Carnegie Mellon

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

- What does “self-consistent” mean? This refers to the design of the algorithm that ensures that the polycrystal ensemble satisfies the boundary conditions of the imposed strain rate (velocity gradient), perhaps combined with certain stress boundary conditions.
- What does “visco-plastic” mean? This refers to the use of a strain-rate sensitive yield function at the single slip system scale, i.e., the shear (slip) rate is proportional to the RSS/CRSS raised to a power. The exponent is typically in the range 10 to 50.
- What improvement does VPSC offer over the Taylor model? The VPSC model allows each grain to deviate from the polycrystal average in a fashion that is consistent (that word again!) with the Eshelby-Kröner inclusion model. The stiffer the interaction, the smaller the deviation (in strain rate).
- For which materials is VPSC most useful? The larger the anisotropy of the single crystal yield surface (think hexagonal versus cubic), the larger the potential deviation of an individual grain from the polycrystal (homogeneous medium).

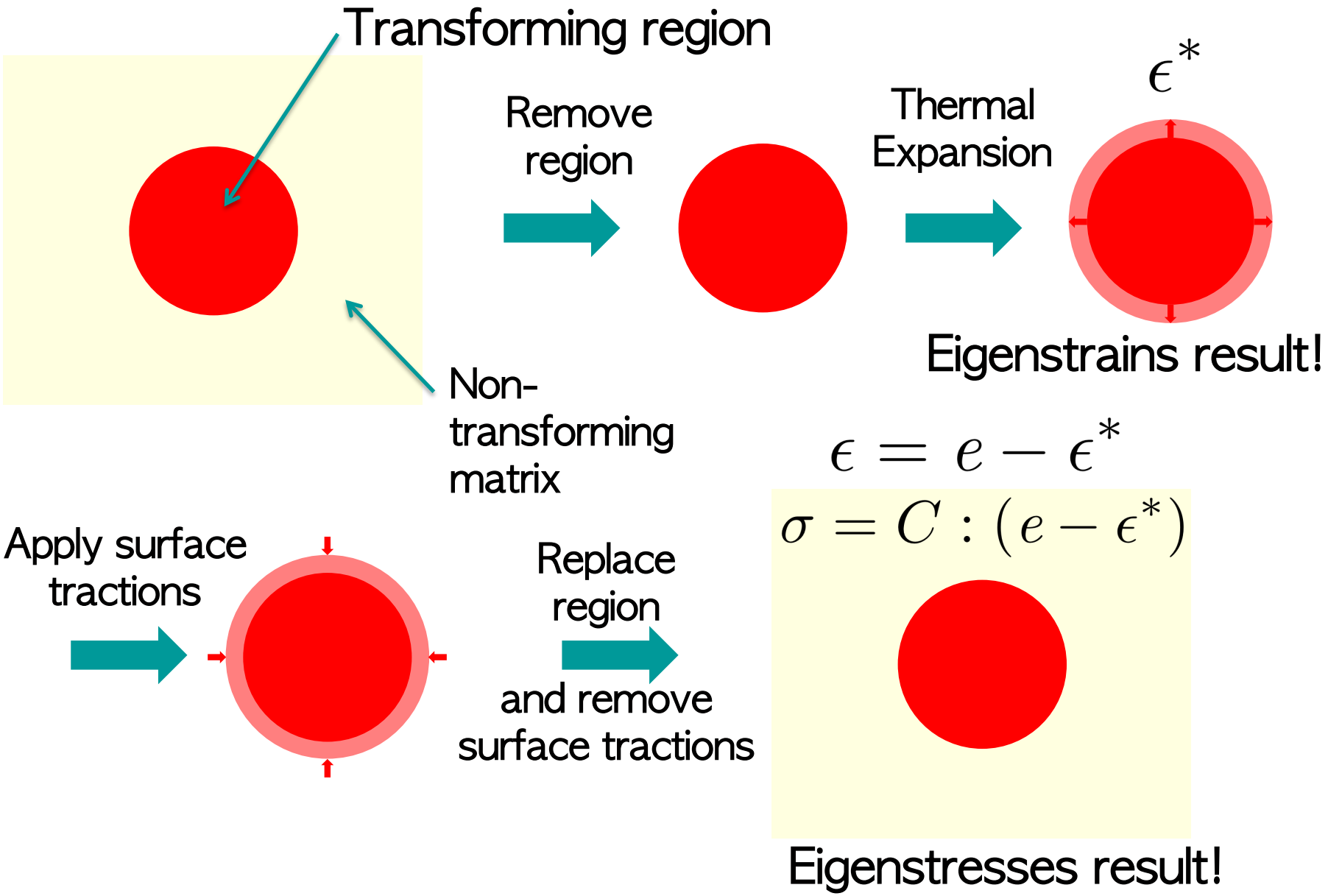
References

- *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.
- Eshelby, JD, "The Determination of the Elastic Field of an Ellipsoidal Inclusion and Related Problems", Proceedings of the *Royal Society of London Series A - Mathematical Physical and Engineering Sciences*, **A241**, 376–396 (1957).
- 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.
- Gurtin: *An Introduction to Continuum Mechanics*, Academic Press, 1981.

Background, Concepts

- The original Taylor model is a pure strain-based boundary condition on the grains. Commonly known as the “full constraints” (FC) model.
- Mecking developed a “relaxed constraints” (RC) model. This was mainly directed at rolling (plane strain compression) that develops strongly flattened grains such that two shear components could be non-zero with only a small penalty in compatibility. Adoption of the RC model resulted in improved agreement between simulated and measured textures.
- The essential idea behind the (viscoplastic) self-consistent (VPSC) model is to compute the stress in each grain as if it were an inclusion embedded in an otherwise homogeneous medium. The “medium” is simply the averaged polycrystal in terms of plastic stiffness.
- A later variant is known as the elasto-viscoplastic self-consistent model (ESCP) in which the effects of elastic anisotropy are included.

