Microstructure Mechanics

Crystal Mechanics

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Contact, website and class days

Date / Location	Topics	Lecturer
15. April 2016 **IMM / RWTH**	Introduction to materials micromechanics, multiscale problems in micromechanics, case studies, crystal structures and defects, relation to products and manufacturing	Raabe
22. April 2016 **IMM / RWTH**	Crystal structures, dislocation statics, crystal dislocations, dislocation dynamics	Raabe
29. April 2016 **IMM / RWTH**	Dislocations, crystalline anisotropy and crystal mechanics in hexagonal metals	Sandlöbes
6. May 2016 **IMM / RWTH**	No classes	-
13. May 2016 **IMM / RWTH**	Fracture mechanics Introduction to FEM	Shanthraj
20. May 2016 **IMM / RWTH**	Athermal phase transformations in micromechanics	Wong
27. May 2016 **IMM / RWTH**	No classes	-
3. June 2016 **IMM / RWTH**	Crystal micromechanics, single crystal mechanics, yield surface mechanics, polycrystal models, Taylor model, Integrated micromechanical experimentation and simulation for complex alloys, hydrogen embrittlement	Raabe
10. June 2016 **IMM / RWTH, 12:15**	Micromechanics of polymers and biological (natural) composites	Raabe
17. June 2016 **IMM / RWTH, 12:15**	Applied micromechanics: multiphase and composite material design	Springer

Overview

- Single crystal yield surface
- Empirical yield surface
- Taylor model for the mechanics of polycrystals
- Examples

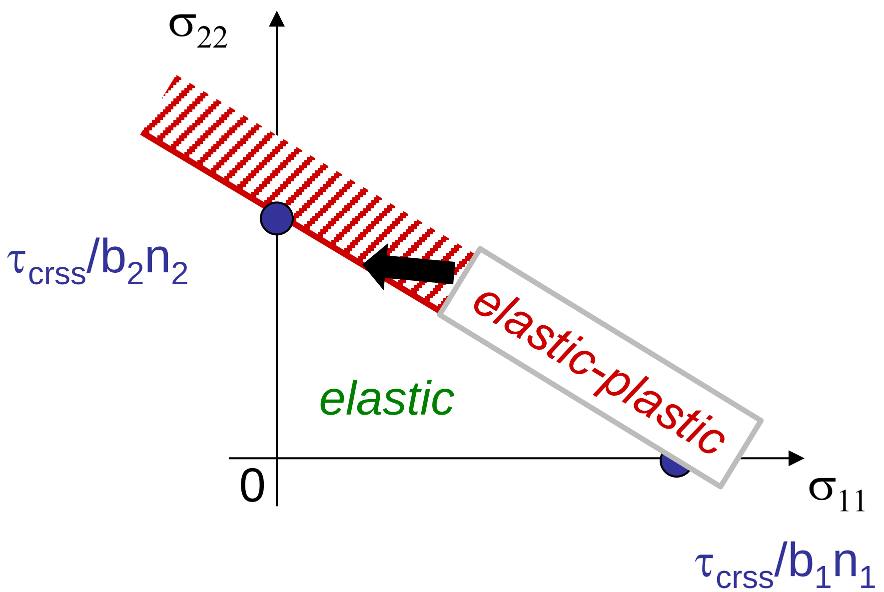
Single crystal plasticity: constructing the yield surface

- Yield criterion for single slip:

$$\sigma_{ij} b_i n_j = \tau_{crss}$$

- In 2D this becomes ($\sigma_1 \equiv \sigma_{11}$:

$$\sigma_{11} b_1 n_1 + \sigma_{22} b_2 n_2 = \tau_{crss}$$



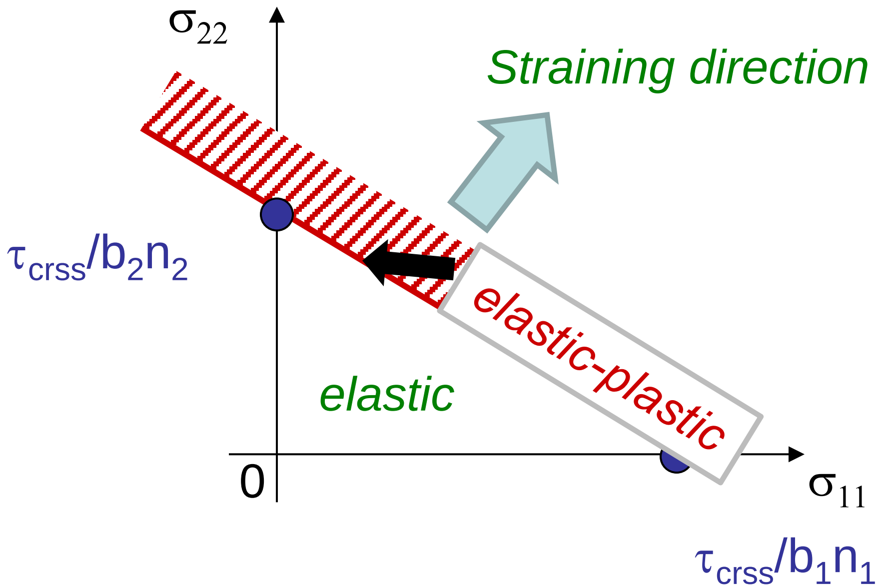
What is the straining direction?
The strain increment is given by:

$$d\varepsilon = \Sigma_s \, d\gamma^{(s)} b^{(s)} n^{(s)}$$

2D case:

$$d\varepsilon_1 = d\gamma \, b_1 n_1; \; d\varepsilon_2 = d\gamma \, b_2 n_2$$

vector perpendicular to the line for yield

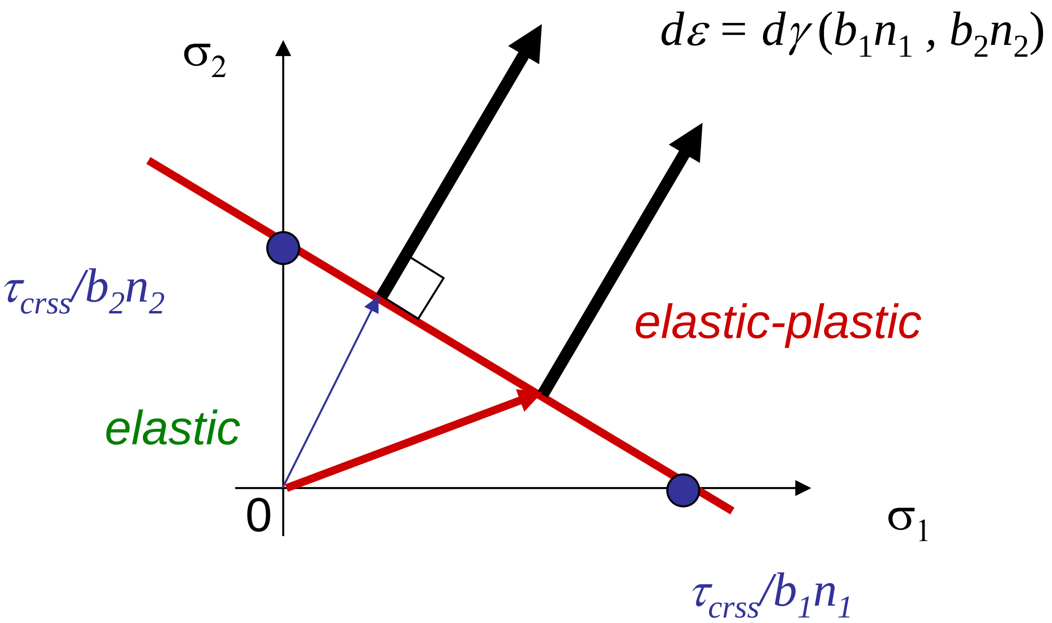


Single crystal plasticity: constructing the yield surface

straining direction in stress space

normality rule for crystallographic slip

Any given stress state can in a crystal in large-strain elasto-plasticity act only in the form of shear (except hydrostatic effects)

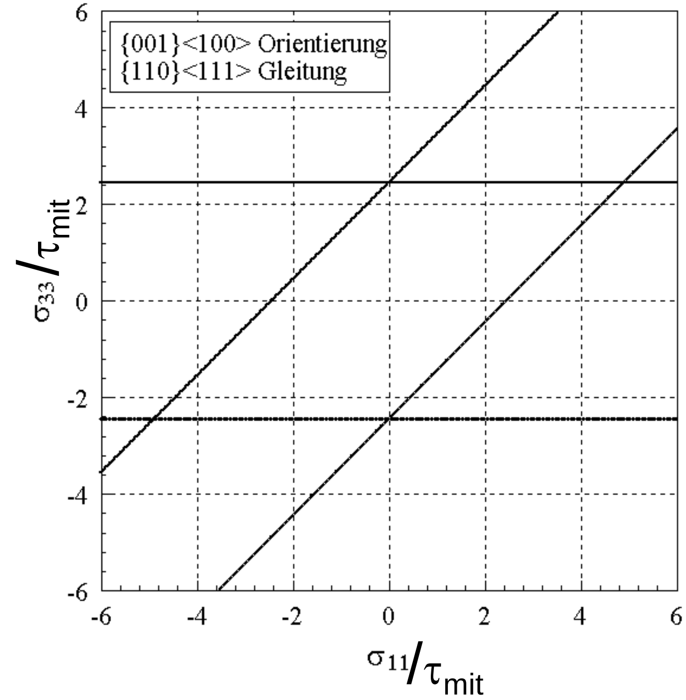


slip system s

$$n_i^s \,,\, b_i^s$$

orientation factor for s

$$m_{ij}^s = n_i^s \, b_j^s$$



symmetric part

$$m_{ij}^{sym,s} = \frac{1}{2}\left(n_i^s \, b_j^s + n_j^s \, b_i^s\right)$$

rotate crystal into sample

$$m_{kl}^s = a_{ki}^c \, n_i^s \; a_{lj}^c \, b_j^s$$

symmetric part

$$m_{kl}^{sym,s} = \frac{1}{2}\left(a_{ki}^c \, n_i^s \; a_{lj}^c \, b_j^s + a_{lj}^c \, n_j^s \; a_{ki}^c \, b_i^s\right)$$

yield surface
(active systems)

