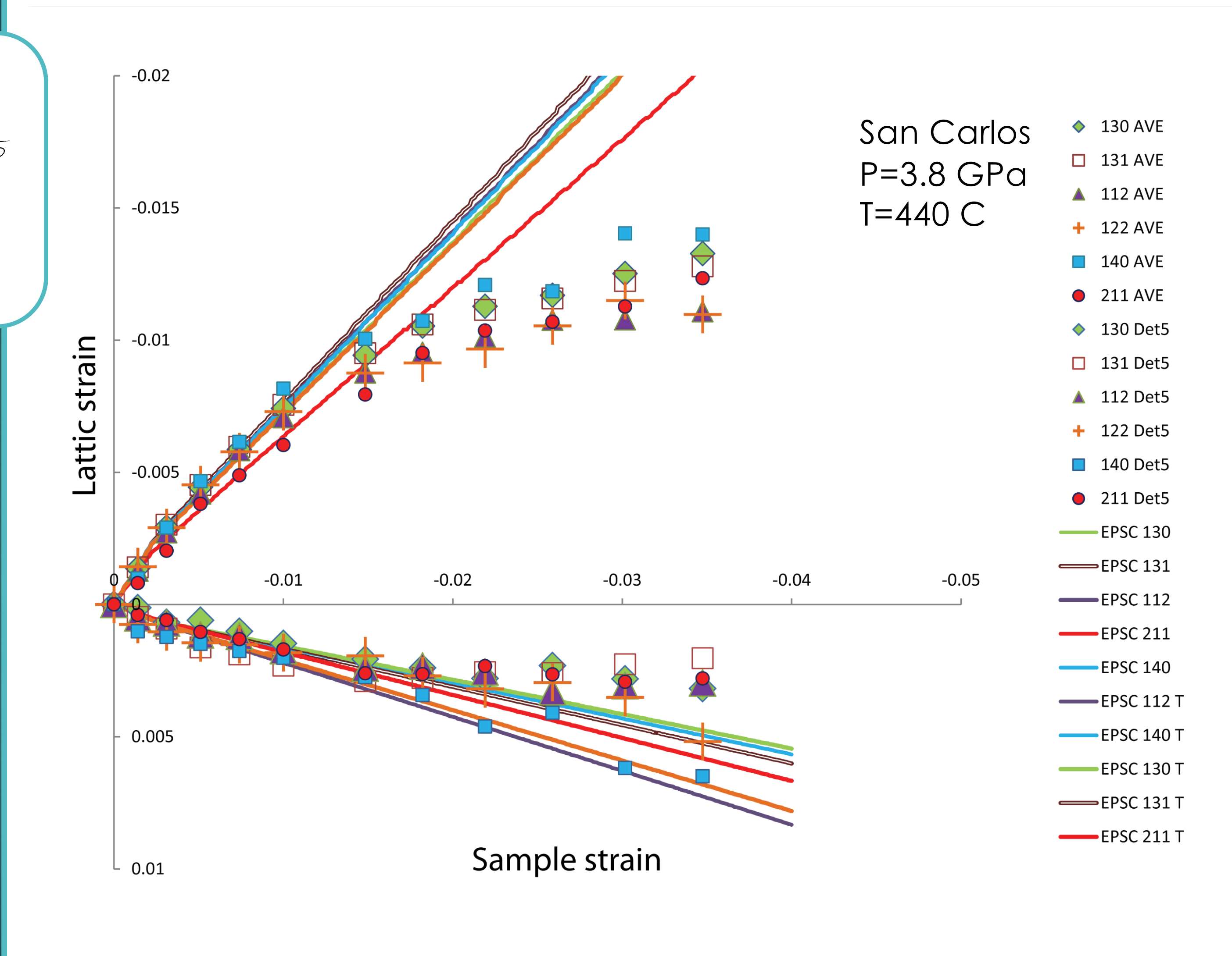
(Burnley & Kaboli, 2019)