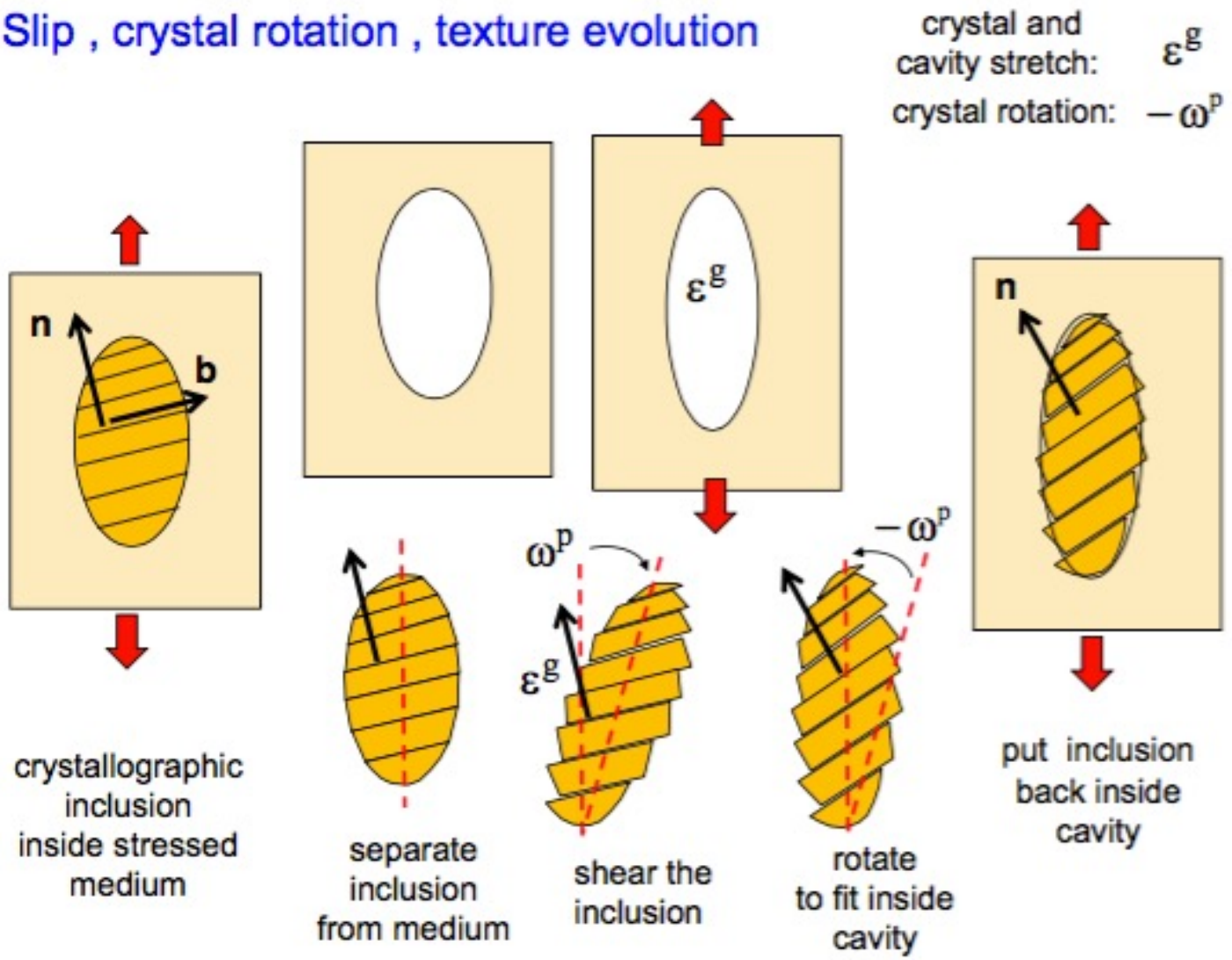
Eigenstrains and Eigenstresses



Self-Consistent Model

- Following slides contain information about a more sophisticated model (than the Taylor 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



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 the 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

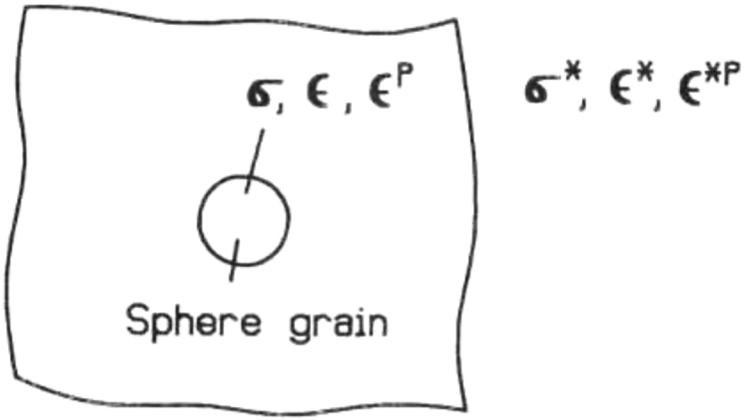


Fig. 11.6 Simple model of polycrystals

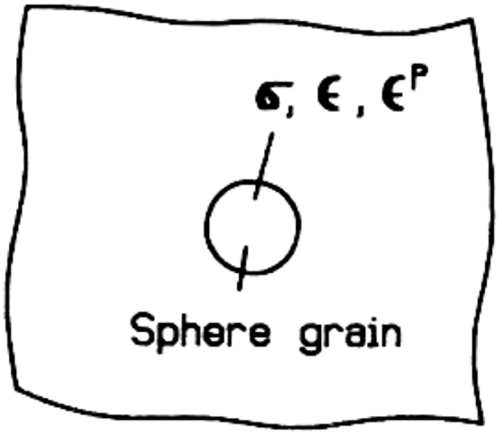
Budiansky and Wu's Model

- 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:

- Sphere (single crystal grain) embedded in a homogeneous polycrystal matrix.
- The grain and the matrix are elastically isotropic.



Khan & Huang

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

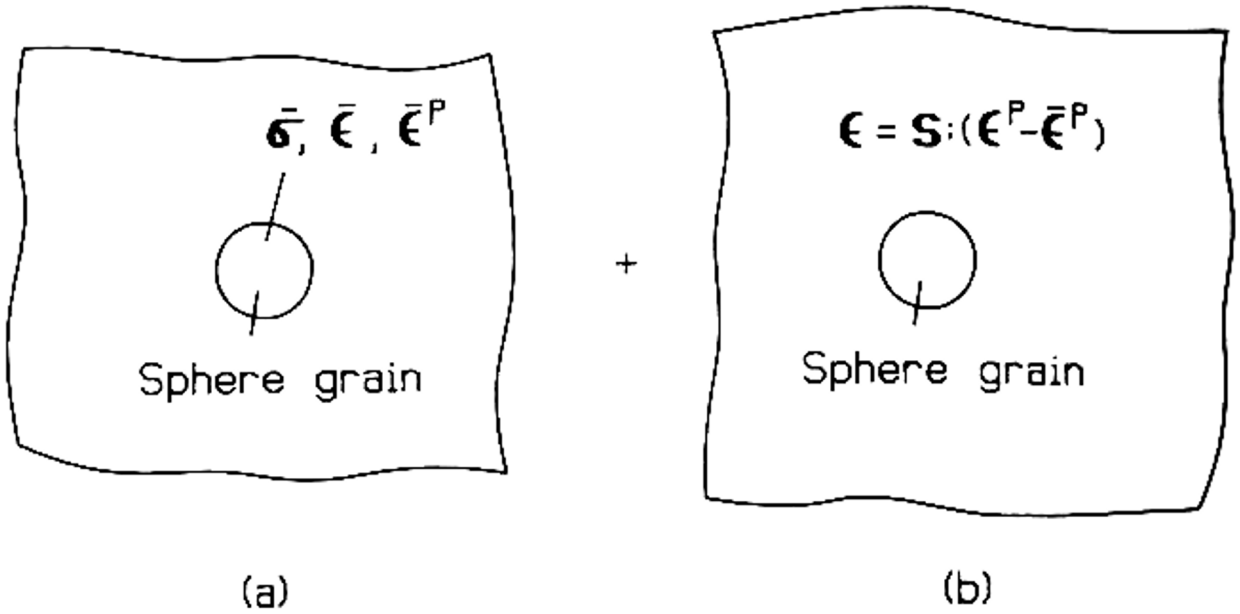
Fig. 11.6 Simple model of polycrystals

- 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, where the overbar indicates the polycrystal ave. and S is an Eshelby tensor



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:

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

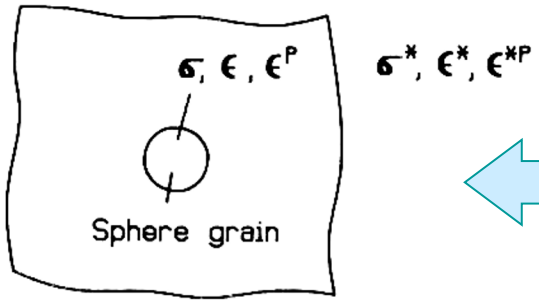


Fig. 11.6 Simple model of polycrystals

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

Khan & Huang

Kröner, Budiansky and Wu's Model

1.b – The sphere

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

- 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).