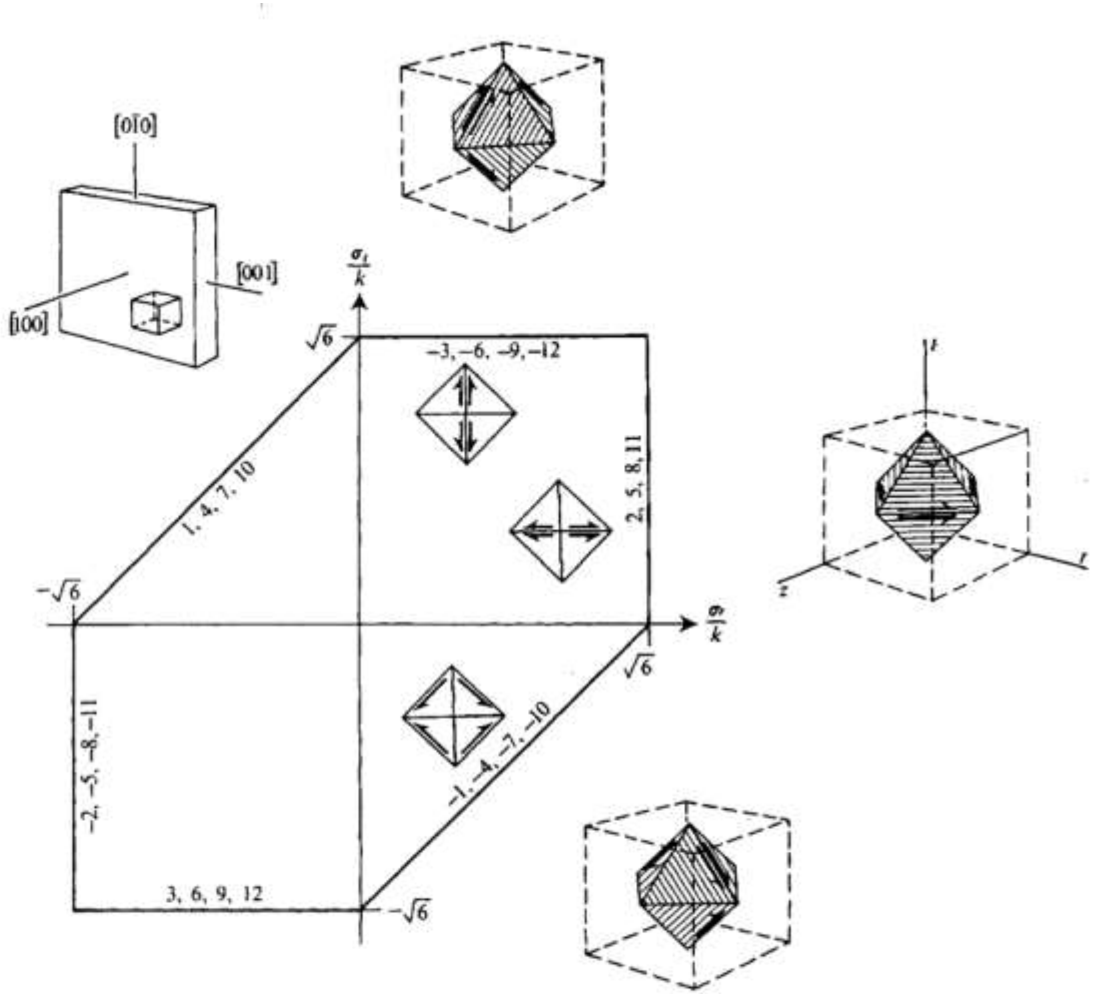
$$m_{kl}^{sym,s=aktiv} \sigma_{kl} = \sigma_{aufg}^s = \tau_{krit,(+)}^{s=aktiv}$$

$$m_{kl}^{sym,s=aktiv} \sigma_{kl} = \sigma_{aufg}^s = \tau_{krit,(-)}^{s=aktiv}$$

(non-active systems)

$$m_{kl}^{sym,s=inaktiv} \sigma_{kl} = \sigma_{aufg}^s < \tau_{krit,(\pm)}^{s=inaktiv}$$

Cube texture component:
(001)[100]



Active slip system:

$$\tau^{\alpha} = \tau_{\text{crit}}$$

$$\tau^{\alpha} \approx \boldsymbol{T}_{\text{e}} \cdot \boldsymbol{S}_0{}^{\alpha}$$

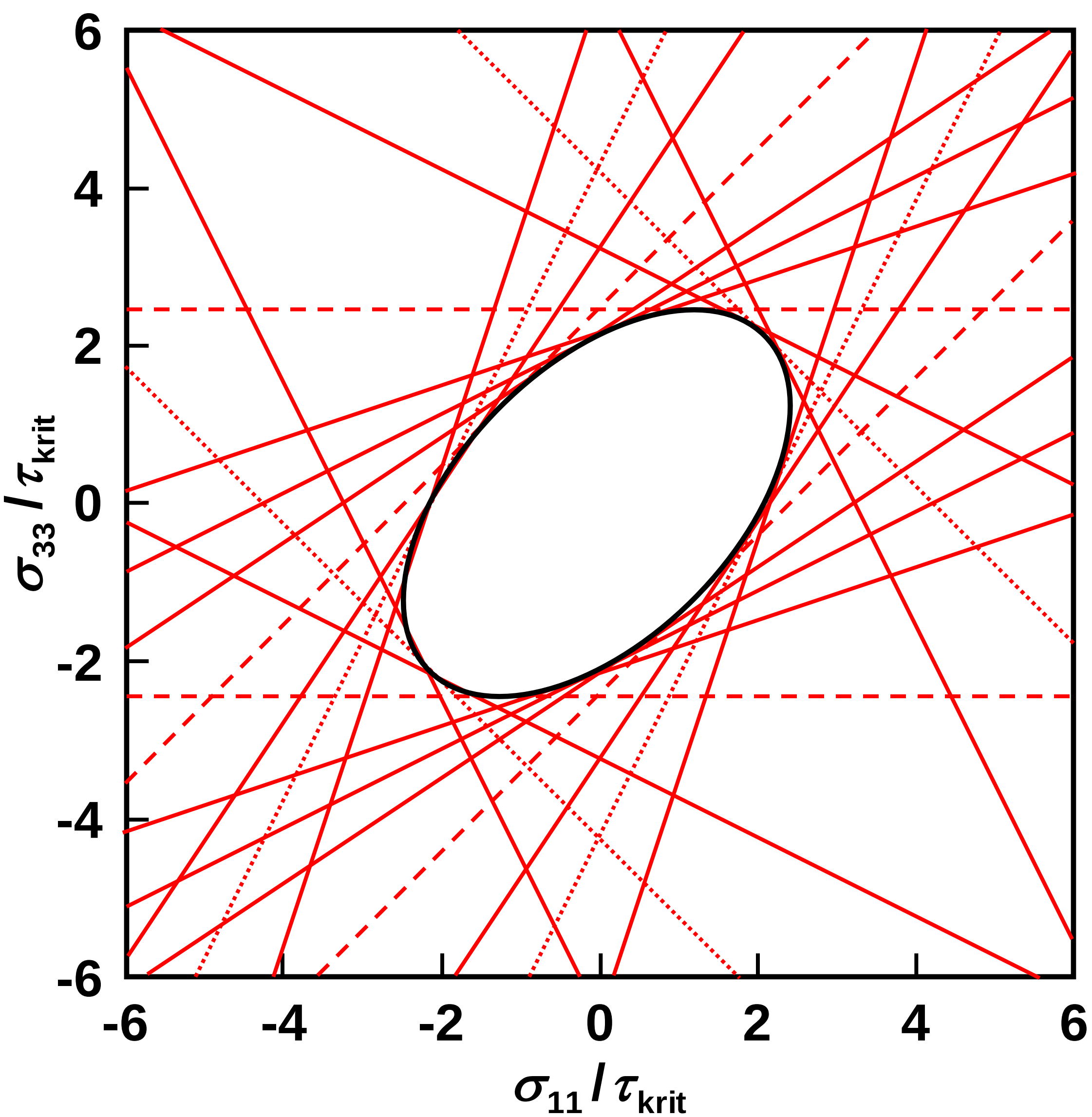
with $\boldsymbol{S}_0{}^{\alpha} = \boldsymbol{m}_0{}^{\alpha} \otimes \boldsymbol{n}_0{}^{\alpha}$