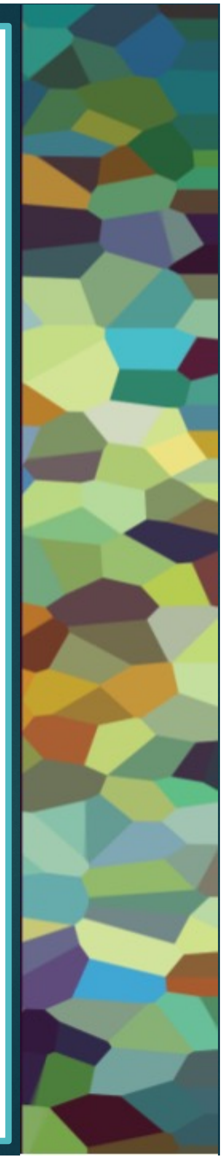


San Carlos
P=3.8 GPa
T=440 C
Lattic strain
Sample strain
-0.02
-0.015
-0.01
-0.005
0
0.005
0.01
0
-0.01
-0.02
-0.03
-0.04
-0.05
130 AVE
131 AVE
112 AVE
122 AVE
140 AVE
211 AVE
130 Det5
131 Det5
112 Det5
122 Det5
140 Det5
211 Det5
EPSC 130
EPSC 131
EPSC 112
EPSC 211
EPSC 140
EPSC 112 T
EPSC 140 T
EPSC 130 T
EPSC 131 T
EPSC 211 T

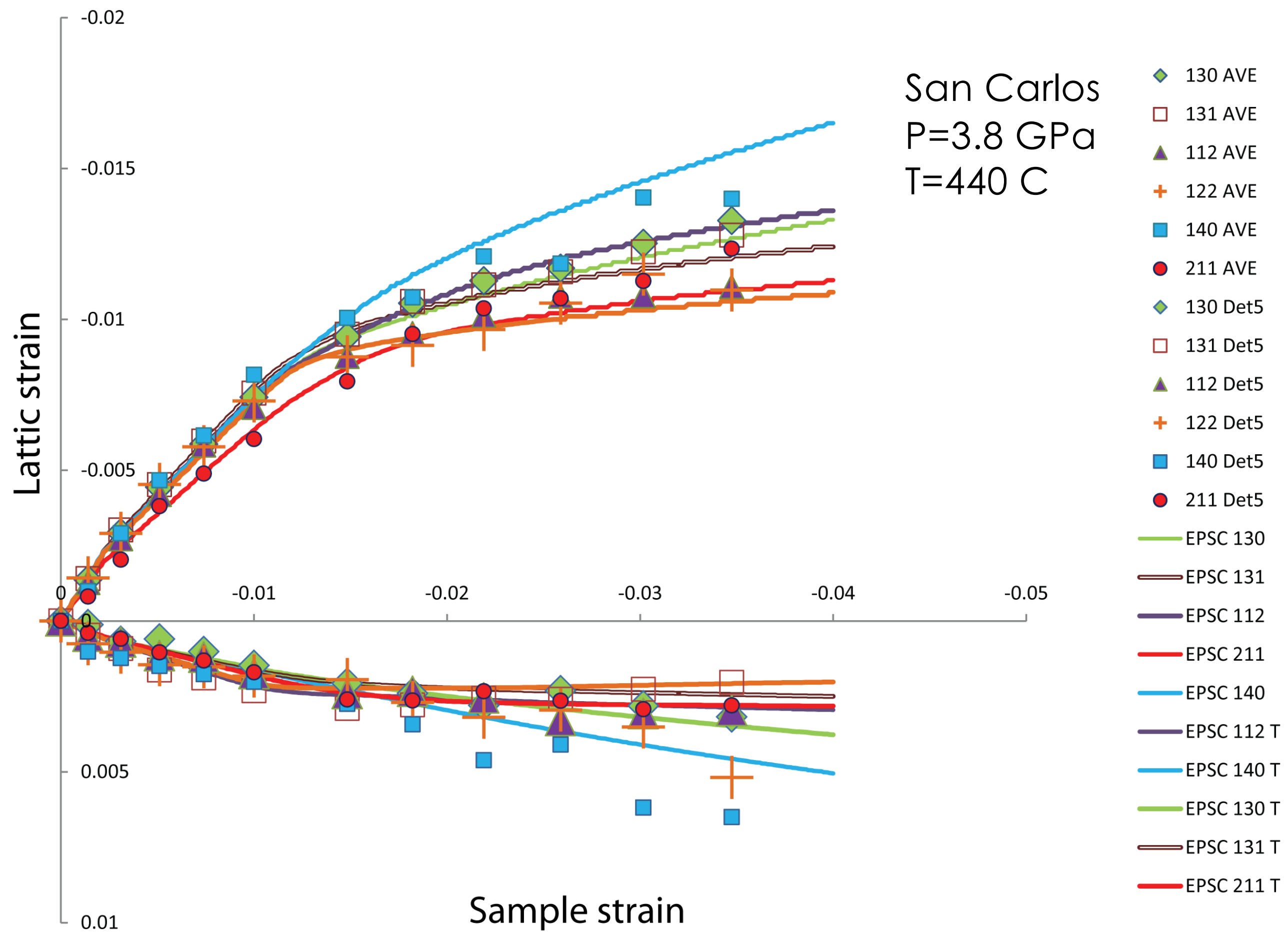
Add "grain boundary" slip system:

- Schmid factor ~0.5 for all
- Work hardening

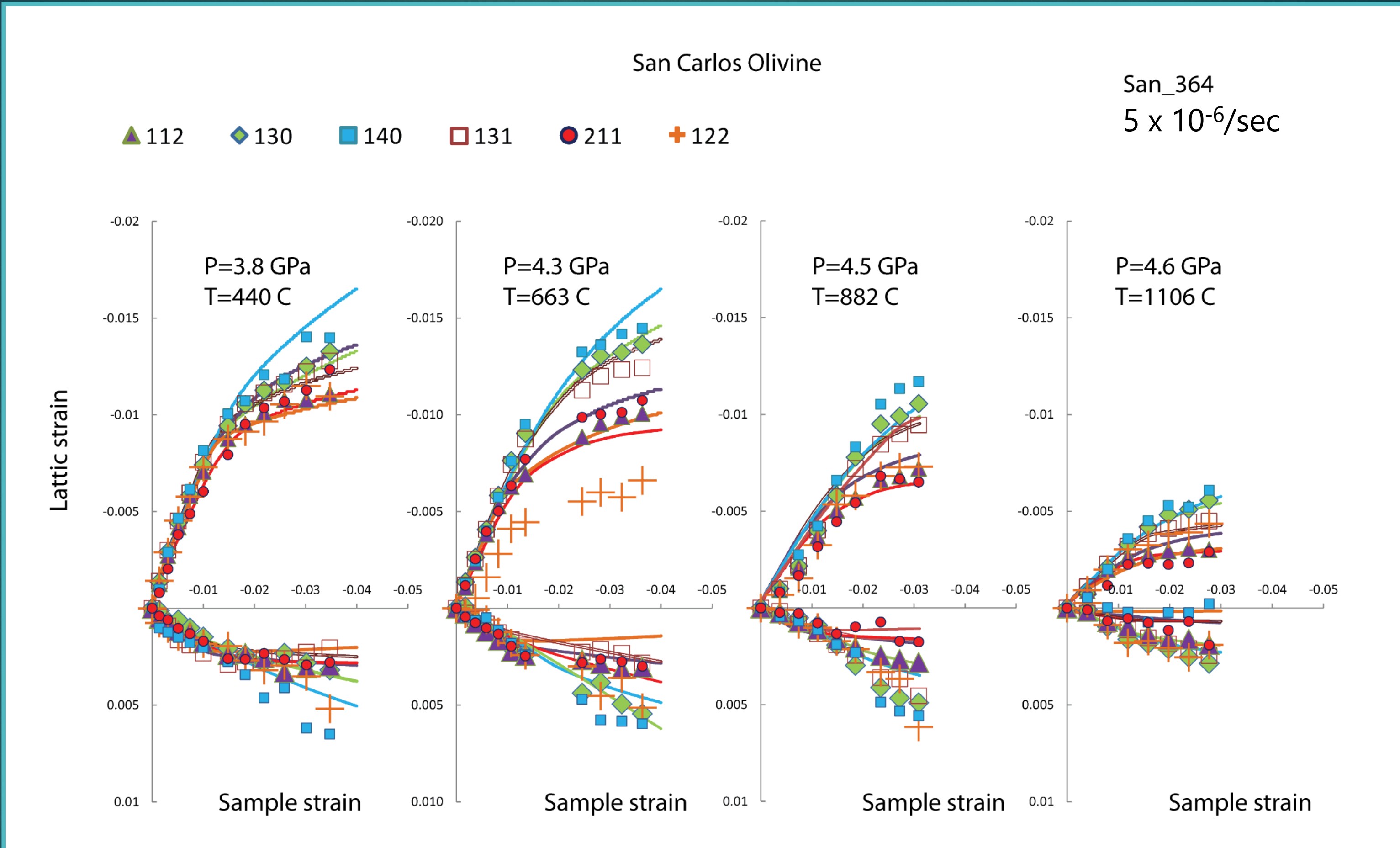




Finish up with real slip systems