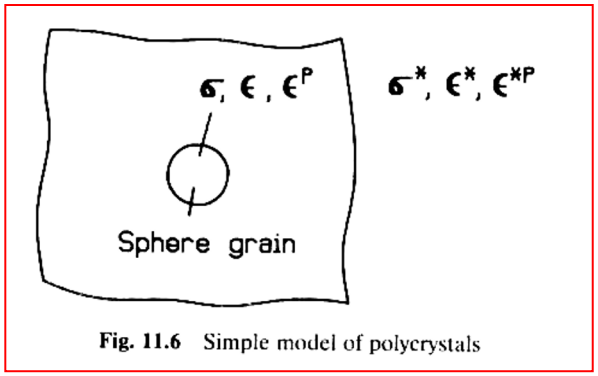
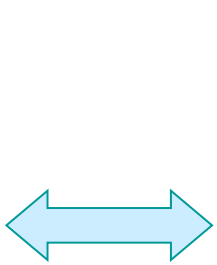


Fig. 11.6 Simple model of polycrystals



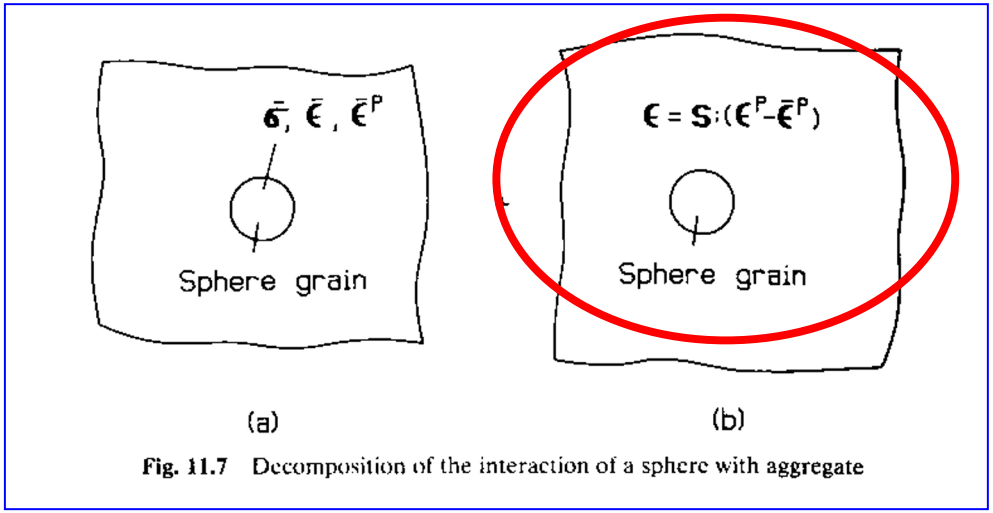


Fig. 11.7 Decomposition of the interaction of a sphere with aggregate

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

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

Where,

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

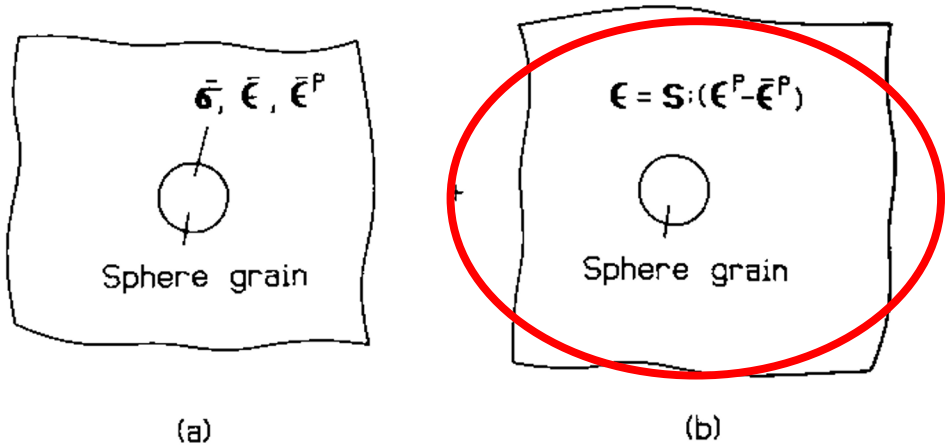


Fig. 11.7 Decomposition of the interaction of a sphere with aggregate

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

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

Given that,

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

where

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

The fraction β was shown earlier as S_{1212}

This leads to

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

Kröner, Budiansky and Wu's Model

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

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

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

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

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

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

ViscoPlastic-SelfConsistent code (VPSC)

- VPSC is based on the Taylor model (uniform plastic strain across a polycrystal) but modified to allow for interactions between each grain and the polycrystal in which it is embedded.
- There is *no microstructure* in VPSC: it works with just a set (list) of orientations. Therefore, there is no local interaction between a grain and some set of neighbor grains, only with the homogeneous effective medium (HEM).
- The modification allows the deformation of each grain to deviate from that of the polycrystal. The constraint on each grain is computed with Eshelby theory (for inclusions).
- Compared to any full-field (FE or FFT) computation with crystal plasticity, VPSC is an order of magnitude more efficient. For example, it is very useful for fitting Voce hardening parameters to experimental data. It is also very efficient for determining constitutive parameters such as CRSS values that evolve with strain for fitting to experimental texture data.

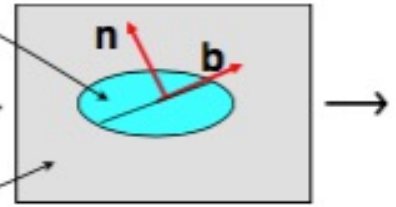
VPSC

- 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:

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 $\bar{\dot{\varepsilon}}'_{ij} = \bar{M}_{ijkl} \bar{\sigma}'_{kl}$



Solve stress equilibrium equation for inclusion in the homogeneous medium $\longrightarrow \sigma_{ij,j} = \frac{\partial \sigma_{i1}}{\partial x_1} + \frac{\partial \sigma_{i2}}{\partial x_2} + \frac{\partial \sigma_{i3}}{\partial x_3} = 0$

Connection between stress in inclusion/grain versus average stress

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

Avg stress= Macroscopic stress → Self consistent

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

Source: Carlos Tome, EFRC Summer School 2012

Assumptions for VPSC

Kocks, Tomé, Wenk: Ch. 8

(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.