bcc 48 slip systems
orientation {001}<100>

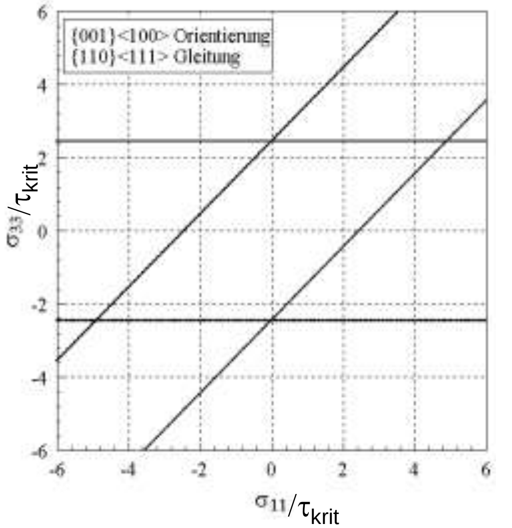
12 x {110}<111> (dashed line)

12 x {112}<111> (dotted line)

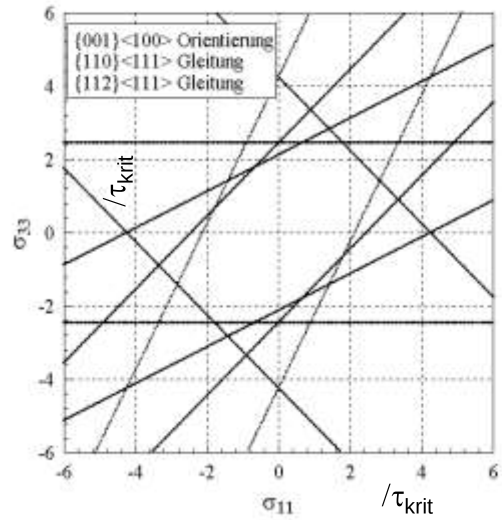
24 x {123}<111> (solid line)



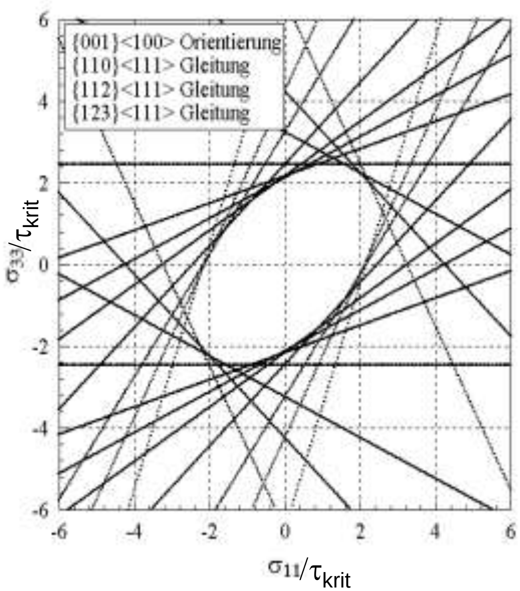
Single crystal plasticity: constructing the yield surface



FCC, BCC
12 systems
section



BCC
24 systems
section



BCC
48 systems
section

yield surface, bcc

single crystal, bcc, (001)[100]

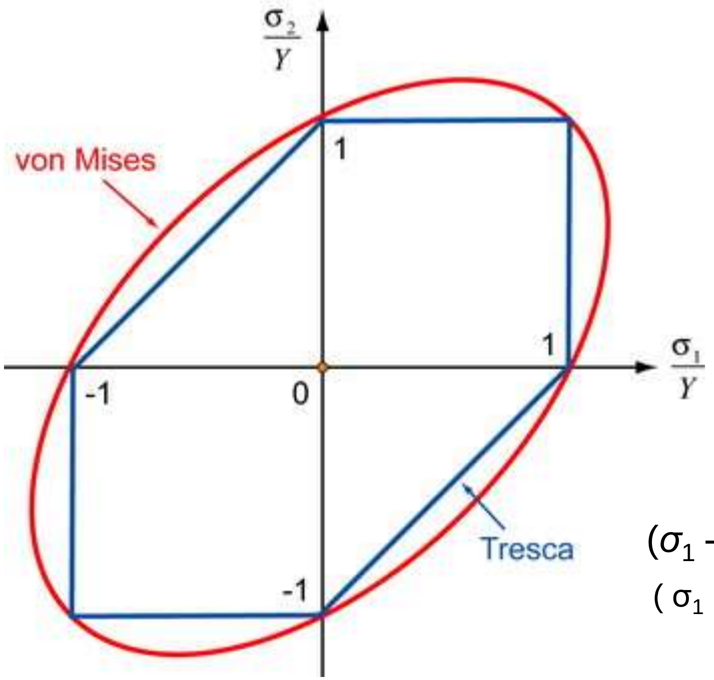
Macroscopic – empiricial yield criteria

Yield criterion: determine the critical stress required to cause permanent deformation