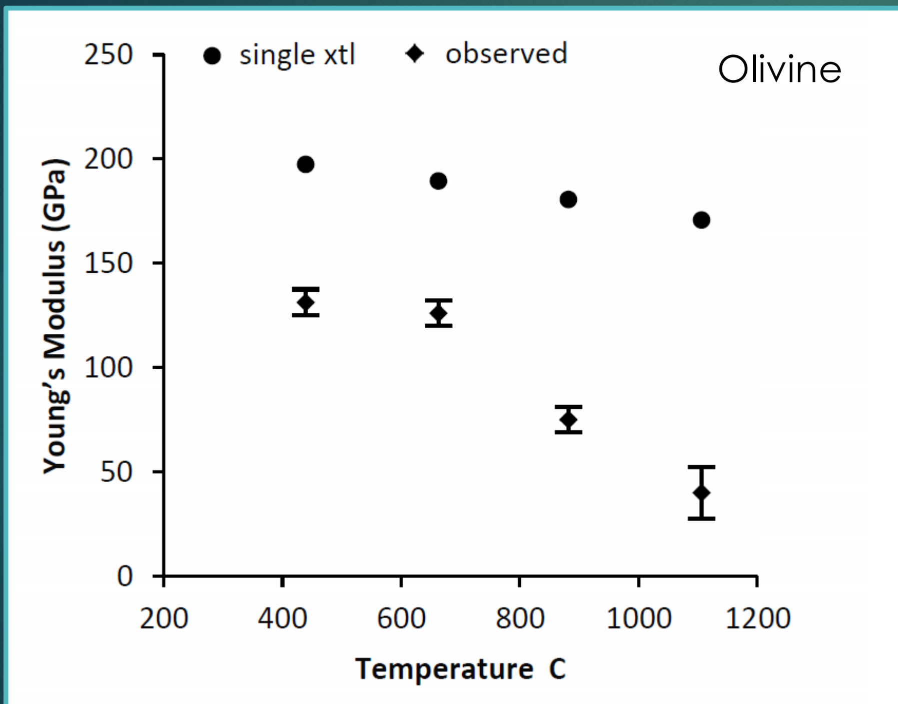


EPSC model fit

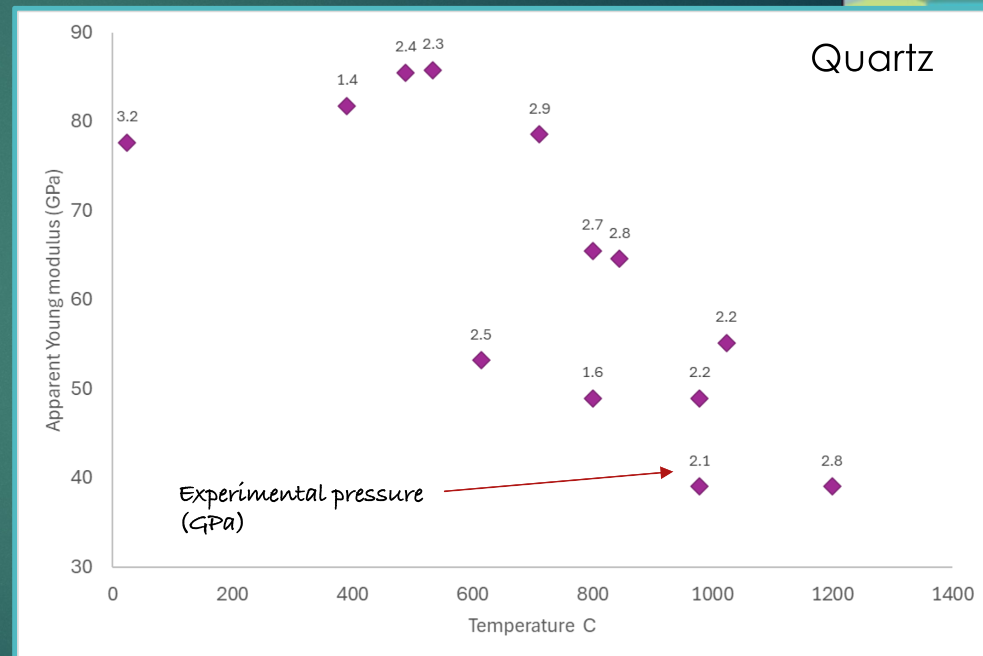


(Burnley & Kaboli, 2019)

