Polycrystal Plasticity - Self-Consistent Model

27-731 (normally, 27-750)
Texture, Microstructure & Anisotropy
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MSE

Objective

- The objective of this lecture is to explain how we can use Eshelby's theory of interaction between an inclusion and its surrounding matrix to model anisotropic deformation.

- Further, to show how to calculate the stresses and distribution of slips in each grain of a polycrystal using the **V**isco**p**lastic **S**elf**c**onsistent code, **VPSC**.

Requirements:

- A basic understanding of how polycrystal plasticity works based on multiple slip in each grain.
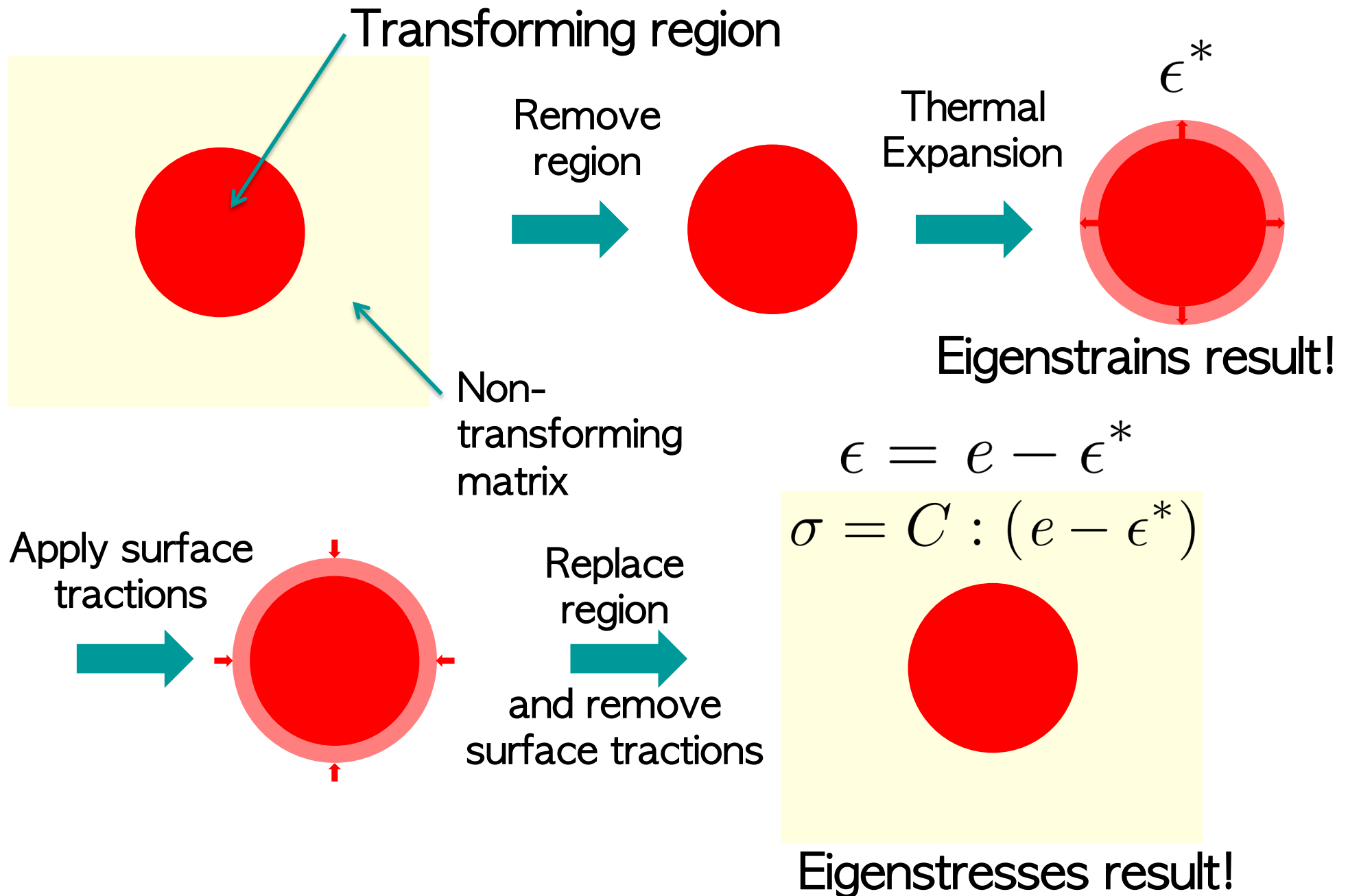
Questions & Answers

References

- Key Paper:
  Lebensohn RA and Tome CN (1993) "A Self-Consistent Anisotropic Approach for the Simulation of Plastic-Deformation and Texture Development of Polycrystals - Application to Zirconium Alloys" *Acta Metall. Mater.* **41** 2611-2624.

- Taylor G (1938) "Plastic strain in metals", *J. Inst. Metals* (U.K.) **62** 307 ;
  Bishop J and Hill R (1951), *Phil. Mag*. **42** 1298;
  Van Houtte P (1988), *Textures and Microstructures* **8 & 9** 313-350;
  Kocks, Tomé & Wenk: *Texture & Anisotropy* (Cambridge); chapter 8, 1996. Detailed analysis of plastic deformation and texture development.

- Reid: *Deformation Geometry for Materials Scientists,* 1973. Older text with many nice worked examples. Be careful of his examples of calculation of Taylor factor because, like Bunge & others, he does not use von Mises equivalent stress/strain to obtain a scalar value from a multiaxial stress/strain state.

- Hosford: *The Mechanics of Crystals and Textured Polycrystals*, Oxford, 1993. Written from the perspective of a mechanical metallurgist with decades of experimental and analytical experience in the area.

- Khan & Huang: *Continuum Theory of Plasticity*, Wiley-Interscience, 1995. Written from the perspective of continuum mechanics.

- De Souza Neto, Peric & Owen: *Computational Methods for Plasticity*, 2008 (Wiley). Written from the perspective of continuum mechanics.

- Gurtin: *An Introduction to Continuum Mechanics*, ISBN 0123097509, Academic Press, 1981.
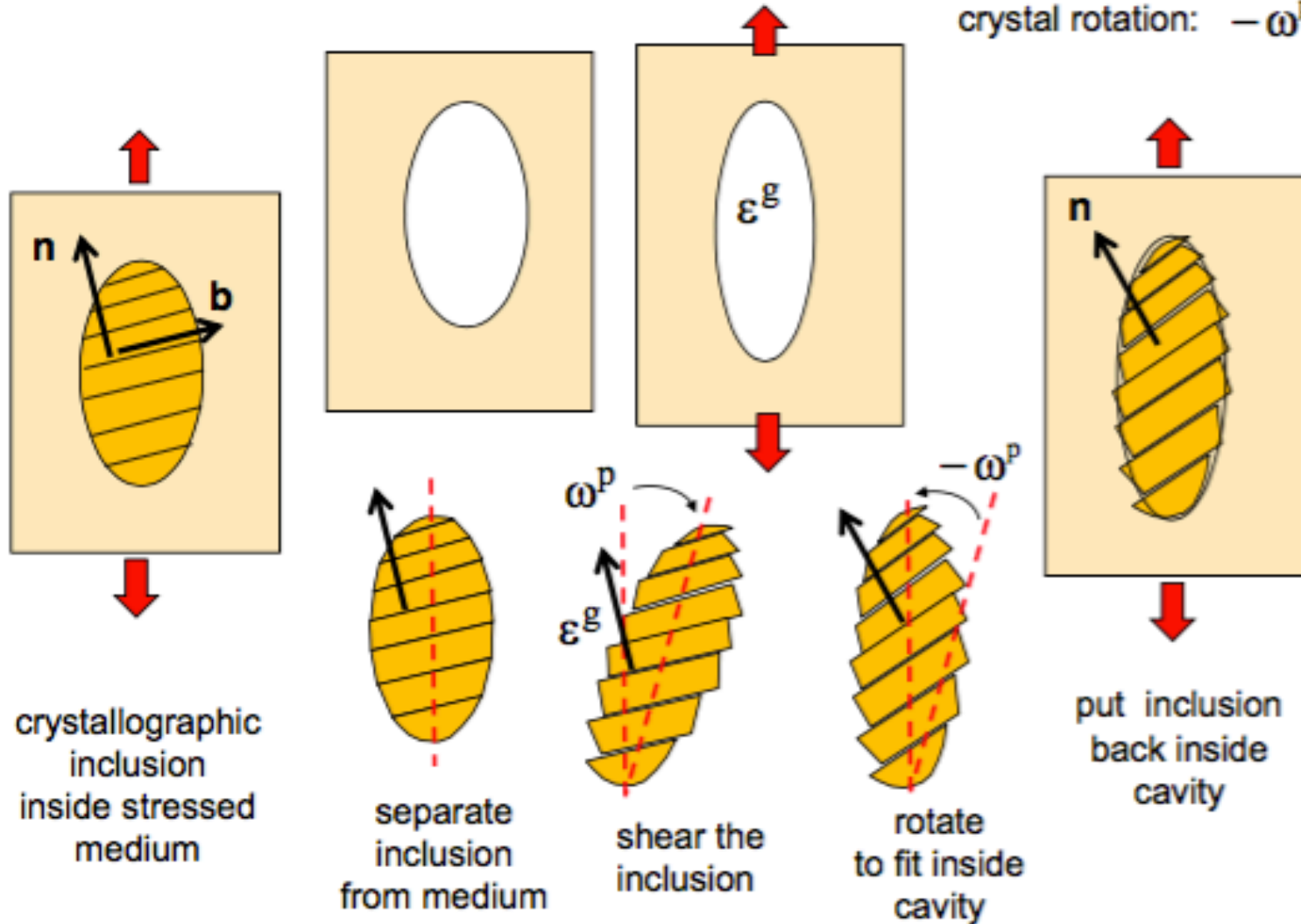
Background, Concepts

Eigenstrains and Eigenstresses

Transforming region

Remove region

Thermal Expansion

ϵ^*

Eigenstrains result!

Non-transforming matrix

Apply surface tractions

Replace region

and remove surface tractions

$$\epsilon = e - \epsilon^*$$

$$\sigma = C : (e - \epsilon^*)$$

Eigenstresses result!