Many different macroscopic yield criteria

σ_{ij} stress acting on a solid
σ1, σ2, σ3 principal values of stress tensor
Y yield stress of the material in uniaxial tension

$$(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_3-\sigma_1)^2=\text{constant}$$

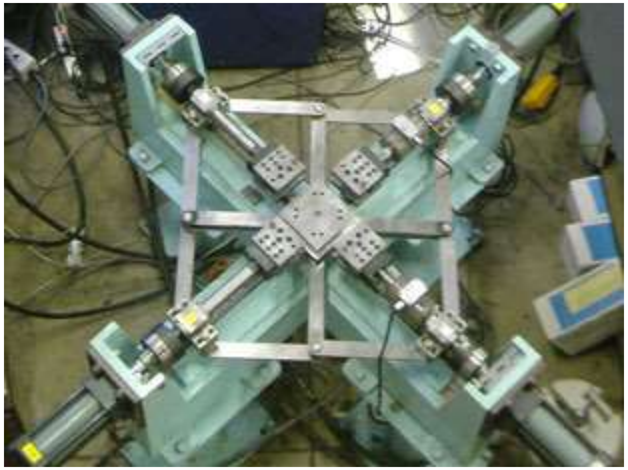


$$(\sigma_1-\sigma_3)=Y$$

$$(\sigma_1>\sigma_2>\sigma_3)$$

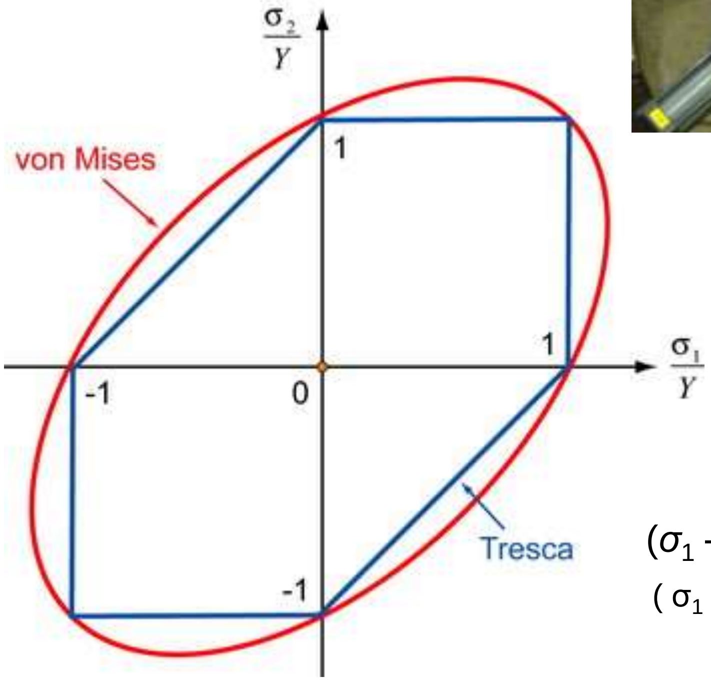
Yield criterion: determine the critical stress required to cause permanent deformation