Temperature dependence of low strain anelastic behavior

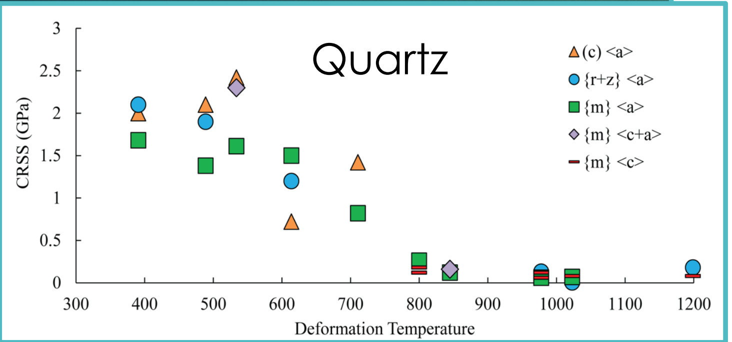


(Burnley and Kaboli, 2019)



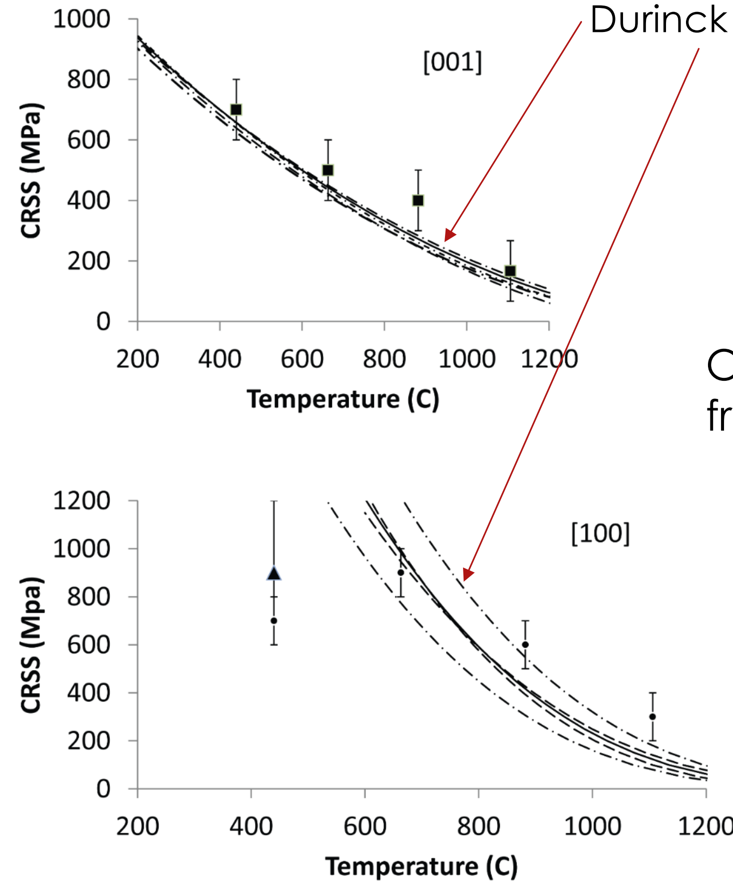
(Medina et al, in prep)

- Applications
  - Investigate other deformation mechanisms
  - Measure CRSS
    - Depends on uniqueness of slip systems



(Medina et al, in prep)