Self-Consistent Model

- Following slides contain information about a more sophisticated model for crystal plasticity, called the *self-consistent model*.

- It is based on a finding a mean-field approximation to the environment of each individual grain.

- This provides the basis for the popular code VPSC made available by Tomé and Lebensohn (Lebensohn, R. A. and C. N. Tome (1993). "A Self-Consistent Anisotropic Approach for the Simulation of Plastic-Deformation and Texture Development of Polycrystals - Application to Zirconium Alloys." *Acta Metallurgica et Materialia* **41** 2611-2624).

VPSC: Inclusion

Slip , crystal rotation , texture evolution

crystal and cavity stretch: ε^g

crystal rotation: $-\omega^p$

ε^g

ω^p

ε^g

$-\omega^p$

crystallographic inclusion inside stressed medium

separate inclusion from medium

shear the inclusion

rotate to fit inside cavity

put inclusion back inside cavity

Eshelby Theory

- Eshelby analyzed the situation of an ellipsoidal inclusion within an infinite matrix that has undergone some eigenstrain. A thermoelastic potential may be defined for inclusions in a matrix with thermal eigen- strains and used to compute the resultant thermal stresses. The potential is employed to determine the displacement at all locations within the solid. Eshelby used this formulation to compute surface integrals at the inclusion surface, which he later simplified to what are known today as Eshelby tensors. These Eshelby tensors transform the local thermoelastic eigenstrain tensors to local total strain tensors.

$$\epsilon_{ij}(x) = S_{ijkl}(x)\ \epsilon^*_{kl}(x)$$

- One of the most significant conclusions from Eshelby's approach is the finding that surface integrals are independent of location within the inclusion itself, and thus, the stress and strain states are constant. For spherical symmetry, the 3 independent tensors are computed as shown on the right.

$$S_{1111} = \frac{7 - 5\nu}{15\,(1 - \nu)},$$

$$S_{1122} = \frac{5\nu - 1}{15\,(1 - \nu)},$$

$$S_{1212} = \frac{4 - 5\nu}{15\,(1 - \nu)},$$

Kröner, Budiansky and Wu's Model

Taylor Model
- compatibility across grain boundary
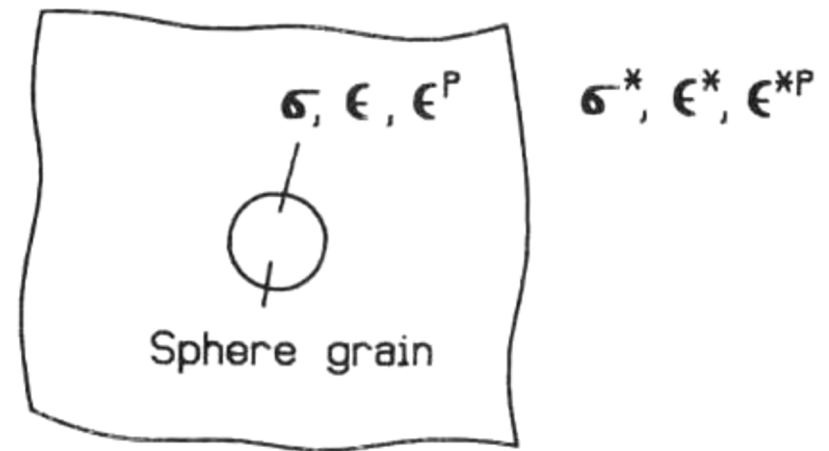- violation of the equilibrium between the grains
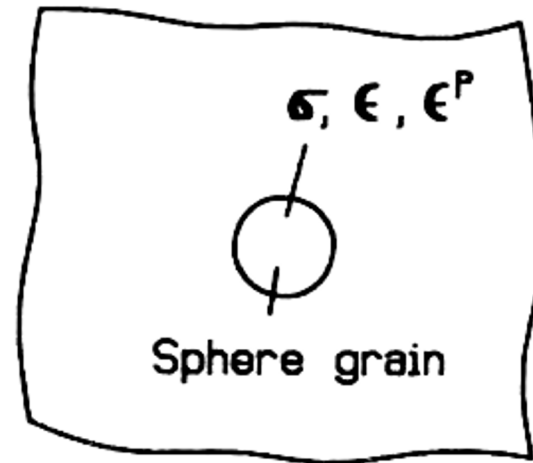

Fig. 11.6 Simple model of polycrystals

Budiansky and Wu's Model
- Self-consistent model
- Ensures both compatibility and equilibrium conditions on grain boundaries
- Based on the Eshelby inclusion model

Kröner, Budiansky and Wu's Model

The model:

Khan & Huang

$\sigma^*, \epsilon^*, \epsilon^{*P}$

$\sigma, \epsilon, \epsilon^{P}$

Sphere grain

Fig. 11.6   Simple model of polycrystals

❖ Sphere (single crystal grain) embedded in a homogeneous polycrystal matrix.

❖ The grain and the matrix are elastically isotropic.

❖ Can be described by an elastic stiffness tensor C, which has an inverse C^{-1}.

❖ The matrix is considered to be of infinite extent.

❖ The overall quantities σ^*, ε^* and ε^{*p} are considered to be the average values of the local quantities σ, ε and ε^{p} over all randomly distributed single crystal grains.

Kröner, Budiansky and Wu's Model

The initial problem can be solved by the following approach

1 – split the proposed scheme into two others as follows
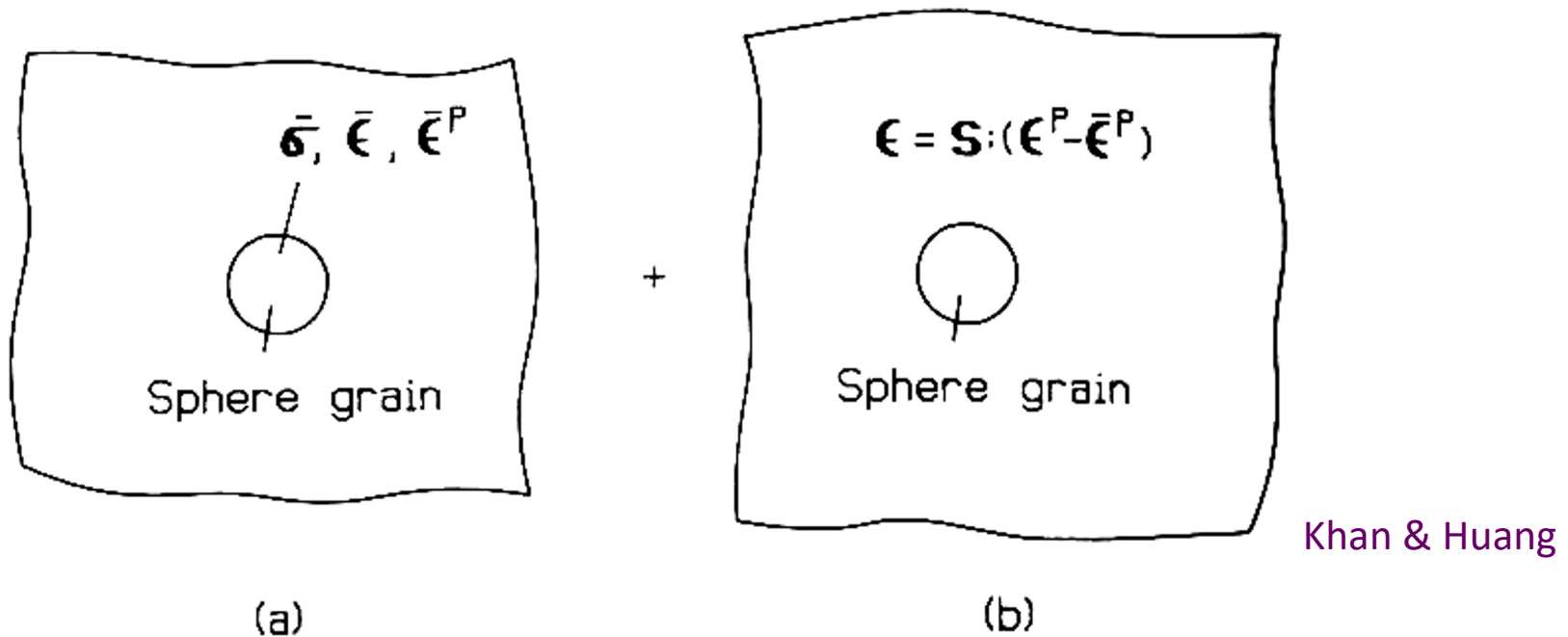
$\bar{\sigma}, \bar{\epsilon}, \bar{\epsilon}^P$

Sphere grain

(a)

+

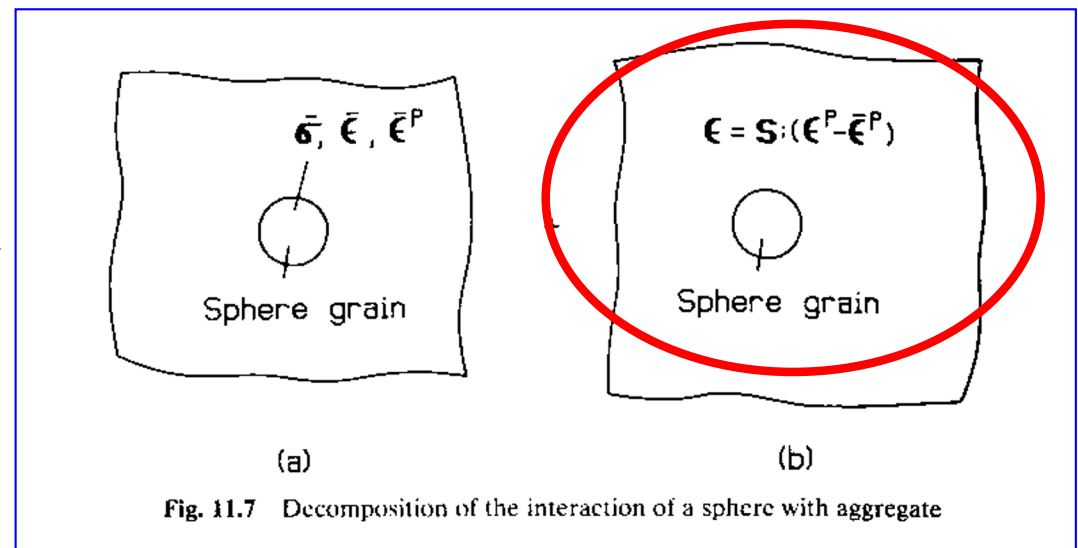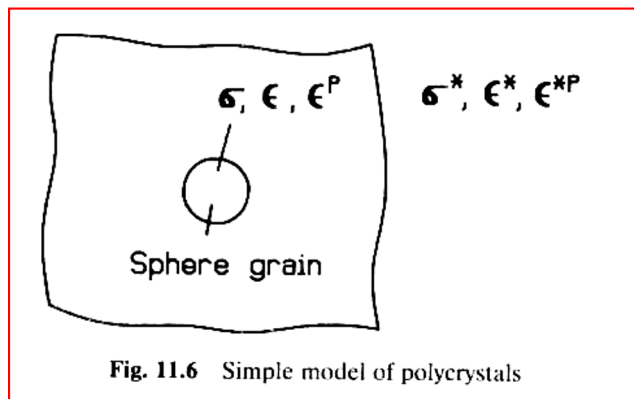$\epsilon = S:(\epsilon^P - \bar{\epsilon}^P)$