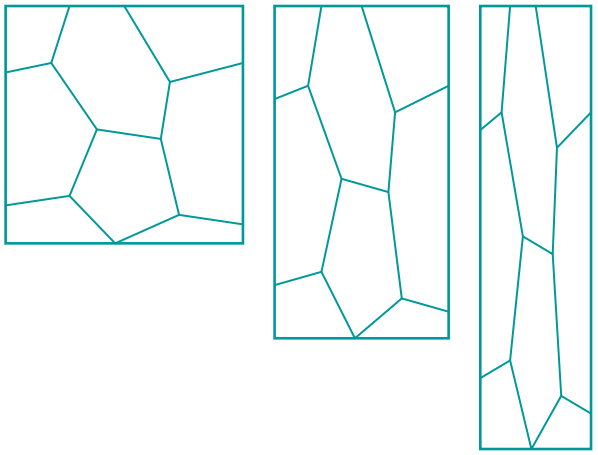
(iii) The deformation of the inclusion (or cluster) embedded in an effective medium has to fulfill local equilibrium and compatibility. In practice, except for the exact Eshelby solution for ellipsoidal inclusions in linear media (see the Appendix), these conditions cannot be fulfilled exactly for non-ellipsoidal 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

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

• 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

Source: Carlos Tome, EFRC Summer School 2012

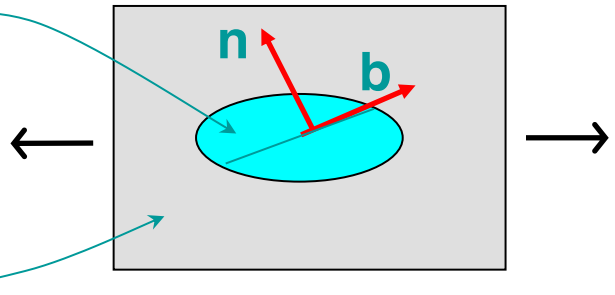
VISCO-PLASTIC SELF-CONSISTENT (VPSC) POLYCRYSTAL MODEL [1]

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

- Deviatoric constitutive response:

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

Homog. medium $\bar{\dot{\varepsilon}}'_{ij} = \bar{M}_{ijkl} \bar{\sigma}'_{kl}$



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

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

Source: Carlos Tome, EFRC Summer School 2012

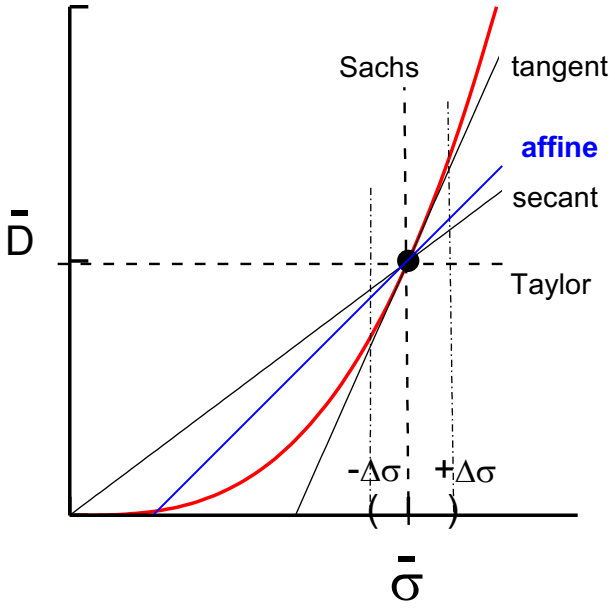
VPSC model → interaction equation

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

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

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

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



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

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 (different choices in vpsc7.in)

Source: Carlos Tome, EFRC Summer School 2012

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:

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

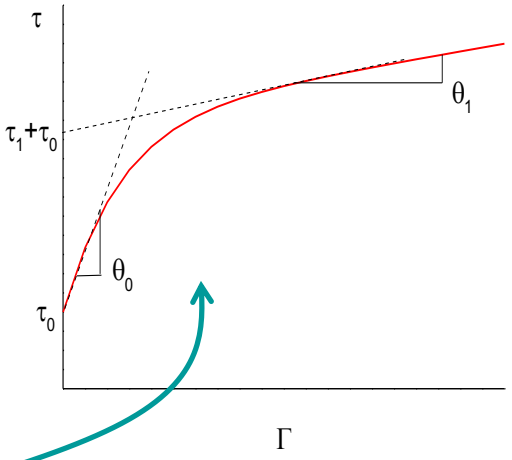
Source: Carlos Tome, EFRC Summer School 2012

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

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

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

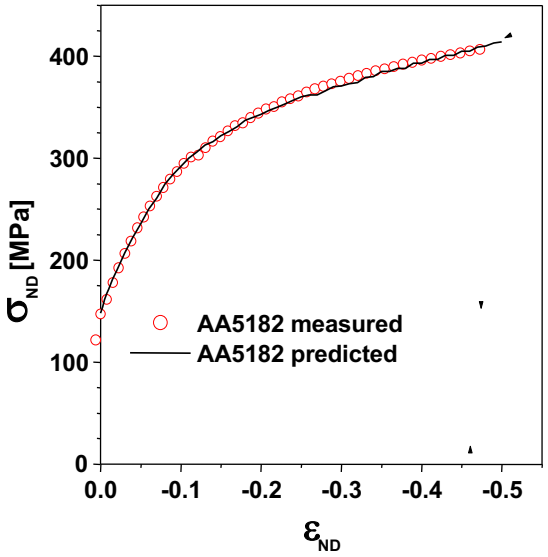


If latent hardening parameters h are considered the CRSS is incrementally updated as:

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

else:

$$\Delta\tau^s = \frac{d\hat{\tau}(\Gamma)}{d\Gamma} \Delta\Gamma$$



Source: Carlos Tome, EFRC Summer School 2012

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)

Source: Carlos Tome, EFRC Summer School 2012

Running VPSC → control file VPSC7.IN

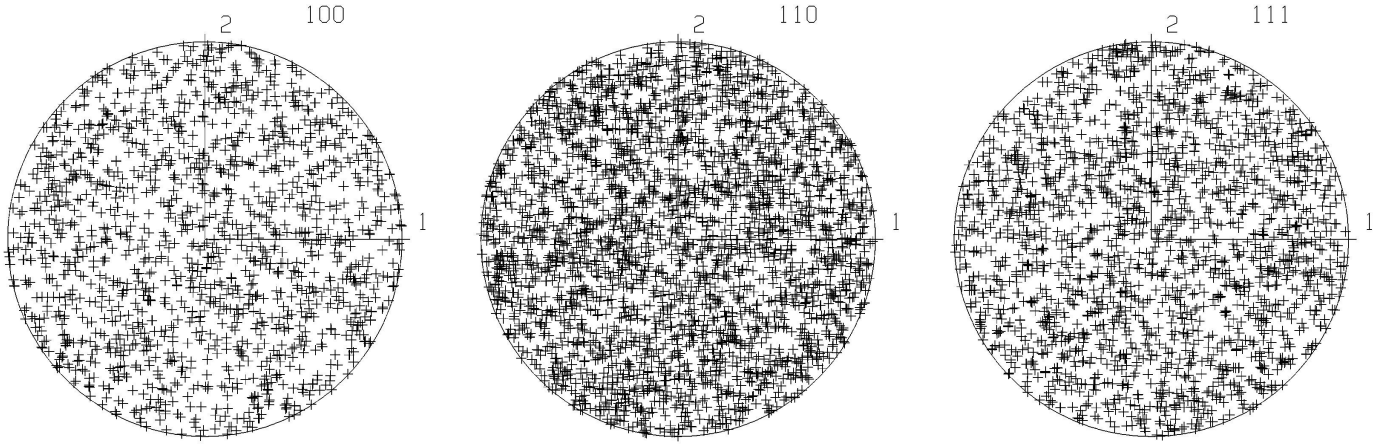
```
. . . . . .
0                       grain shape and orient ctrl (ishape=0 to 4)
1.0  1.0  1.0           initial ellipsoid ratios (dummy if ishape=4)
0.0  0.0  0.0           init Eul ang ellips axes (dummy if ishape=3,4)
* name and path of texture file (filetext)
example1\rand500.tex
* name and path 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
```