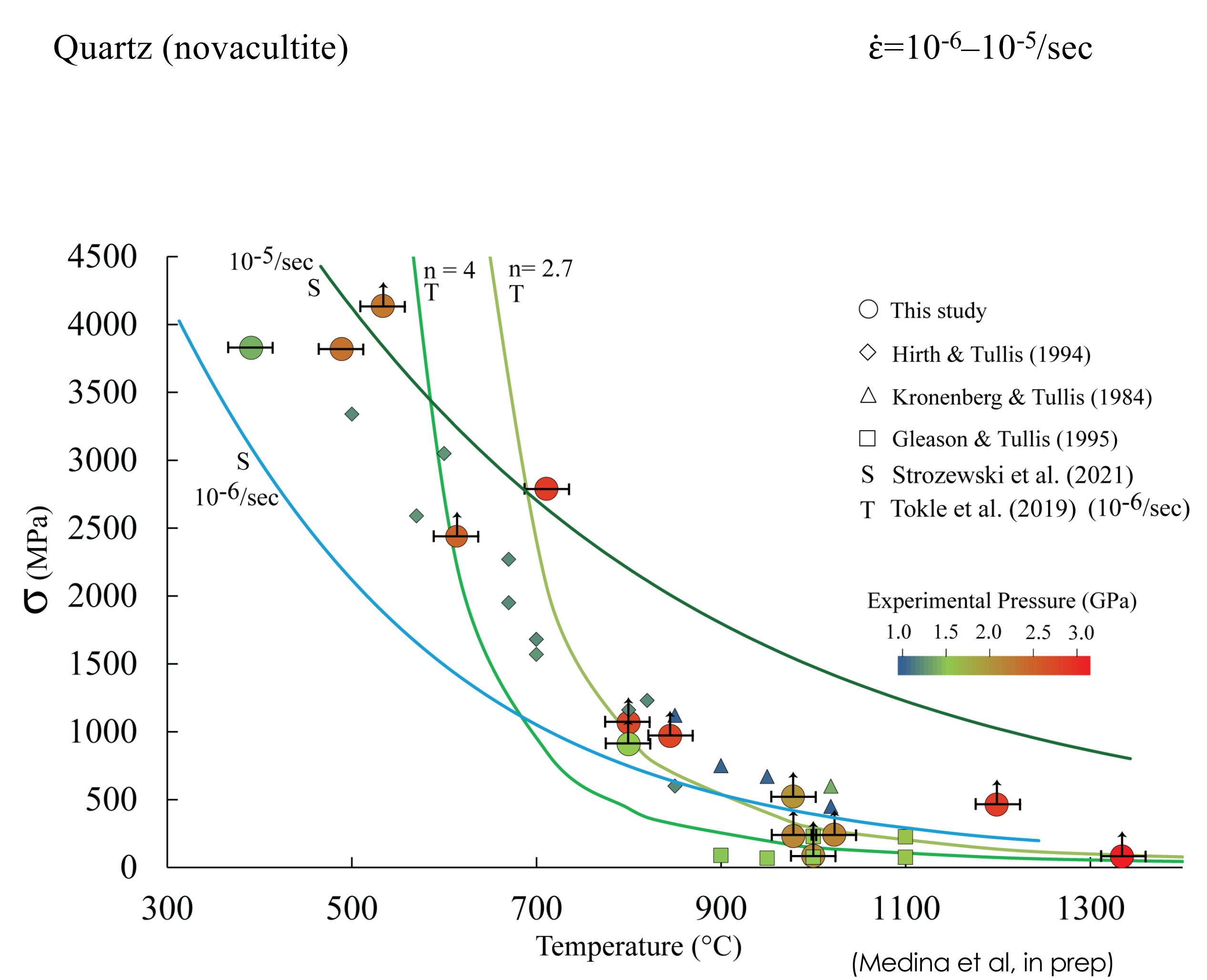
Data from olivine single crystal studies compiled by Durinck et al. 2007