Sphere grain

(b)

Khan & Huang

Fig. 11.7 Decomposition of the interaction of a sphere with aggregate

Kröner, Budiansky and Wu's Model

1.a – The aggregate and grain are subject to the overall quantities $\overline{\sigma}, \overline{\varepsilon}$ and $\overline{\varepsilon}^{p}$. In this case the total strain is given by the sum of the elastic and plastic strains:

$$\varepsilon = \mathbf{C}^{-1} : \overline{\sigma} + \overline{\varepsilon}^{p}$$
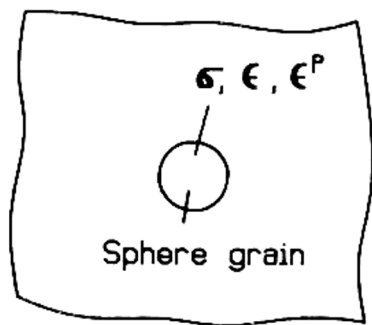
Fig. 11.6   Simple model of polycrystals
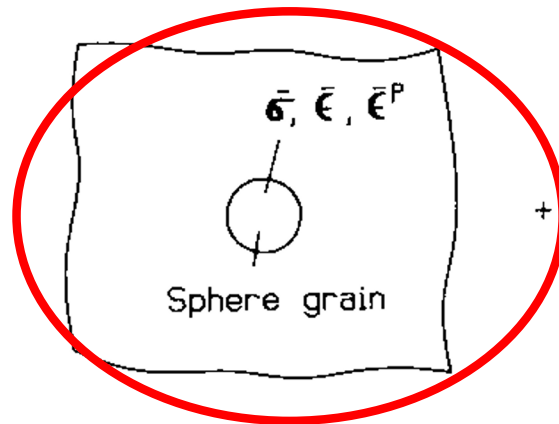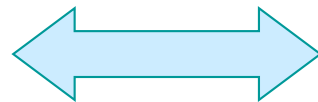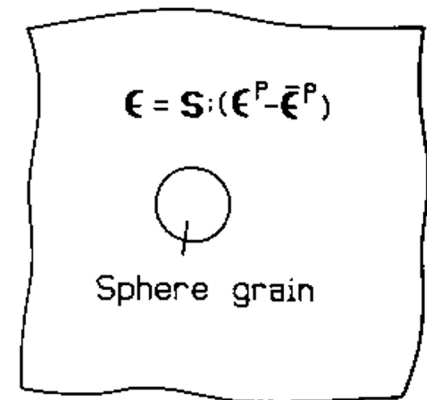
Fig. 11.7   Decomposition of the interaction of a sphere with aggregate

Khan & Huang

Kröner, Budiansky and Wu's Model

1.b – The sphere

$$\varepsilon' = \varepsilon^{\mathrm{p}} - \bar{\varepsilon}^{\mathrm{p}}{}_{composite}$$

❖ has a stress-free transformation strain, ε', which originates in the difference in plastic response of the individual grain from the matrix as a whole. This transformation strain is an eigenstrain.

❖ has the same elastic property as the aggregate.

❖ is small when compared with the aggregate (the aggregate is considered to extend to infinity).

Fig. 11.6 Simple model of polycrystals

(a)   (b)

Fig. 11.7 Decomposition of the interaction of a sphere with aggregate

Kröner, Budiansky and Wu's Model

The strain inside the sphere due to the elastic interaction between the grain and the aggregate caused by ε' is given by

$$\varepsilon = S : \varepsilon' = S : (\varepsilon^p - \bar{\varepsilon}^p)$$

Where,

S is the Eshelby tensor (*not* a compliance tensor) for a spherical inclusion in an isotropic elastic matrix
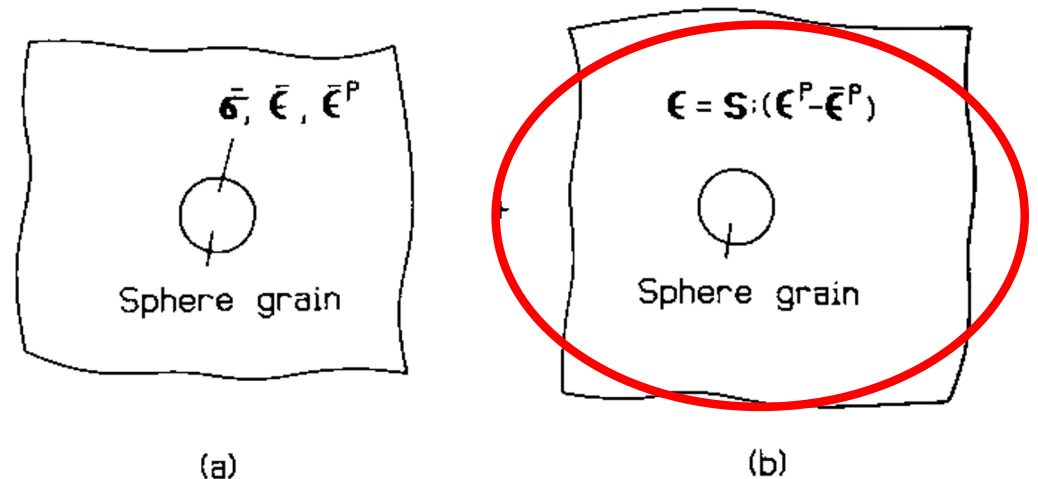

Fig. 11.7   Decomposition of the interaction of a sphere with aggregate

Kröner, Budiansky and Wu's Model

Then the actual strain inside the sphere is given by the sum of the two representations (1a and 1b) as follows

$$\varepsilon = \mathbf{C}^{-1} : \overline{\sigma} + \overline{\varepsilon}^{\mathrm{p}} + S : (\varepsilon^{\mathrm{p}} - \overline{\varepsilon}^{\mathrm{p}})$$

Given that,

$$S : (\varepsilon^{\mathrm{p}} - \overline{\varepsilon}^{\mathrm{p}}) = \beta(\varepsilon^{\mathrm{p}} - \overline{\varepsilon}^{\mathrm{p}})$$

where

$$\beta = \frac{2(4 - 5v)}{15(1 - v)}$$

The fraction was shown earlier as S_{1212}

This leads to

$$\varepsilon = \mathbf{C} : \overline{\sigma} + \overline{\varepsilon}^{\mathrm{p}} + \beta(\varepsilon^{\mathrm{p}} - \overline{\varepsilon}^{\mathrm{p}})$$

Kröner, Budiansky and Wu's Model

From the previous equation, it follows that the stress inside the sphere is given by

$$\sigma = \mathbf{C} : \varepsilon^{e} = \boldsymbol{C} : (\varepsilon - \varepsilon^{p}) =$$

$$= \overline{\sigma} - 2G(1 - \beta)(\varepsilon^{p} - \overline{\varepsilon}^{p})$$

Kröner, Budiansky and Wu's Model

In incremental form

$$\dot{\sigma} = \overline{\dot{\sigma}} - 2G(1 - \beta)(\dot{\varepsilon}^{\mathrm{p}} - \overline{\dot{\varepsilon}}^{\mathrm{p}})$$

where

$$\overline{\sigma} = (\sigma)_{\mathrm{ave}}, \qquad \overline{\dot{\sigma}} = (\dot{\sigma})_{\mathrm{ave}}$$

$$\overline{\varepsilon}^{\mathrm{p}} = (\varepsilon^{\mathrm{p}})_{\mathrm{ave}}, \qquad \overline{\dot{\varepsilon}}^{\mathrm{p}} = (\dot{\varepsilon}^{\mathrm{p}})_{\mathrm{ave}}$$

VPSC

- Each grain is a visco-plastic anisotropic ellipsoidal inclusion embedded in a visco-plastic anisotropic Homogeneous Effective Medium (HEM).
- Eshelby result: Stress and strain rate are uniform inside the inclusion but differ from macroscopic (average) values

- Deviatoric constitutive response:

$$\text{grain} \quad \dot{\varepsilon}'_{ij} = \dot{\gamma}_0 \sum_s m^s_{ij} \left(\frac{m^s : \sigma}{\tau^s} \right)^n = M_{ijkl} \sigma'_{kl}$$

$$\text{medium} \quad \bar{\dot{\varepsilon}}'_{ij} = \bar{M}_{ijkl} \bar{\sigma}'_{kl}$$
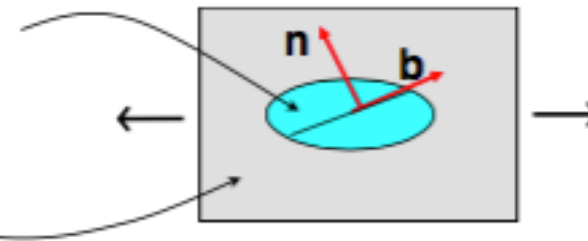
Solve stress equilibrium equation for inclusion in the homogeneous medium $\longrightarrow$ $\sigma_{ij,j} = \dfrac{\partial \sigma_{i1}}{\partial x_1} + \dfrac{\partial \sigma_{i2}}{\partial x_2} + \dfrac{\partial \sigma_{i3}}{\partial x_3} = 0$

Interaction between stress in inclusion with average stress

$$\sigma^g_{ij} = B^g_{ijkl} \bar{\sigma}_{kl} \qquad B^g = (M^g + \tilde{M})^{-1} : (\bar{M} + \tilde{M}) \quad \text{is the localization tensor}$$

Avg stress= Macroscopic stress -> Self consistent

$$\langle \sigma'_{ij} \rangle = \bar{\sigma}'_{ij} \qquad \bar{M}_{ijmn} = \langle M^g_{ijkl} B^g_{klmn} \rangle$$

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Assumptions for VPSC

Kocks,
Tomé,
Wenk

(i) The constitutive equation that describes the local response is non-linear and is known explicitly. The non-linear overall response of the aggregate is approximated using a linearization procedure, which is assumed to represent the material behavior within a certain range of stresses and strain rates.