Source: Carlos Tome, EFRC Summer School 2012

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
. . . . . .
. . . . . .
```



Source: Carlos Tome, EFRC Summer School 2012

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.               |
```

Source: Carlos Tome, EFRC Summer School 2012

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
   ..........     .........
```

Source: Carlos Tome, EFRC Summer School 2012

EXAMPLE 1: TENSION & COMPRESSION of FCC

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:

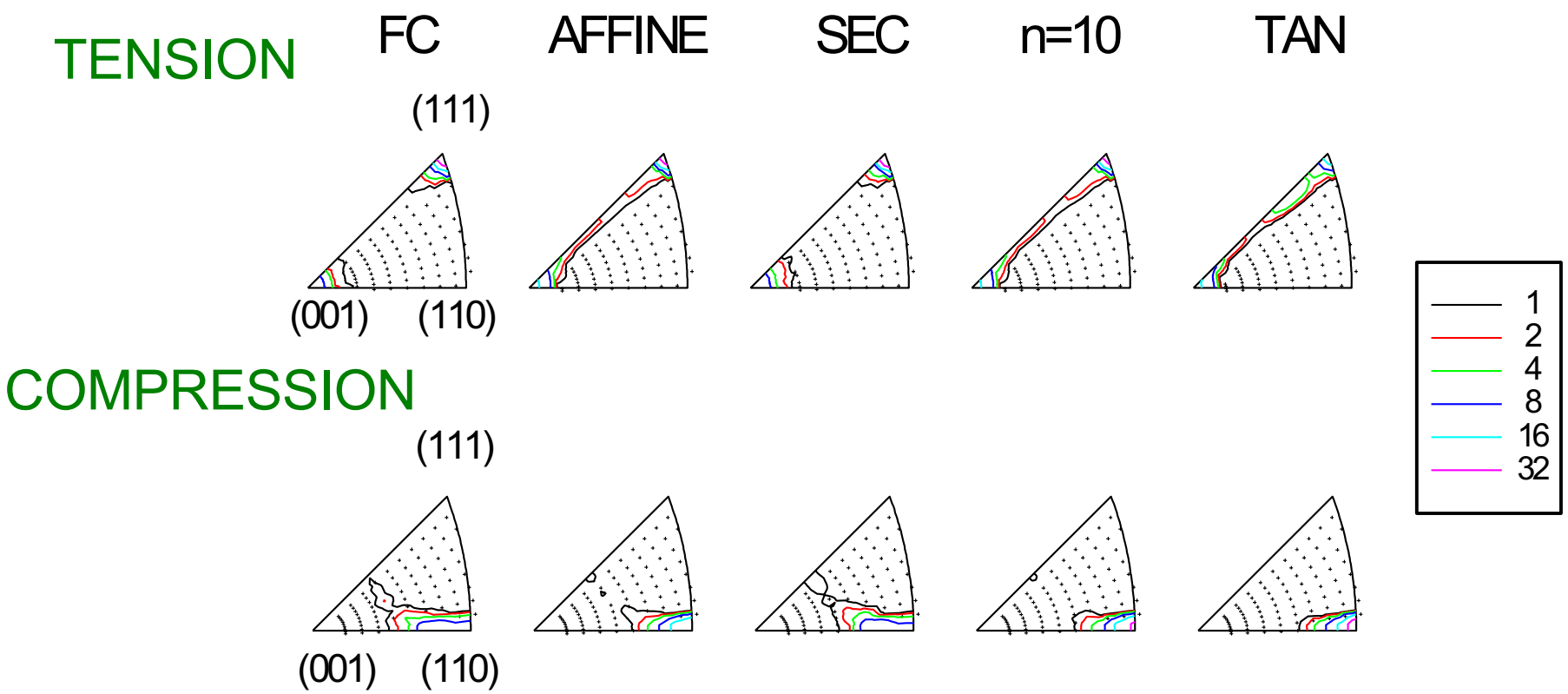
The imposed velocity gradient is symmetric and equal to the strain rate tensor:

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

Source: Carlos Tome, EFRC Summer School 2012

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)



Source: Carlos Tome, EFRC Summer School 2012

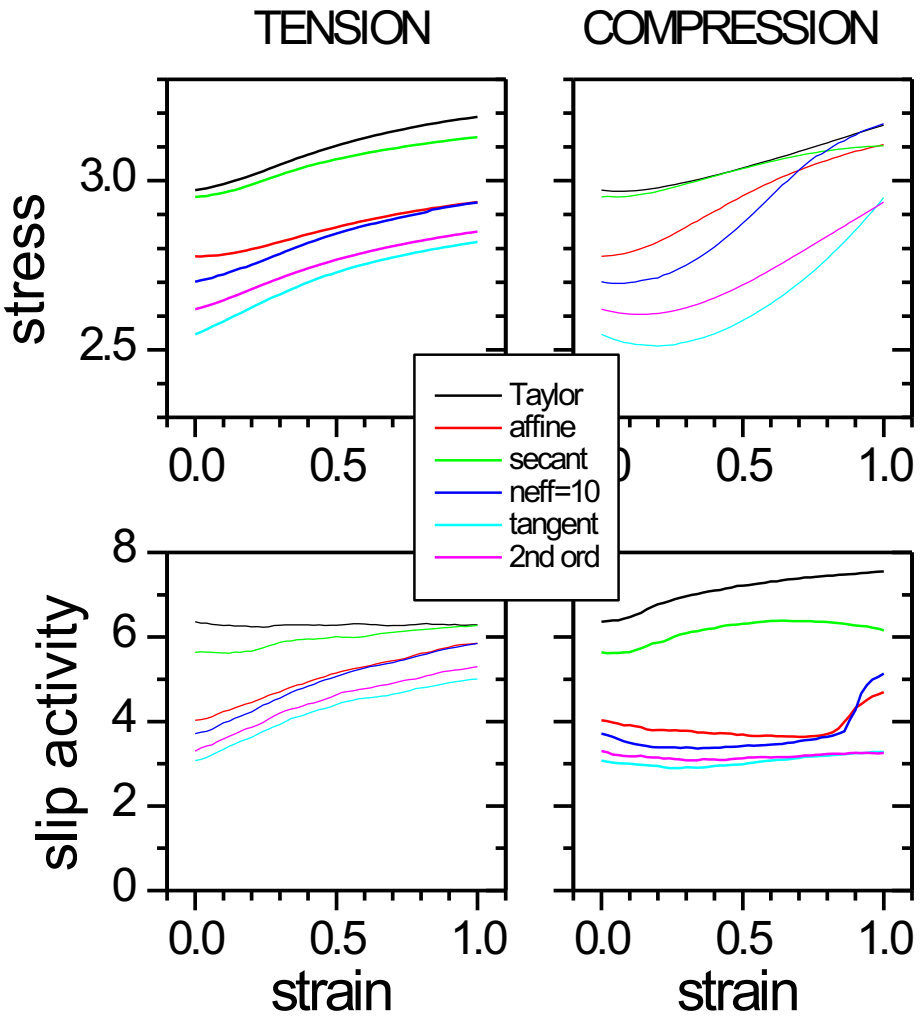
EXAMPLE 1: TENSION & COMPRESSION of FCC → STRESS

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



Source: Carlos Tome, EFRC Summer School 2012

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):

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

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

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

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

Source: Carlos Tome, EFRC Summer School 2012

EXAMPLE 2: ROLLING of FCC → PROCESS FILE

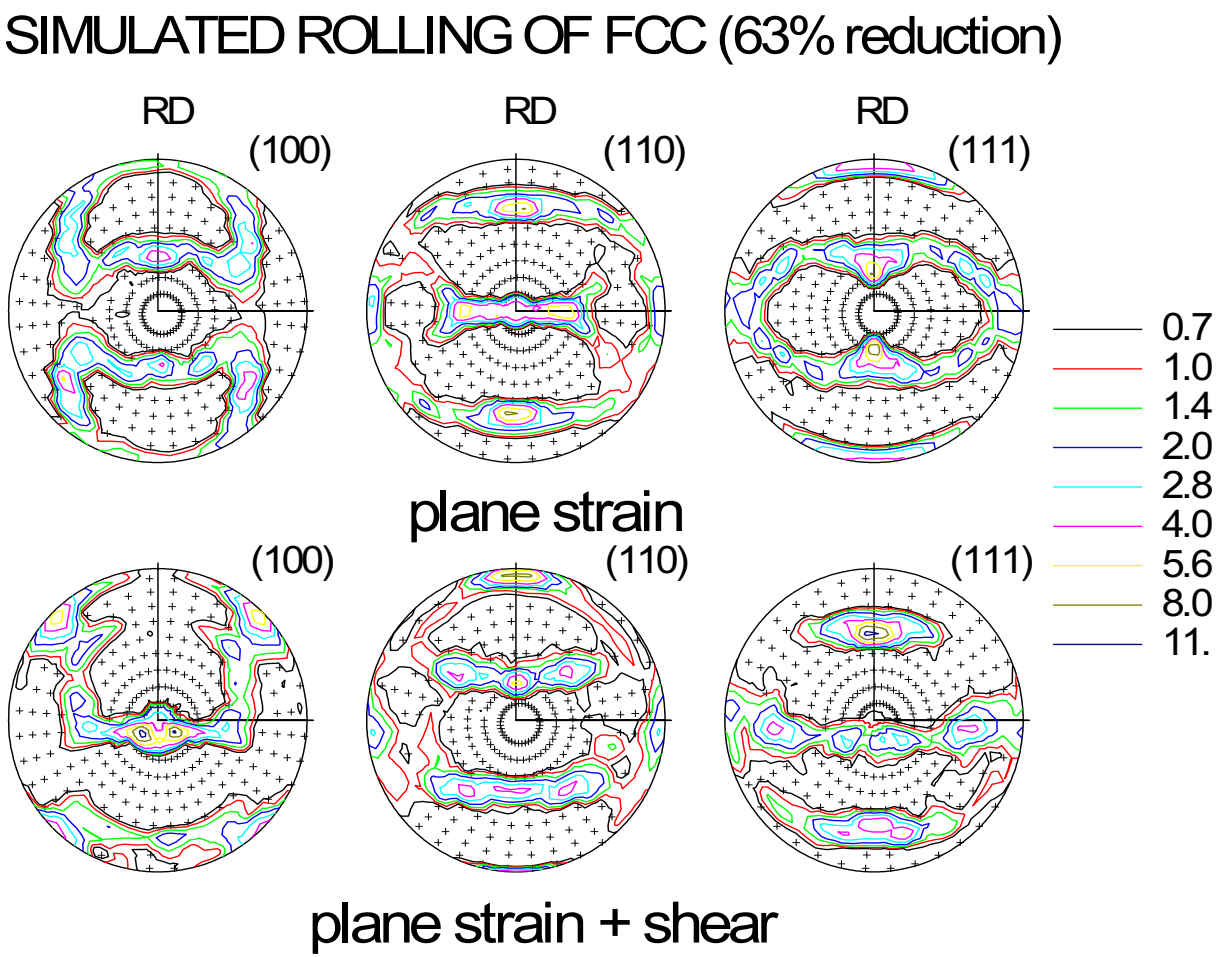
File VPSC7.INa enforces rolling followed by a yield locus calculation and a Lankford and Young modulus calculation.