Many different macroscopic yield criteria



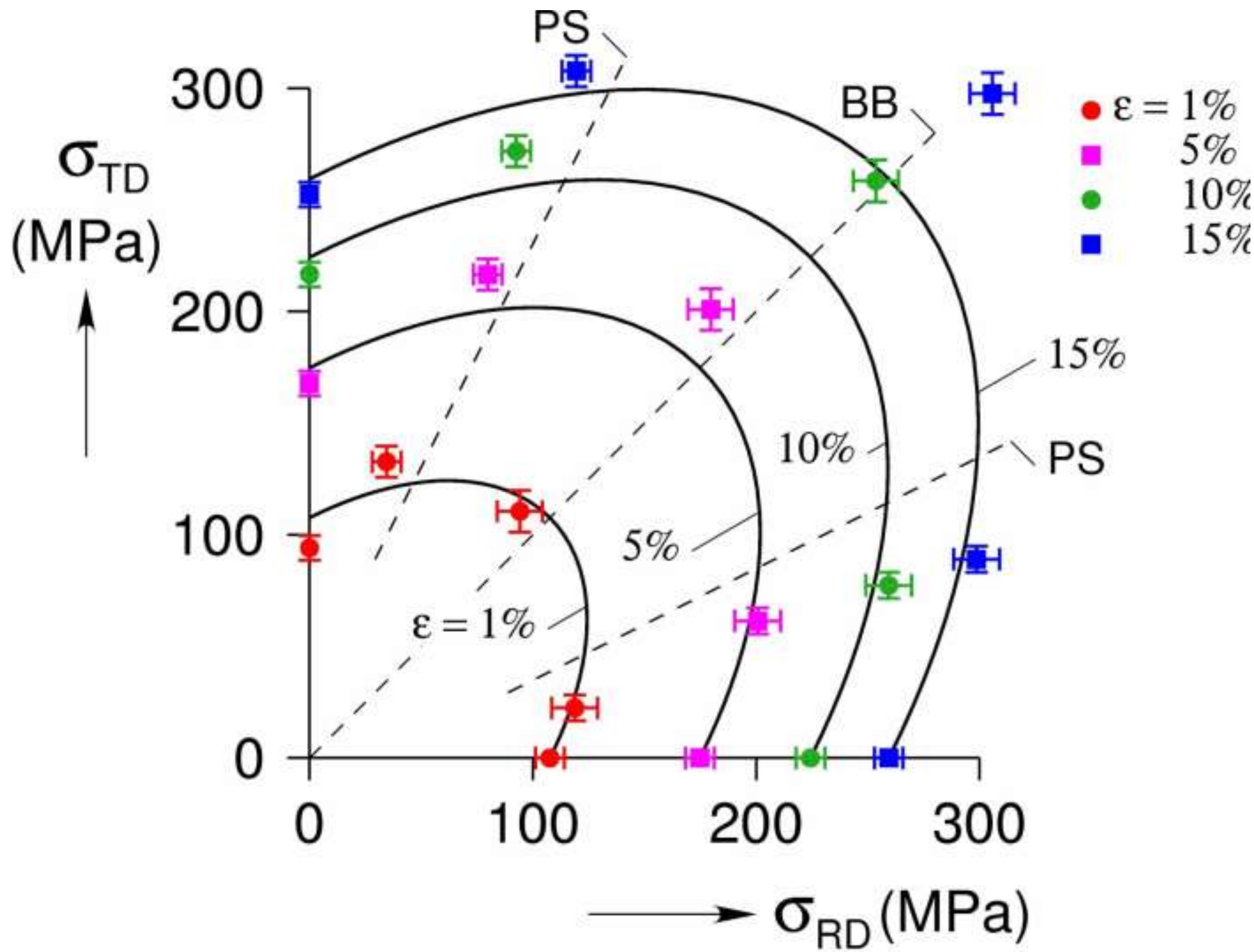
σ_{ij} stress acting on a solid
$\sigma 1$, $\sigma 2$, $\sigma 3$ principal values of stress tensor
Y yield stress of the material in uniaxial tension

$$(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_3-\sigma_1)^2=\text{constant}$$