(ii) Heterogeneity at the grain level leads to localized intergranular interactions, which are nearly impossible to describe realistically. A simplifying hypothesis is to assume a Homogeneous Equivalent Medium (HEM) with uniform properties, whose overall response to external loading conditions is the same as the aggregate's. Each grain (or cluster of grains) is assumed to be embedded in and interacting with such a homogeneous matrix. Each grain is assumed to be representative of all the grains with the same orientation, and the HEM represents the average neighborhood of all these grains. A disadvantage of this approach is that it overlooks topology, correlation and localization effects (such as percolation). This disadvantage is partially addressed by the 'cluster' method to be discussed in Section 6 of this Chapter.

(iii) The deformation of the inclusion (or cluster) embedded in an effective medium has to fulfill local equilibrium and compatibility. In practice, except for the exact Eshelby solution for ellipsoidal inclusions in linear media (see the Appendix), these conditions cannot be fulfilled exactly for non-ellipsoidal inclusions or non-linear media. It is usual, however, to linearize the response of the medium, and to assume that the grain can be characterized as essentially ellipsoidal, which guarantees that the stress and the strain are uniform within the domain of the grain. By extending the Eshelby result it is possible to use the interaction equation, which relates the stress and the strain in the grain to the overall stress and strain in the aggregate. This is an important characteristic of self-consistent models, since it permits one to account for the relative anisotropy of both grain and matrix.

(iv) The previous relation is assumed to apply to every grain (or cluster) considered individually. When combined with the condition that the volume averages of stress and strain must be equal to the macroscopic stress and strain, it leads to a non-linear equation that permits a calculation of the unknown overall moduli that describe the HEM response.

FULL CONSTRAINTS (FC) POLYCRYSTAL MODEL

• Also known as Taylor model. Based on enforcing strain continuity over stress equilibrium. Represents an absolute upper bound for macroscopic stress.
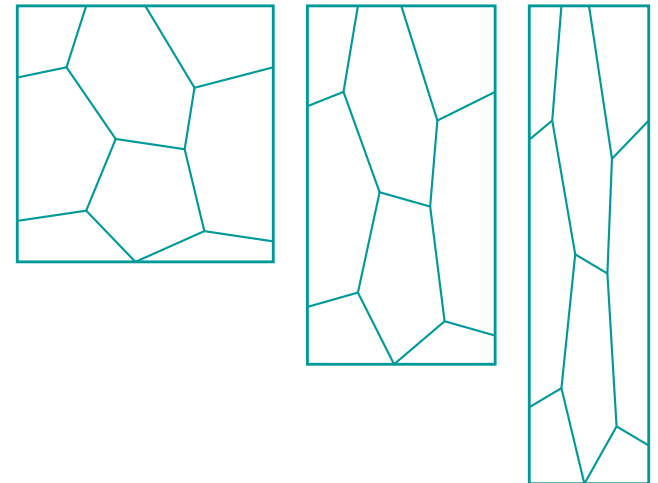
• Imposes the same velocity gradient (plastic strain and plastic spin) to all the grains

grain strain rate

$$\dot{\varepsilon}'_{ij} = \dot{\gamma}_0 \sum_s m^s_{ij} \left(\frac{m^s : \sigma}{\tau^s} \right)^n$$

impose

$$\dot{\varepsilon}'_{ij} = \overline{\dot{\varepsilon}}'_{ij}$$

• solve non-linear equation (typically n=20) for the stress in each grain

• calculate shear rates in every slip system

$$\dot{\gamma}^s = \dot{\gamma}_0 \left(\frac{m^s_{ij} \sigma_{ij}}{\tau^s} \right)^n$$

• update hardening and grain orientation incrementally

*V*ISCO-*P*LASTIC *S*ELF-*C*ONSISTENT (*VPSC*) POLYCRYSTAL MODEL [1]

• Each grain is a visco-plastic anisotropic ellipsoidal inclusion embedded in a visco-plastic anisotropic Homogeneous Effective Medium (HEM).

• Deviatoric constitutive response:

grain
$$\dot{\varepsilon}'_{ij} = \dot{\gamma}_0 \sum_s m^s_{ij} \left(\frac{m^s : \sigma}{\tau^s} \right)^n = M_{ijkl} \sigma'_{kl}$$
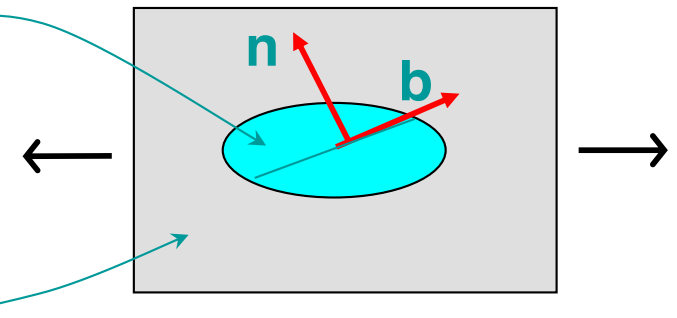
medium
$$\overline{\dot{\varepsilon}}'_{ij} = \overline{M}_{ijkl} \overline{\sigma}'_{kl}$$

Solve stress equilibrium equation for inclusion in the homogeneous medium $\longrightarrow$ $\sigma_{ij,j} = (\sigma'_{ij} + p\delta_{ij})_{,j} = 0$

Eshelby result: stress and strain-rate are uniform inside the inclusion
…but different from the macroscopic stress and strain rate !

[1] R.A. Lebensohn & C.N. Tomé, Acta Materialia **41** (1993) 2611

VPSC model → interaction equation

Solving stress equilibrium equation for the VP inclusion embedded in the VP medium leads to the interaction equation

$$(\dot{\varepsilon}'_{ij} - \bar{\dot{\varepsilon}}'_{ij}) = -\widetilde{M}_{ijkl}(\sigma'_{kl} - \bar{\sigma}'_{kl})$$

where $\widetilde{M}_{ijkl} = (I-S)^{-1}_{ijmn} S_{mnpq} \overline{M}_{pqkl}$

and $S_{(\overline{M})}$ is the Eshelby tensor

M is the compliance of the medium and relates stress with strain rate $\quad \bar{\varepsilon}'_{ij} = \overline{M}_{ijkl}\bar{\sigma}'_{kl}$

M large: the medium is very compliant → stress continuity → Sachs

M small: the medium is very stiff → strain continuity → Taylor

Intermediate cases: secant, affine, tangent
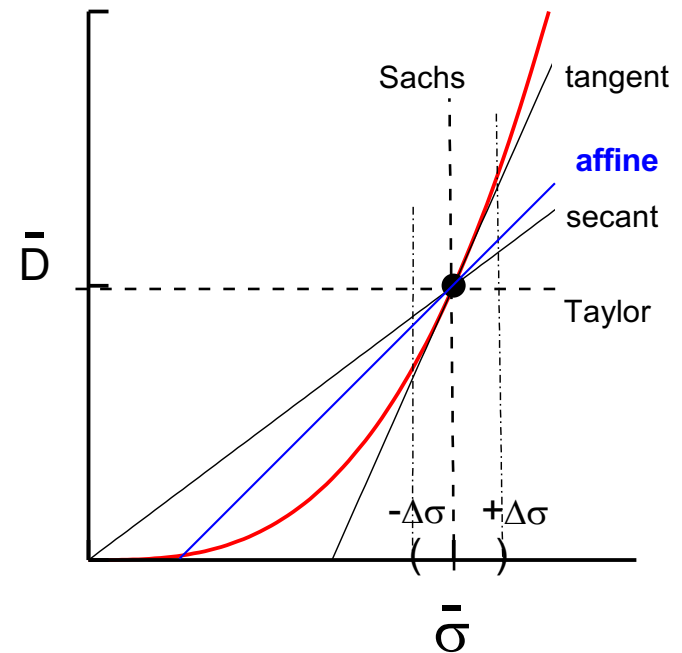
Visco-Plastic Self-Consistent Polycrystal Model

The interaction equation can be written as a localization equation that relates stress in the inclusion with average stress

$$\sigma'_{ij} = B_{ijkl}\overline{\sigma}'_{kl}$$ **B: localization tensor**

Assumption for having a polycrystal model: treat each grain as an inclusion inside the effective macroscopic medium.