```
. . . . . .
. . . . . .
*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
```

Source: Carlos Tome, EFRC Summer School 2012

EXAMPLE 2: ROLLING of FCC → FINAL TEXTURE

The superimposed shear breaks the orthotropic symmetry of the rolling texture



Source: Carlos Tome, EFRC Summer School 2012

EXAMPLE 2: ROLLING of FCC → CHARACTERIZATION

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

the yield locus,

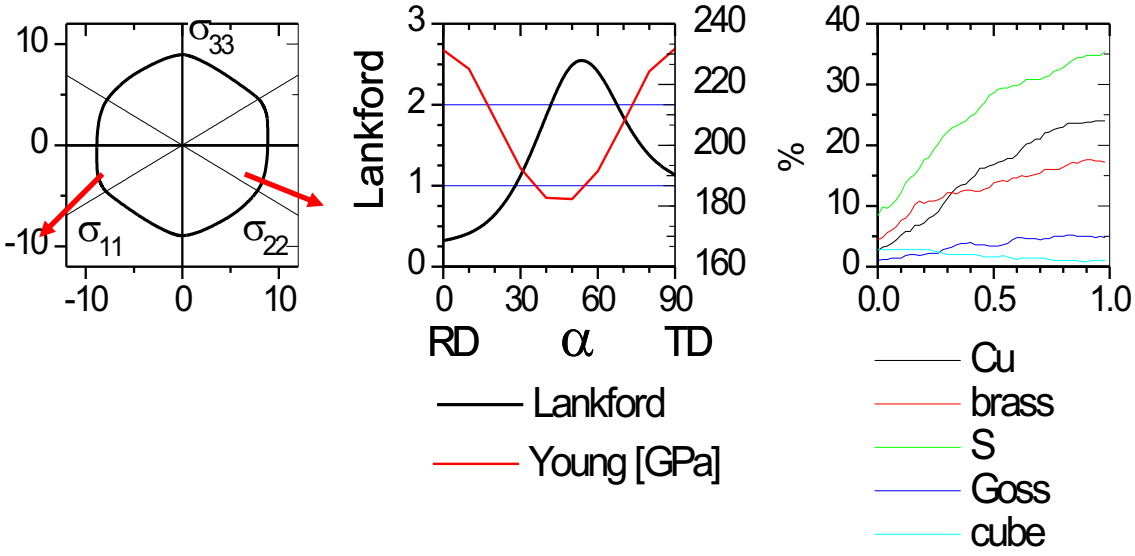
the in-plane anisotropy (Lankford),

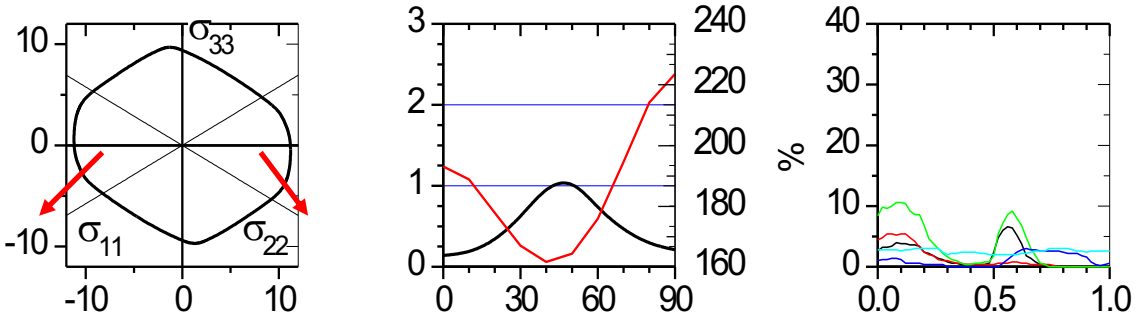
the directional Young modulus,

the final rolling components,

are different.

Plane strain





Plane strain + shear

Source: Carlos Tome, EFRC Summer School 2012

EXAMPLE 5: TORSION of FCC → fixed ends

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

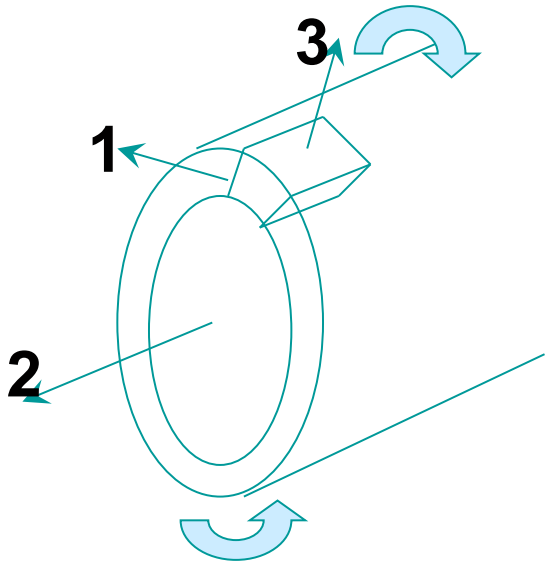
Deformation by slip in the <110> direction and on {111} crystallographic planes, up to $\varepsilon_{12} = 2.0$

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 $\varepsilon_{22} = 0.$
the hoop and radial stress components are imposed to zero

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

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



Source: Carlos Tome, EFRC Summer School 2012

EXAMPLE 5: TORSION of FCC → process sequence

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
```