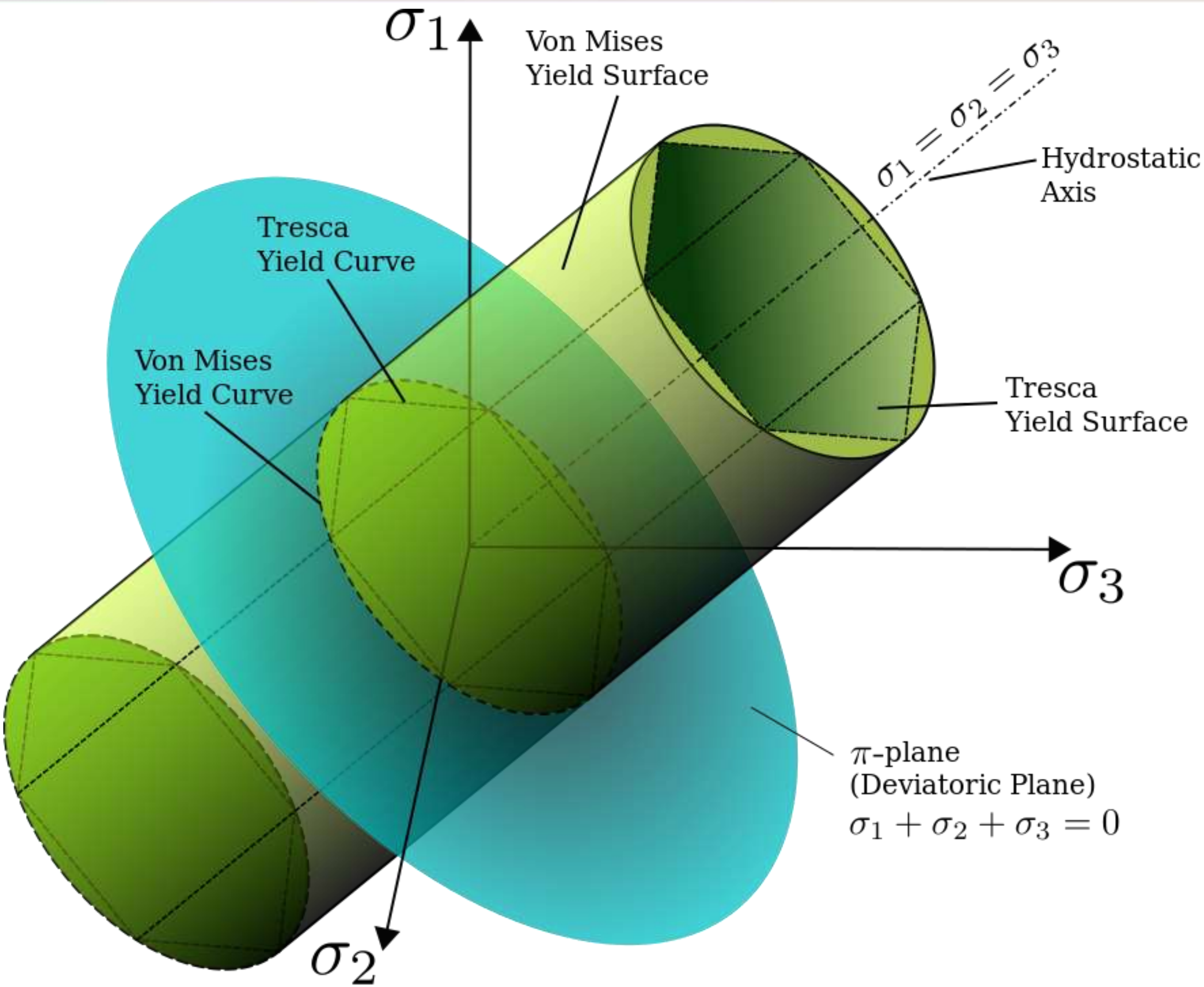
$$(\sigma_1 - \sigma_3) = Y$$

$$(\sigma_1 > \sigma_2 > \sigma_3)$$



PS
BB
$\varepsilon = 1\%$
5%
10%
15%
σ_{TD} (MPa)
σ_{RD} (MPa)
0
100
200
300

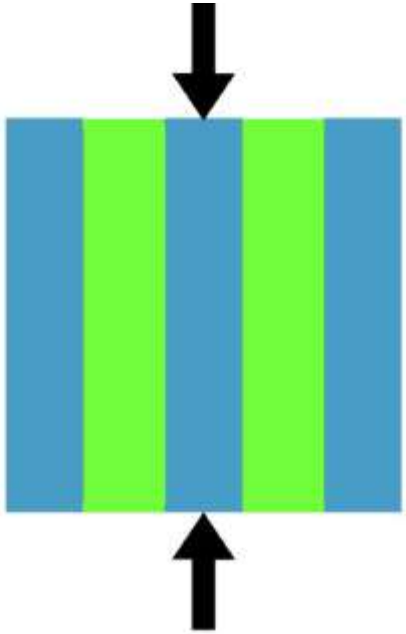
Macroscopic yield criteria



- How does that work for bicrystals ?
- Two extreme cases :
- iso-strain (Taylor)
- iso-stress (Schmid)

Roters et al. Acta Mater. 58 (2010)

Iso-stress and iso-strain: general approach

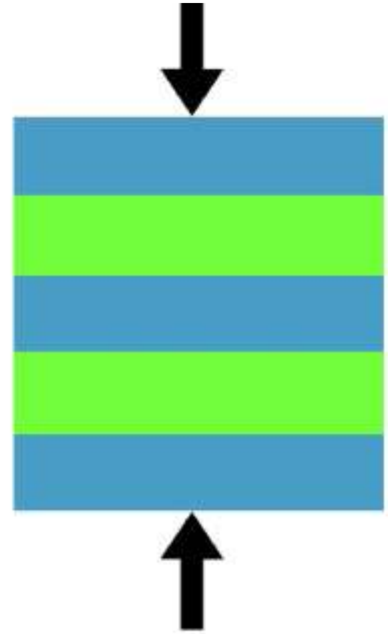


Isostrain

$$\varepsilon = \varepsilon_s = \varepsilon_d$$

$$\sigma = \sigma_s + \sigma_d$$

Displacement continuity across layers



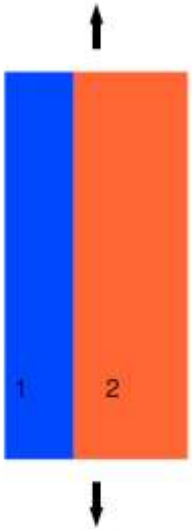
Isostress

$$\varepsilon = \varepsilon_s + \varepsilon_d$$

$$\sigma = \sigma_s = \sigma_d$$

Stress continuity across layers

Bounding Case - Isostrain



$$\epsilon_1=\epsilon_2=\epsilon_{tot}$$
$$\sigma_1=E_1\epsilon_1=E_1\epsilon_{tot} \quad ; \quad \sigma_2=E_2\epsilon_2=E_2\epsilon_{tot}$$
$$P_1=A_1\sigma_1=A_1E_1\epsilon_{tot} \quad ; \quad P_2=A_2\sigma_2=A_2E_2\epsilon_{tot}$$
$$P_{tot}=P_1+P_2=\epsilon_{tot}(A_1E_1+A_2E_2)$$
$$\sigma_{tot}=\frac{P_{tot}}{A_1+A_2}=\epsilon_{tot}\left(\frac{A_1}{A_1+A_2}E_1+\frac{A_2}{A_1+A_2}E_2\right)$$
$$\sigma_{tot}=(f_1E_1+f_2E_2)\epsilon_{tot}$$
$$\boxed{E_{tot}=f_1E_1+f_2E_2}$$

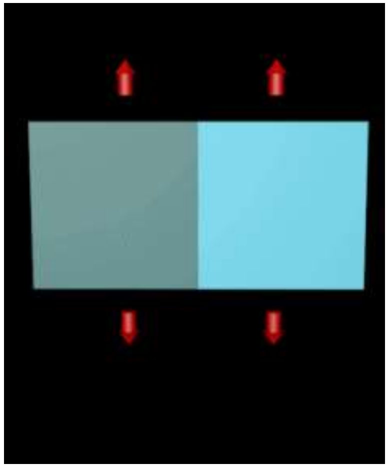
P_1, P_2 are the loads on 1 and 2.
f_1, f_2 are the volume fractions of 1 and 2.

Bounding Case - Isostress

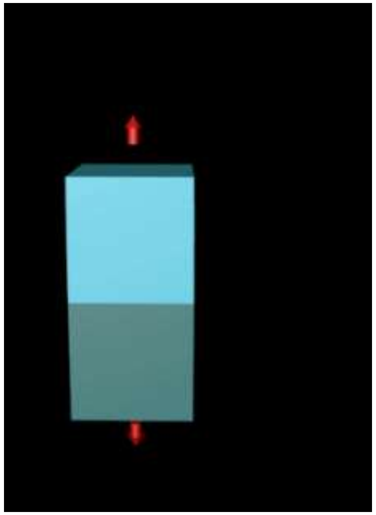
$$\sigma_1=\sigma_2=\sigma_{tot}$$
$$\sigma_1=E_1\epsilon_1 \quad ; \quad \sigma_2=E_2\epsilon_2$$
$$\epsilon_{tot}=f_1\epsilon_1+f_2\epsilon_2=f_1\frac{\sigma_{tot}}{E_1}+f_2\frac{\sigma_{tot}}{E_2}$$
$$\boxed{E=\frac{\sigma_{tot}}{\epsilon_{tot}}=\frac{1}{\frac{f_1}{\epsilon_1}+\frac{f_2}{\epsilon_2}}=\frac{E_1E_2}{f_1E_2+f_2E_1}}$$