The condition that the average stress over all grains has to be equal to the macroscopic stress …

$$\left\langle \sigma'_{ij} \right\rangle = \overline{\sigma}'_{ij}$$

…leads to a self-consistent equation for the plastic moduli of the aggregate:

$$\overline{M}_{ijmn} = \left\langle M_{ijkl}B_{klmn} \right\rangle$$

Hardening of slip modes inside VPSC

An 'extended Voce' law is used in VPSC to describe the hardening of slip and twin systems vs accumulated shear in grain Γ

$$\dot{\varepsilon}_{ij} = \dot{\gamma}_0 \sum_{s} m_{ij}^s \left(\frac{m_{kl}^s \sigma_{kl}}{\tau^s} \right)^n$$

$$\hat{\tau}(\Gamma) = \tau_0 + (\tau_1 + \theta_1 \Gamma)\left\{ 1 - \exp\left(-\frac{\Gamma|\theta_0|}{\tau_1} \right) \right\}$$

If latent hardening parameters h are considered the CRSS is incrementally updated as:

$$\Delta\tau^s = \frac{d\hat{\tau}(\Gamma)}{d\Gamma} \sum_{s'=1}^{N} h^{ss'} \Delta\gamma^{s'}$$

else:

$$\Delta\tau^s = \frac{d\hat{\tau}(\Gamma)}{d\Gamma} \Delta\Gamma$$
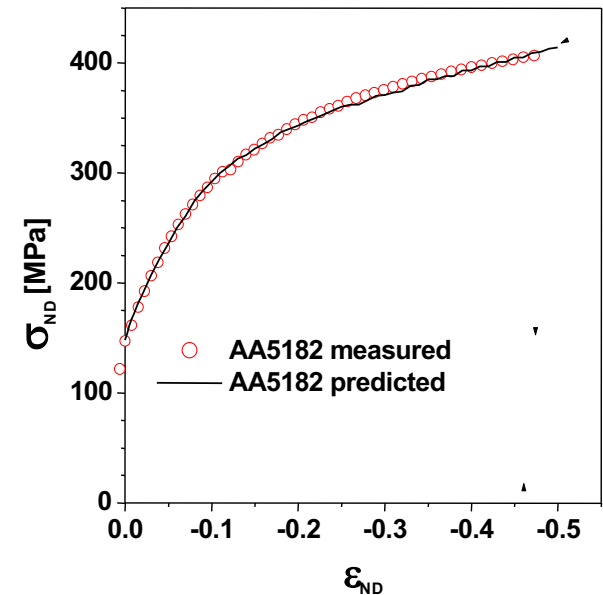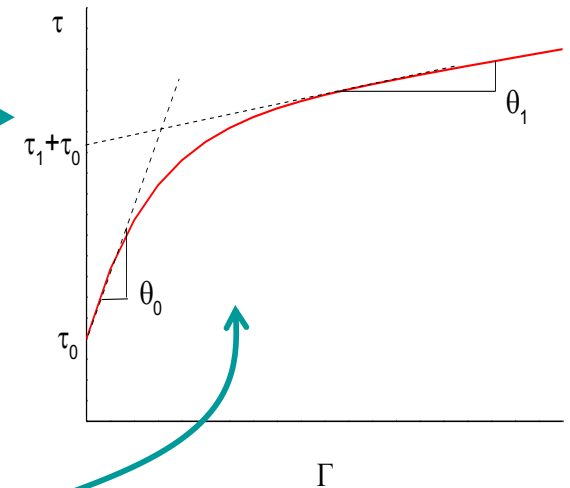
Running the code VPSC: input & output

INPUT:

- **Parameters of the run and names of datafiles (file VPSC7.IN)**
  INITIAL TEXTURE (discrete orientation file)
  ACTIVE SLIP AND TWIN SYSTEMS (hardening parameters)
  MACROSCOPIC VELOCITY GRADIENT (strain history)

OUTPUT:

- **Parameters of the run and input data (file RUN_LOG.OUT)**
  FINAL TEXTURE (discrete orientation file → TEX_PH1.OUT)
  STRESS-STRAIN RESPONSE (hardening → STR_STR.OUT)
  STATISTICS (system activity, twin fractions → ACT_PH1.OUT)

```
. . . . . . .
0                    grain shape and orient ctrl (ishape=0 to 4)
1.0  1.0  1.0        initial ellipsoid ratios (dummy if ishape=4)
0.0  0.0  0.0        init Eul ang ellips axes (dummy if ishape=3,4)
* name and path of texture file (filetext)
example1\rand500.tex
* name and path of single crystal file (filecrys)
example1\fcc.sx
. . . . . . . .
. . . . . . .
*MODELING CONDITIONS FOR THE RUN
0        ihardlaw (0:Voce, 1:MTS, 2:composite grain)
1        iratesens (0:rate insensitive, 1:rate sensitive)
0        interaction (0:FC,1:affine,2:secant,3:neff=10,4:tangent,5:SO)
1  1  1  iupdate: update orient, grain shape, hardening
. . . . . . .
*NUMBER OF PROCESSES
1
*IVGVAR AND PATH\NAME OF FILE FOR EACH PROCESS
0
example1\tension.3
```

Running VPSC7 → TEXTURE file

RAND500.TEX → a file containing 500 randomly generated orientations

```
dummy
dummy
random texture generated by RANDTEXT.FOR (23/01/97)
B   500
   102.74    119.56     33.65  1.000000
   219.06     36.21     70.51  1.000000
   166.66     28.59     45.80  1.000000
   149.74     86.13     38.68  1.000000
. . . . . . . .
. . . . . .
```
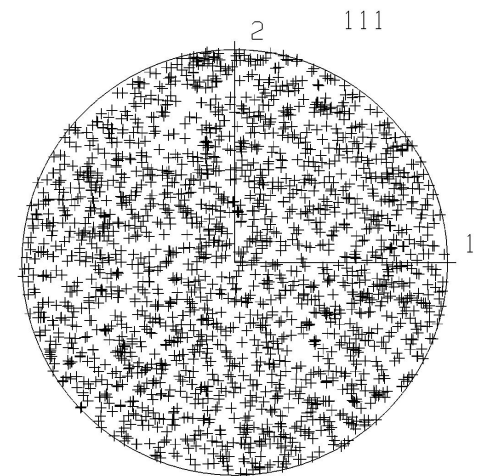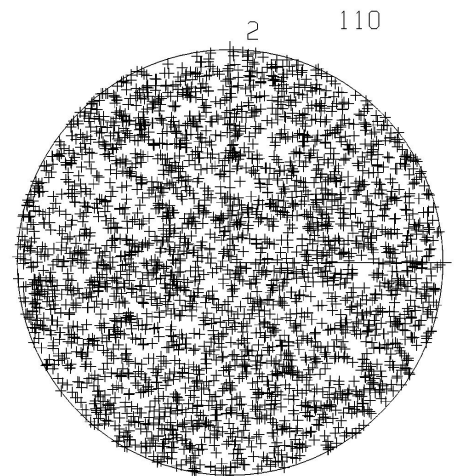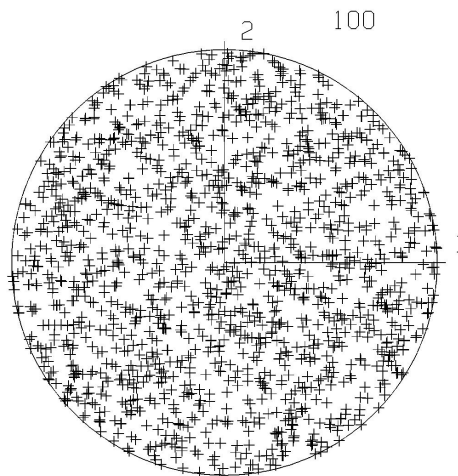
Running VPSC7 → PROCESS file

TENSION.3 → 50 steps of 2% axial strain along direction 3

```
50  3  0.02   298.        nsteps  ictrl  eqincr  temp
* boundary conditions
  1      1      1          iudot |   flag for vel.grad.
  1      1      1                |   (0:unkn-1:known)
  1      1      1                |

 -0.5    0.     0.          udot |   vel.grad
  0.    -0.5    0.                |
  0.     0.     1.0              |

  0      0      0          iscau |   flag for Cauchy
         0      0                |   (0:unkn-1:known)
                0                |

  0.     0.     0.       scauchy |   Cauchy stress
         0.     0.                |
                0.                |
```

Running VPSC7 → SINGLE CRYSTAL FILE

FCC.SX → slip systems and hardening parameters for FCC

```
*Material: AUSTENITIC STEEL
 cubic         crysym
  1.  1.  1.     90. 90.  90.    unit cell axes and angles
 Elastic stiffness (single crystal [GPa])
 205.0  138.0  138.0  000.0  000.0  000.0

 ….
*Info about slip & twinning modes in this file:
 2         nmodesx    (total # of modes listed in file)
 1         nmodes     (# of modes to be used in the calculation)
 1         mode(i)    (label of the modes to be used)
 <111>{110} SLIP
 1  12  20   1                      modex,nsmx,nrsx,iopsysx
 0.000  0      0.000  0.000         twshx,isectw,thres1,thres2
 1.0    0.0    0.0    0.0    0.  0.  tau0,tau1,thet0,thet1 ,hpfac,gndfac
     1.0    1.0                     hlat(nmodes)
  1 1 1      0 1 -1
  1 1 1      1 0 -1
  1 1 1      1 -1  0
   ……….   ………
```

Simulate axial tension and compression of an initially random FCC aggregate.

Deformation by slip in the <110> direction and on {111} crystallographic planes. The CRSS = τ^s = constant = 1

The Voce hardening is rigid perfectly plastic:

The imposed velocity gradient is symmetric and equal to the strain rate tensor:

$$\overline{L}_{i,j} = \overline{\dot{\varepsilon}}_{ij} = \begin{bmatrix} -0.5 & 0 & 0 \\ 0 & -0.5 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \text{axial tensile rate}$$

EXAMPLE 1: TENSION & COMPRESSION of FCC → TEXTURE

Predicted textures after 100% axial tension and compression using different grain-matrix interaction and compression (INTERACTION=0,1,2,3,4)

Stress (Taylor factor) evolution and Average Number of Active Systems per Grain using different grain-matrix interaction assumptions.

TAYLOR (FC):
upper bound and more than 6 active systems

TANGENT:
lower bound, about 4 active systems in tension and 3 in compression.