Source: Carlos Tome, EFRC Summer School 2012

EXAMPLE 5: TORSION of FCC → free ends

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

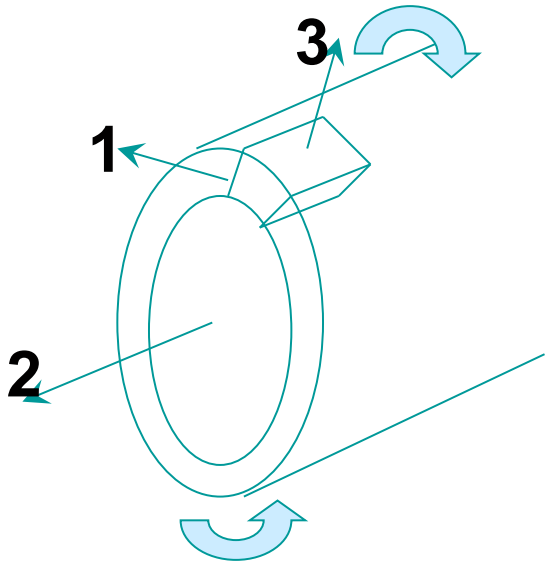
Deformation by slip in the <110> direction and on {111} crystallographic planes, up to $\varepsilon_{12} = 2.0$

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

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

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

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

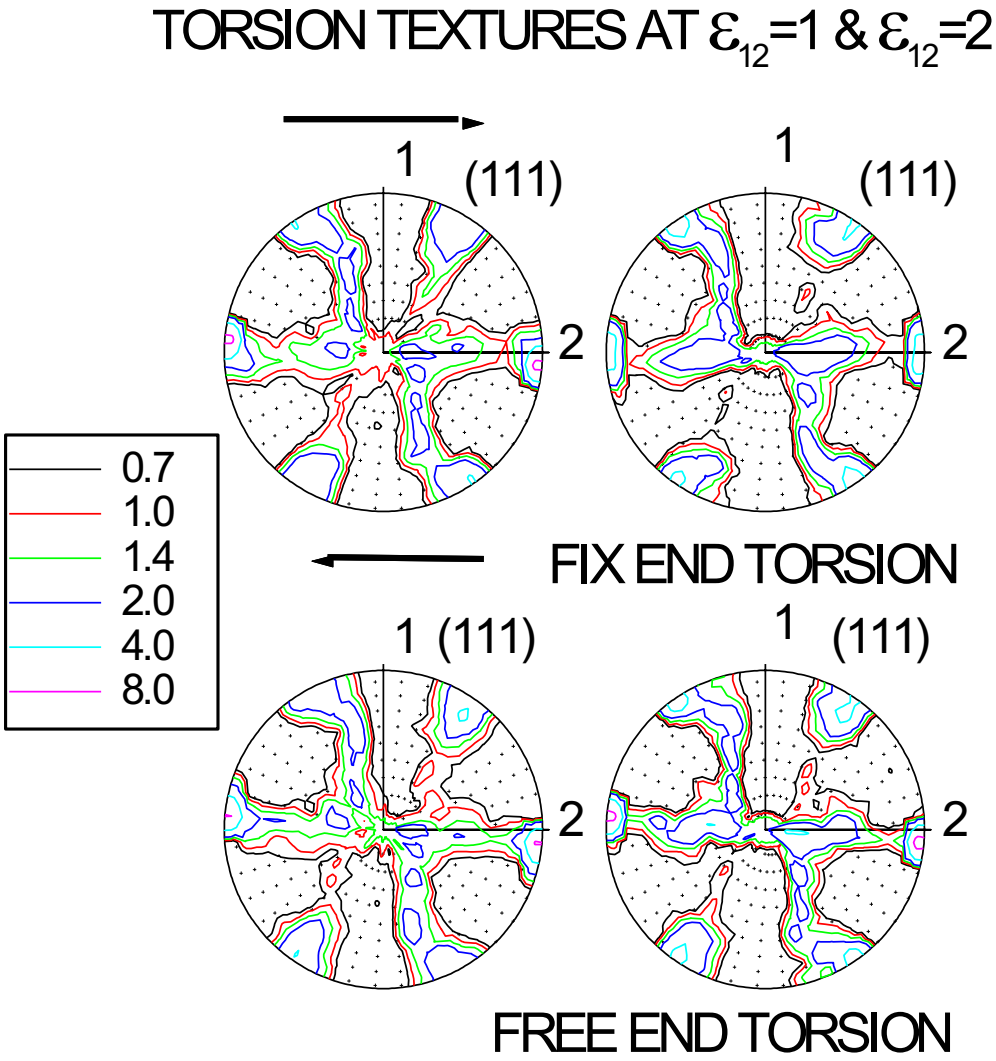


Source: Carlos Tome, EFRC Summer School 2012

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.