Olivine CRSS derived from EPSC models

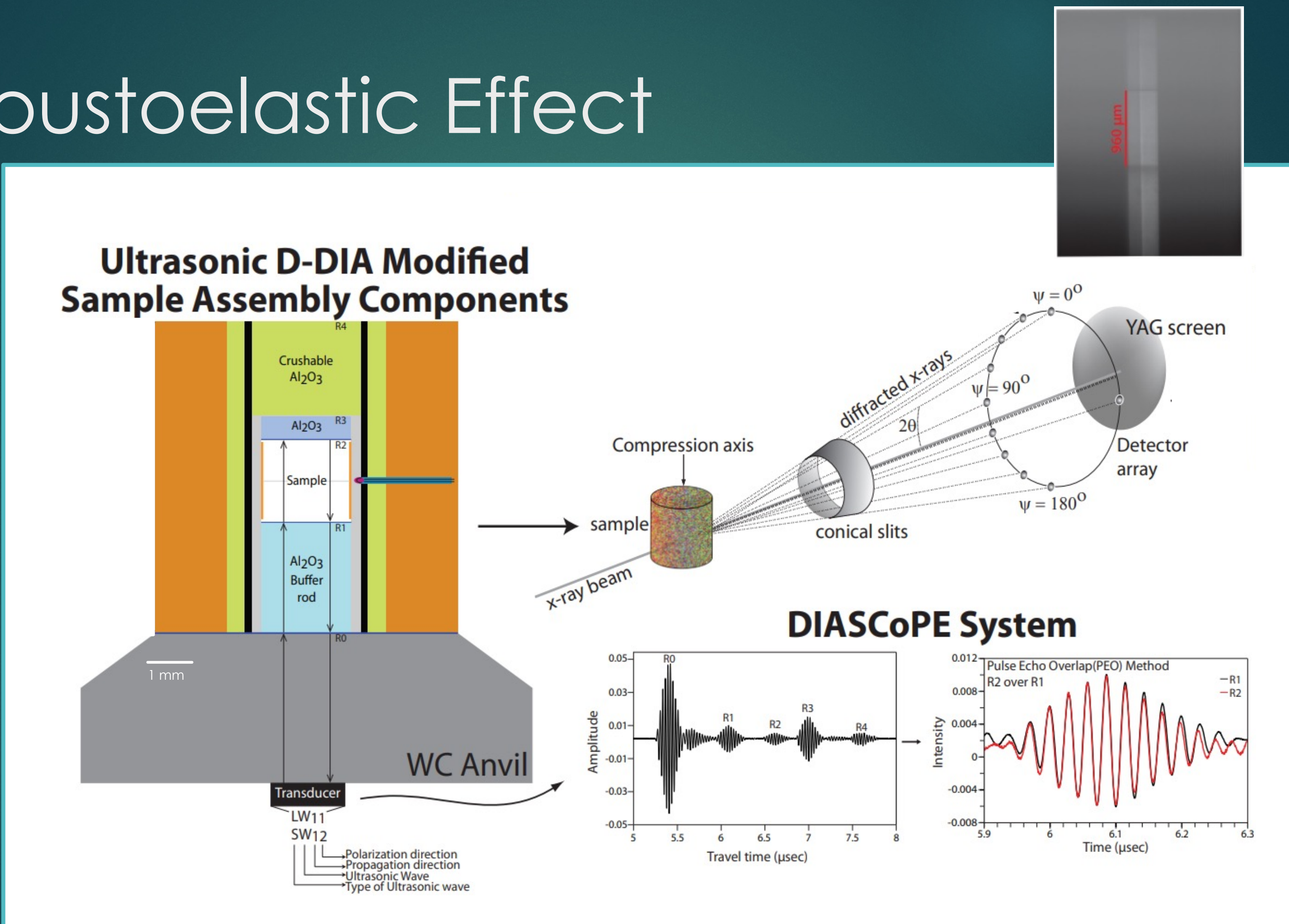
(Burnley & Kaboli, 2019)

- Applications
  - Investigate other deformation mechanisms
  - Measure CRSS
  - Measure sample strength



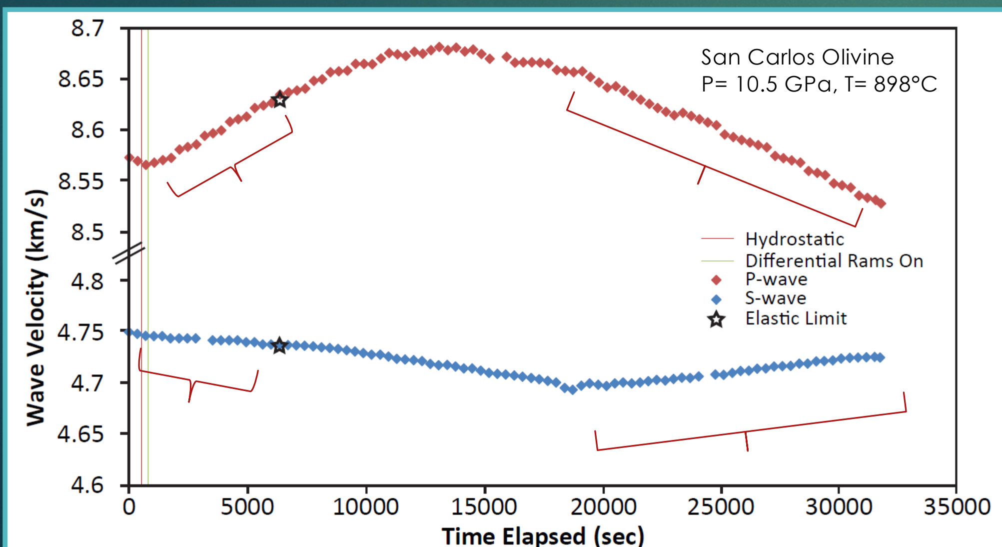
(Medina et al, in prep)