In general: Self-Consistent leads to plane strain deformation of individual grains

TENSION   COMPRESSION

Legend:
- Taylor
- affine
- secant
- neff=10
- tangent
- 2nd ord

stress axis: 2.5, 3.0

slip activity axis: 0, 2, 4, 6, 8

strain axis: 0.0, 0.5, 1.0
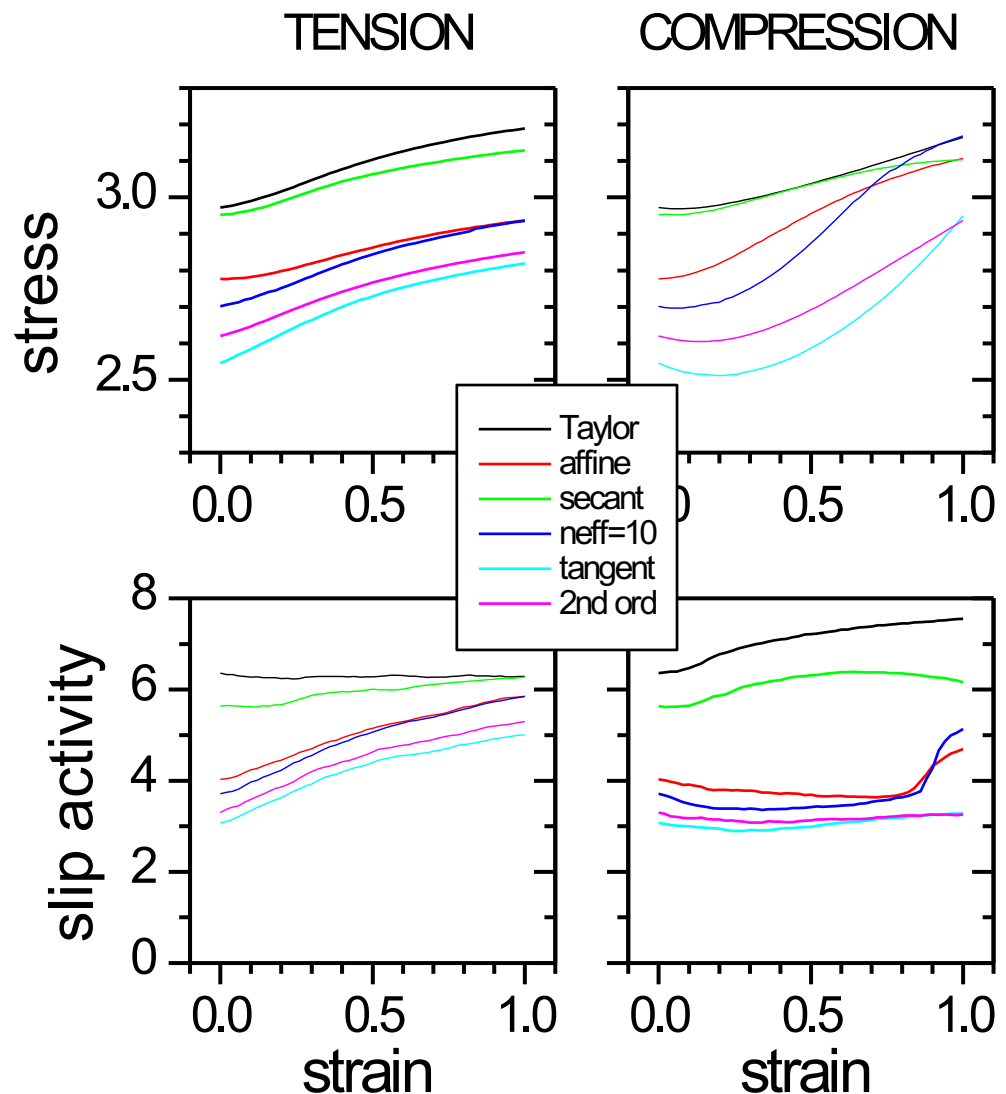
EXAMPLE 2: ROLLING of FCC

Simulate plane strain deformation of an initially random FCC aggregate.

Deformation by slip in the <110> direction and on {111} crystallographic planes, up to E33=100% (63% reduction).

The Voce hardening is linearly increasing: $\tau_0 = \theta_0 = \theta_1 = 1$, $\tau_1 = 0$

The imposed velocity gradient is plane strain (EXAMPLE 2a):

$$\overline{L}_{ij} = \overline{\dot{\epsilon}}_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad \text{plane strain rate}$$

We also run plane strain with superimposed shear (EXAMPLE 2b):

$$\overline{L}_{ij} = \begin{bmatrix} 1 & 0 & L_{13} \\ 0 & 0 & 0 \\ L_{13} & 0 & -1 \end{bmatrix} \quad \text{plane strain} + \text{shear} / \text{reverse shear}$$

$$\text{where} \quad L_{13} = 1.25 \sin(2\pi\epsilon_{33})$$

EXAMPLE 2: ROLLING of FCC → PROCESS FILE

File VPSC7.INa enforces rolling followed by a yield locus calculation and a Lankford and Young modulus calculation.

. . . .
. . . . . .
*NUMBER OF PROCESSES
3
*IVGVAR AND PATH\NAME OF FILE OR STRESS SUBSPACE OR ANG INCREM

0   ivgvar=0 will run a monotonic strain path
example2\rolling

2   ivgvar=2 will calculate PCYS at the end
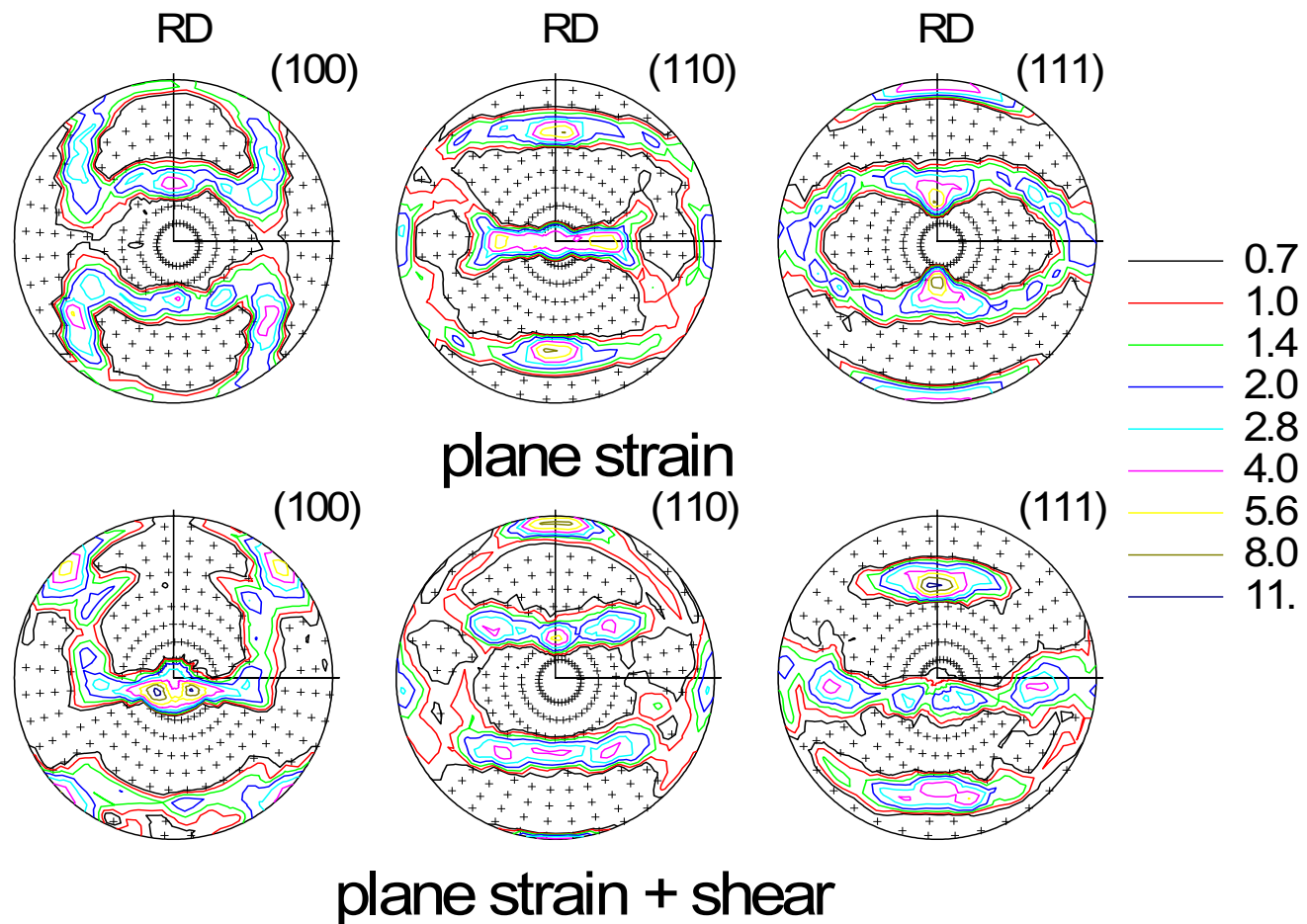1   2   -->   section of stress space

3   ivgvar=3 will calculate Lankford coefficients at the end
10   -->   angular increment for tensile probing