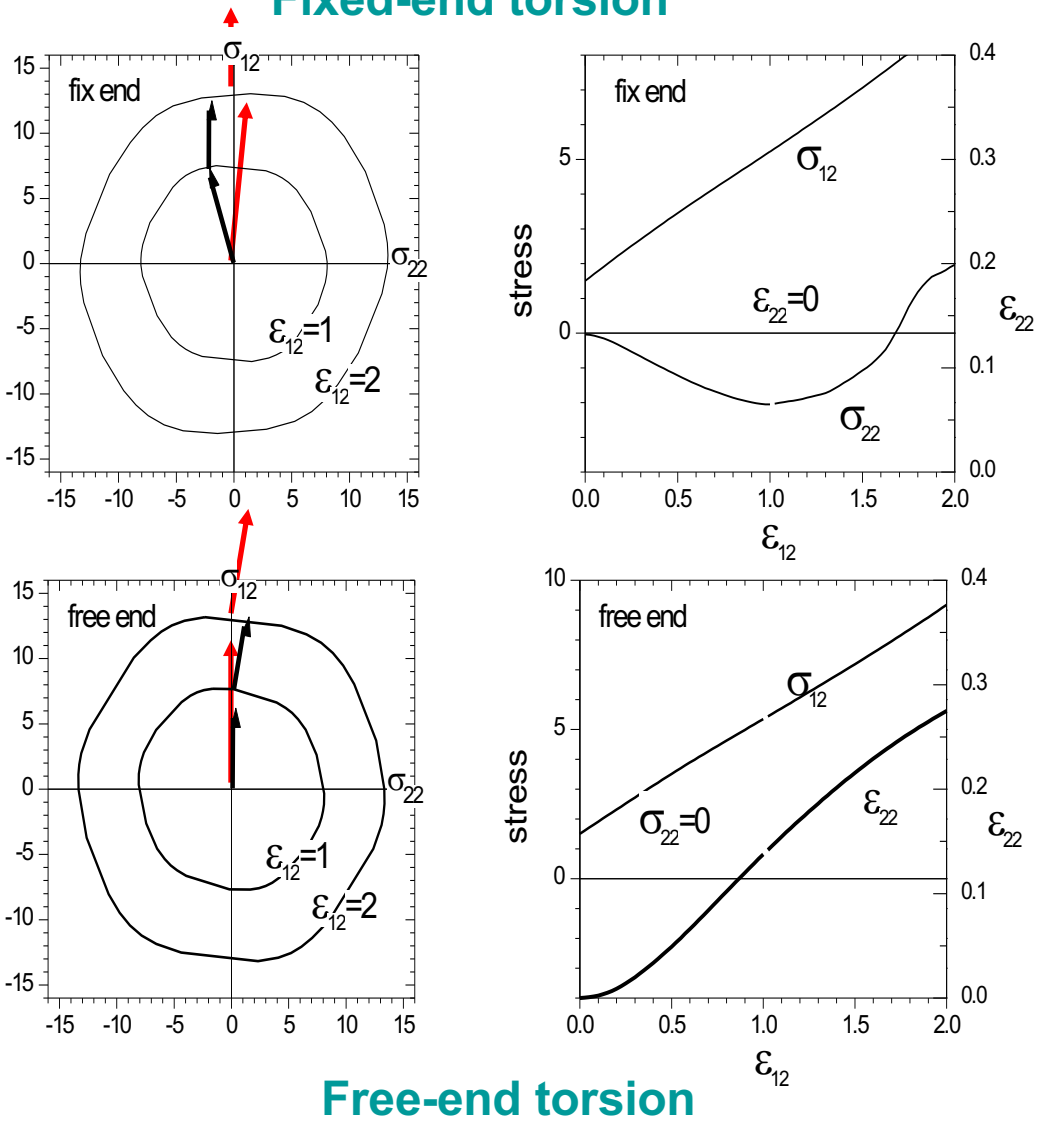
Source: Carlos Tome, EFRC Summer School 2012

EXAMPLE 5: TORSION of FCC → CHARACTERIZATION

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.

Fixed-end torsion



Source: Carlos Tome, EFRC Summer School 2012

Plotting Results from VPSC: packages and installation

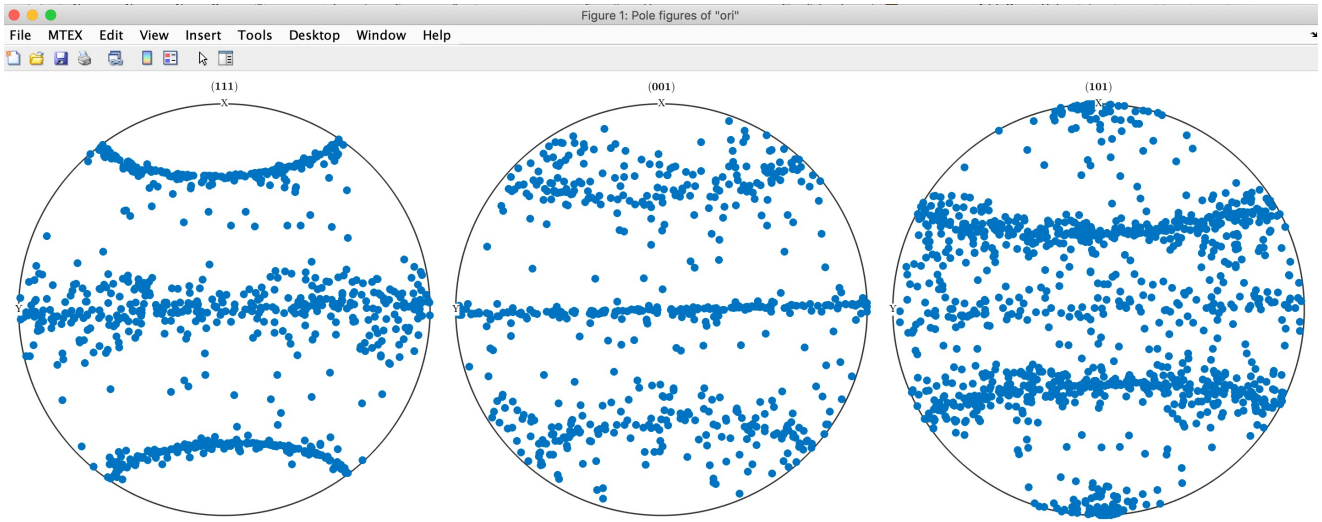
- Suggestion: use MTEX, which is available as an open source package within MATLAB. MATLAB is freely available for academic use for members of CMU.
- Step 1: install MATLAB
- Step 2: search on “github mtex” to find the webpage. Download it as a zip file. Unpack the zip.
- Step 3: open MATLAB and add the path to the MTEX folder.

Specific Directions for M1 Macs

- Here are the directions from the Apple developer website for how to get TF up and running on an M1 mac. It suggests that you use miniconda rather than anaconda, so there might be some complications there. I was running into issues on my intel Mac because python was being compiled on an older version of clang. I would run this line "python -c "import platform; print(platform.mac_ver())"" to see which version of clang python was compiled on the first line needs to be either 11 or 12; I can't totally remember. My version that doesn't work is 10.13 so I think anything higher than that will work because that's when M1 was introduced. I doubt ARM64 compiled python versions would be on any clang from before that, so hopefully, this works for you without too much trouble.
- Courtesy of Gregory Wong, CMU, Feb. 2022

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')