Acoustoelastic Effect

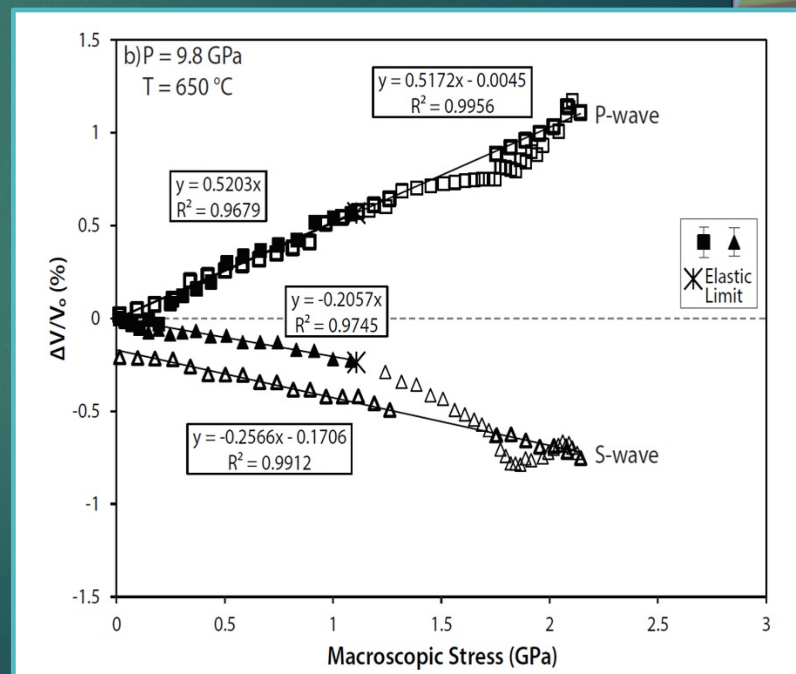


Ultrasound velocity as a function of compressive

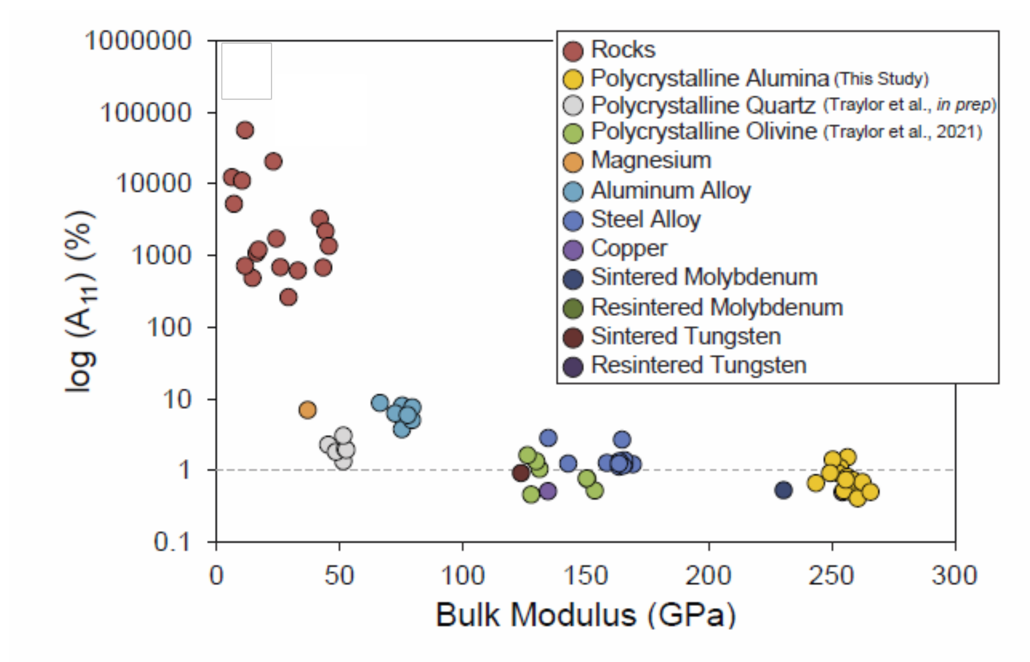
- P-wave velocities increase with compression
- S-wave velocities slightly decrease with compression



- P-wave slope = A_{11}
- S-wave slope = A_{12}



Dependence of acoustoelastic constant A_{11} on bulk modulus



Conclusions

- EPSC forward models of powder x-ray data from D-DIA experiments provides a rich source of information about what is going on inside rocks
- Going forward
  - EPSC/VPSC codes for more than one phase
  - Automated model optimization