EXAMPLE 2: ROLLING of FCC → FINAL TEXTURE

The superimposed shear breaks the orthotropic symmetry of the rolling texture

SIMULATED ROLLING OF FCC (63% reduction)

plane strain

plane strain + shear

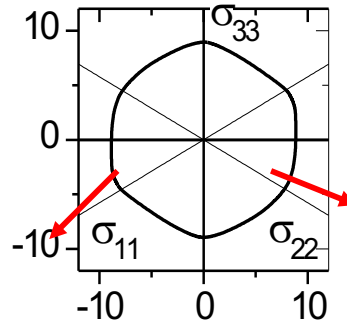The superimposed shear alters the final texture. As a consequence,
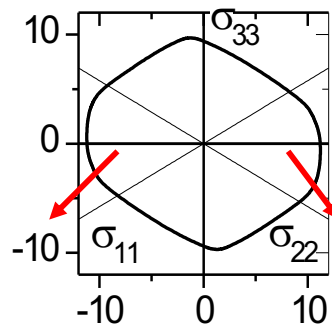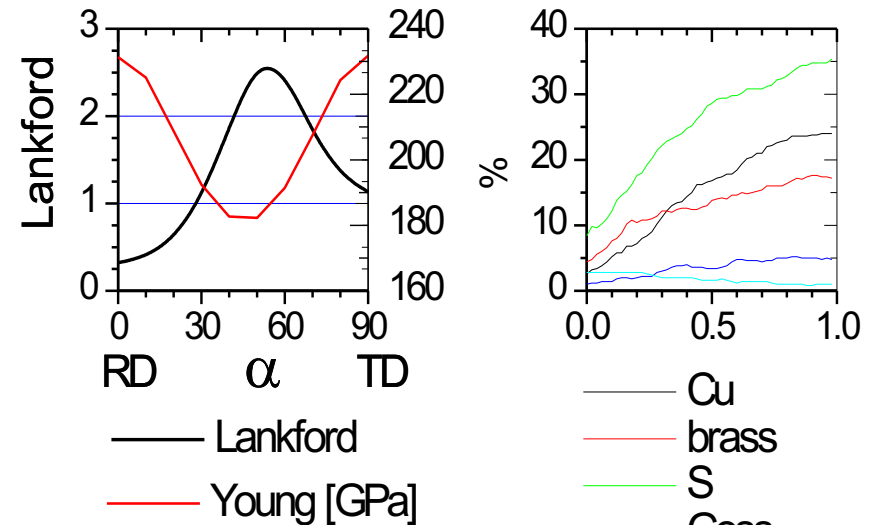
the yield locus,

the in-plane anisotropy (Lankford),

the directional Young modulus,
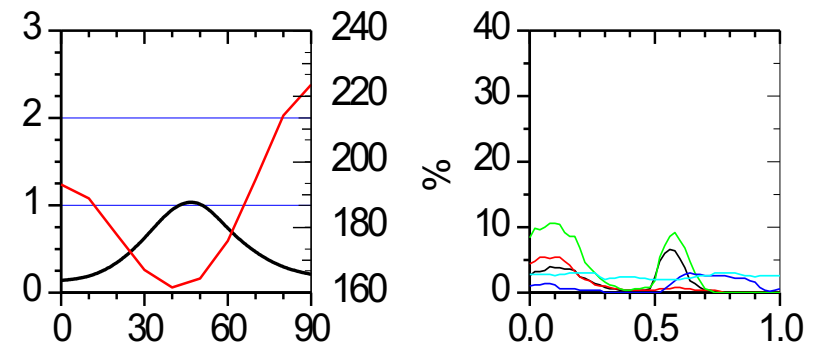
the final rolling components,

are different.

Plane strain

Plane strain + shear

EXAMPLE 5: TORSION of FCC → fixed ends

Simulate torsion (simple shear) of an initially random FCC aggregate.

Deformation by slip in the <110> direction and on {111} crystallographic planes, up to $\varepsilon_{12} = 2.0$
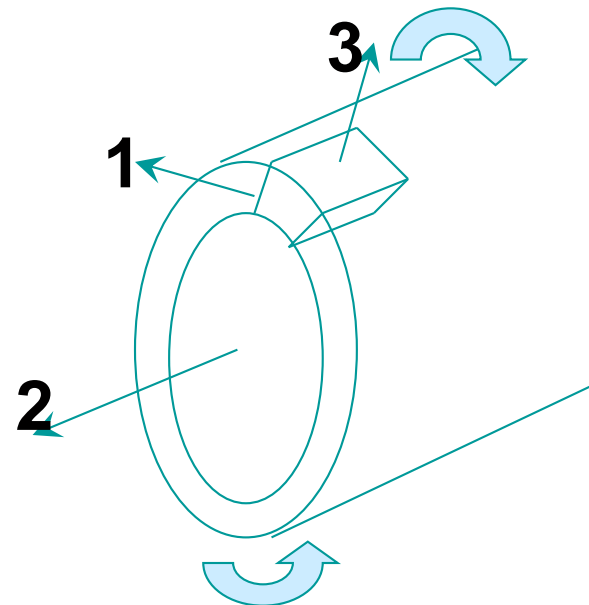
The Voce hardening is linearly increasing: $\tau_0 = \theta_0 = \theta_1 = 1 \,, \tau_1 = 0$

Case 5a: the imposed velocity gradient is fixed-end mode $\dot{\varepsilon} \bar{} = 0.$
 the hoop and radial stress components are imposed to zero

$$\bar{L}_{ij} = \bar{\dot{\varepsilon}}_{ij} = \begin{bmatrix} ? & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & ? \end{bmatrix}$$

$$\bar{\Sigma}_{ij} = \begin{bmatrix} 0 & ? & ? \\ & ? & ? \\ & & 0 \end{bmatrix}$$

The sequence of processes enforced through VPSC7.IN are:

1- 40 steps of $\Delta\varepsilon_{12} = 2.5\%$

2- calculation of intermediate yield surface, projection $(\sigma_{12}, \sigma_{22})$

3- 40 steps of $\Delta\varepsilon_{12} = 2.5\%$

4- calculation of the final yield surface, projection $(\sigma_{12}, \sigma_{22})$

```
*NUMBER OF PROCESSES
4
*IVGVAR AND PATH\NAME OF FILE; STRESS SUBSP OR ANG INCR
0
example5\torsion.a
2       ivgvar=2 will calculate PCYS at the end
1 5          -->   section of stress space
0
example5\torsion.a
2       ivgvar=2 will calculate PCYS at the end
1 5          -->   section of stress space
```

Simulate torsion (simple shear) of an initially random FCC aggregate.

Deformation by slip in the <110> direction and on {111} crystallographic planes, up to $\varepsilon_{12} = 2.0$
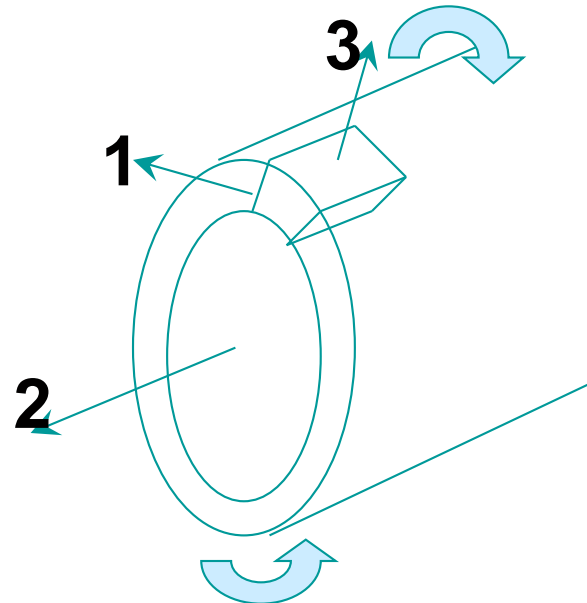
The Voce hardening is linearly increasing: $\tau_0 = \theta_0 = \theta_1 = 1$, $\tau_1 = 0$

Case 5b: the imposed velocity gradient is free-end mode $\sigma_{22} = 0.$
the hoop and radial stress components are imposed as zero

$$\overline{L}_{ij} = \overline{\dot{\varepsilon}}_{ij} = \begin{bmatrix} ? & 1 & 0 \\ 0 & ? & 0 \\ 0 & 0 & ? \end{bmatrix}$$
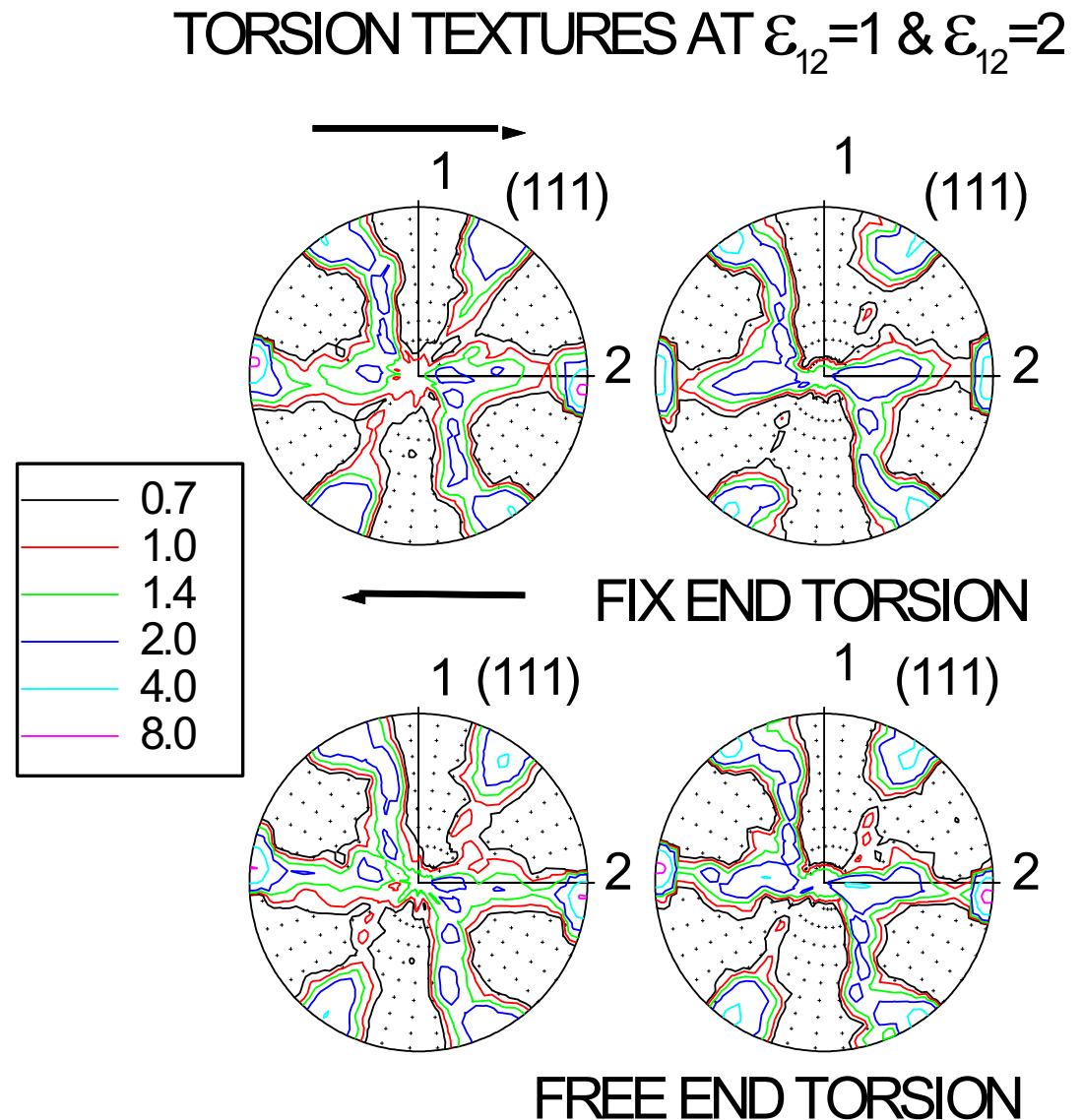
$$\overline{\Sigma}_{ij} = \begin{bmatrix} 0 & ? & ? \\ & 0 & ? \\ & & 0 \end{bmatrix}$$

EXAMPLE 5: TORSION of FCC → FINAL TEXTURE

Textures are typical of shear.

A slight rotation of the texture between fix-end and free-end is responsible for the rotation of the yield locus and the associated change in length.
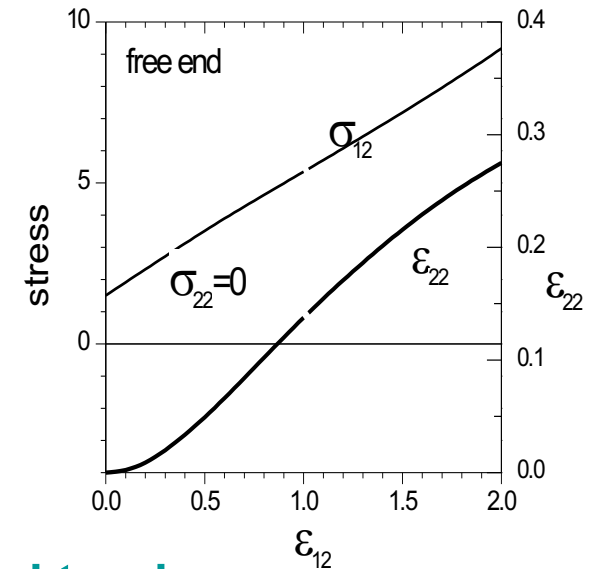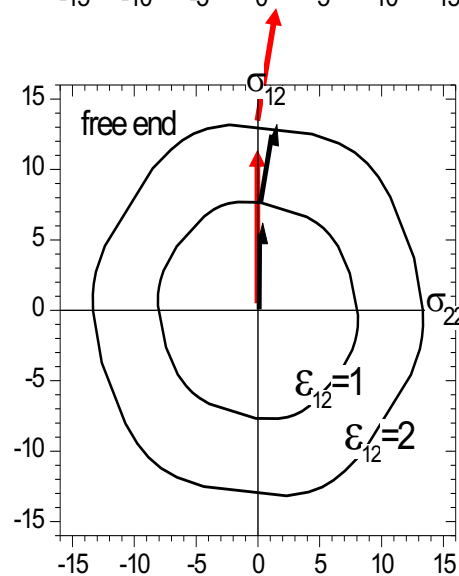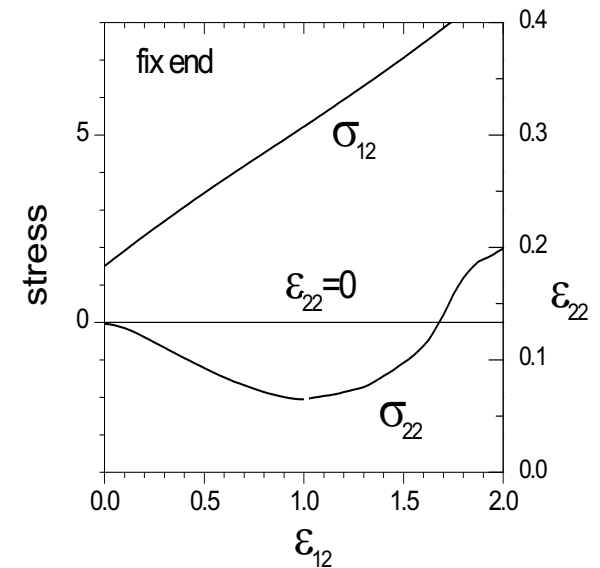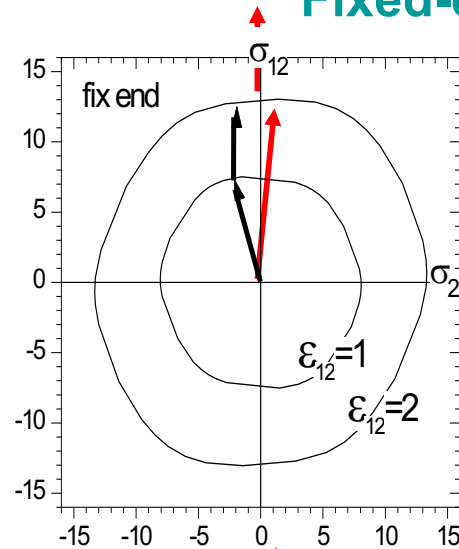
TORSION TEXTURES AT ε_{12}=1 & ε_{12}=2

—	0.7
—	1.0
—	1.4
—	2.0
—	4.0
—	8.0

FIX END TORSION

FREE END TORSION

Fixed-end torsion

FIXED END:
Axial strain is zero → strain rate perpendicular to the yield surface AND vertical.

FREE END:
Axial stress is zero → strain rate perpendicular to the yield surface AND stress vector vertical.

Free-end torsion

Plotting Results from VPSC: packages and installation

- Suggestion: use MTEX, which is available as an open source package within MATLAB. MATLAB is freely available for academic use for members of CMU.

- Step 1: install MATLAB

- Step 2: search on "github mtex" to find the webpage. Download it as a zip file. Unpack the zip.

- Step 3: open MATLAB and add the path to the MTEX folder.

Plotting Results : Using MTEX

- Step 1: edit the file TEX_PH1-compression1.OUT, where the name depends on what you have in the VPSC control file, vpsc7.in. You can always do this by hand but a python/bash script would be worth implementing to automate it.

  - Each texture output has 4 header lines. Insert "#" at the beginning of each of those lines. Add a 5th line that reads " phi1 Phi phi2 weight" so that MTEX can read in appropriate headers for each of the 4 columns of data.

- Go to https://mtex-toolbox.github.io/OrientationImport.html to find an example of how to import lists of orientations.

  - For fcc metals such as Al, use cs = crystalSymmetry.load('Al-Aluminum.cif') to load the correct crystal symmetry

  - Add Folder to the MATLAB path where you have the VPSC results (with the edited TEX list).

  - fname = fullfile('~/code/CarlosTome-self-consistent/vpsc7d_noexe/Al_Rollett ','TEX_PH1-compression1-headers.txt'); note the different path name to the data

  - plotPDF(ori,Miller({1,1,1},{0,0,1},{1,0,1},cs)); note the different set of Miller indices to specify which poles to plot
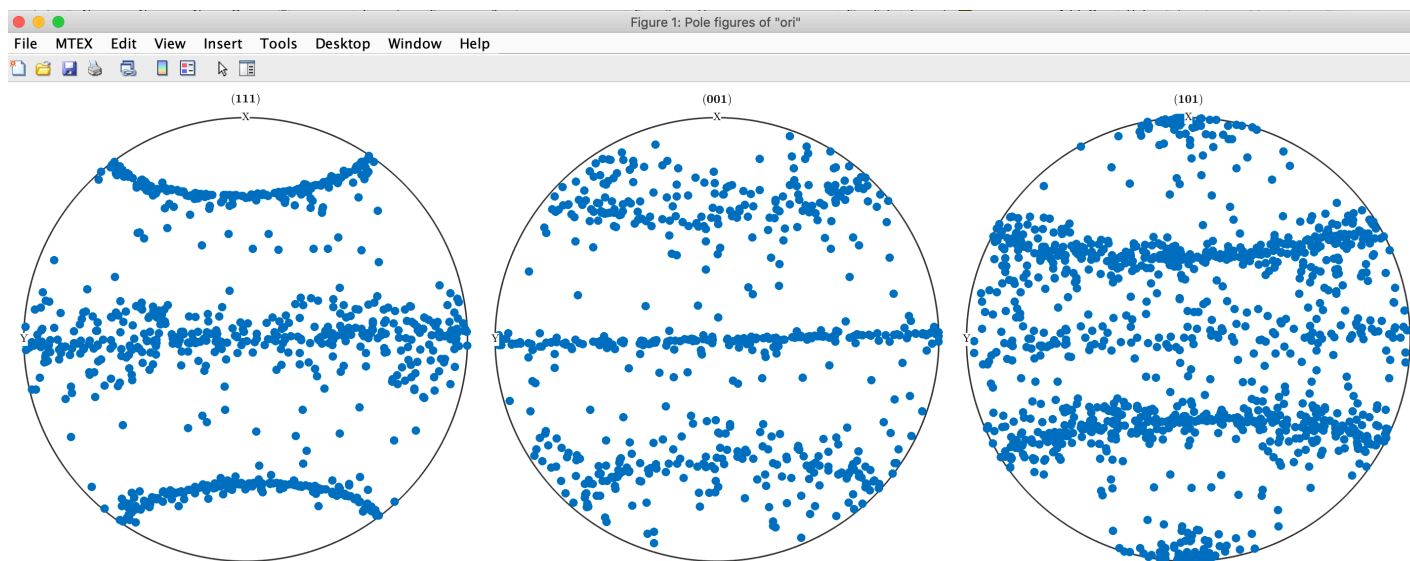
Plotting Results: MTEX, odf

- https://mtex-toolbox.github.io/ODFTutorial.html

- This command should work to compute the odf from the list of orientations:
  odf = calcDensity(ori)

- Assuming that you succeed in computing the odf, many different kinds of plot are possible.

- See https://mtex-toolbox.github.io/orientation.calcDensity.html for more detail of options (kernel width, e.g.)

- pf = calcPoleFigure(odf,Miller({1,1,1},{0,0,1},{1,0,1},cs))

Pole Figures

- https://mtex-toolbox.github.io/PoleFigure.plot.html
- plot(pf,'contourf')