Iso-stress and iso-strain

- iso-strain (Taylor-model)



- iso-stress (Sachs-model)



Roters et al. Acta Mater. 58 (2010)

Iso-stress and iso-strain for polycrystals

Sachs Model (previous lecture on single crystal):

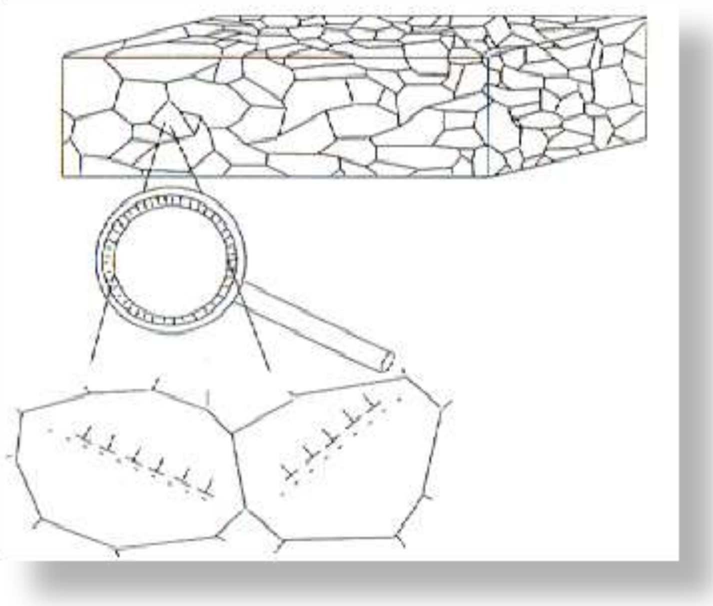
- All grains with aggregate or polycrystal experience the same state of stress;
- Equilibrium condition across the grain boundaries satisfied;
- Compatibility conditions between the grains violated, thus, finite strains will lead to gaps and overlaps between grains;
- Generally most successful for single crystal deformation with *stress boundary conditions on each grain*.

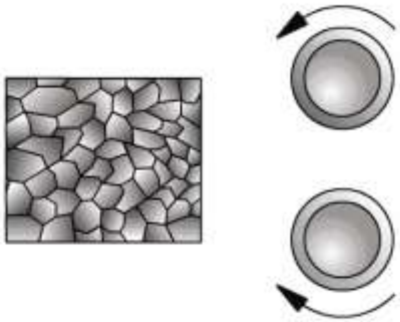
Taylor Model (this lecture):

- All single-crystal grains within the aggregate experience the same state of deformation (strain);
- Equilibrium condition across the grain boundaries violated, because the vertex stress states required to activate multiple slip in each grain vary from grain to grain;
- Compatibility conditions between the grains satisfied;
- Generally most successful for polycrystals with strain boundary conditions on each grain.

- Taylor model for the mechanics of polycrystals

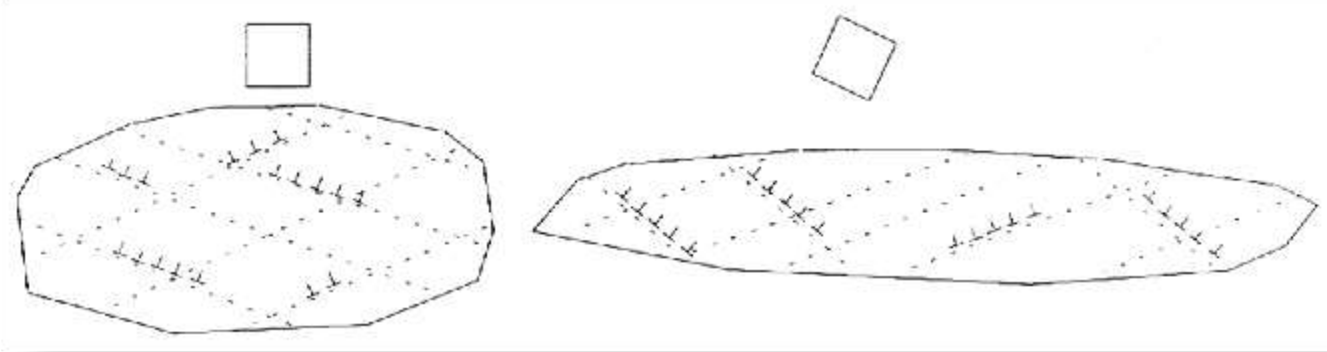
The Taylor Model





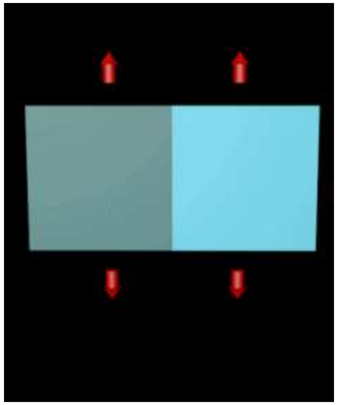
$$\varepsilon_{ij} = \frac{1}{2} \sum_{s=1}^{5} \left(n_i^s b_j^s + n_j^s b_i^s \right) \gamma^s$$

$$\varepsilon_{ij} = \frac{1}{2} \sum_{s=1}^{5} \left(n_i^s b_j^s + n_j^s b_i^s \right) \gamma^s$$

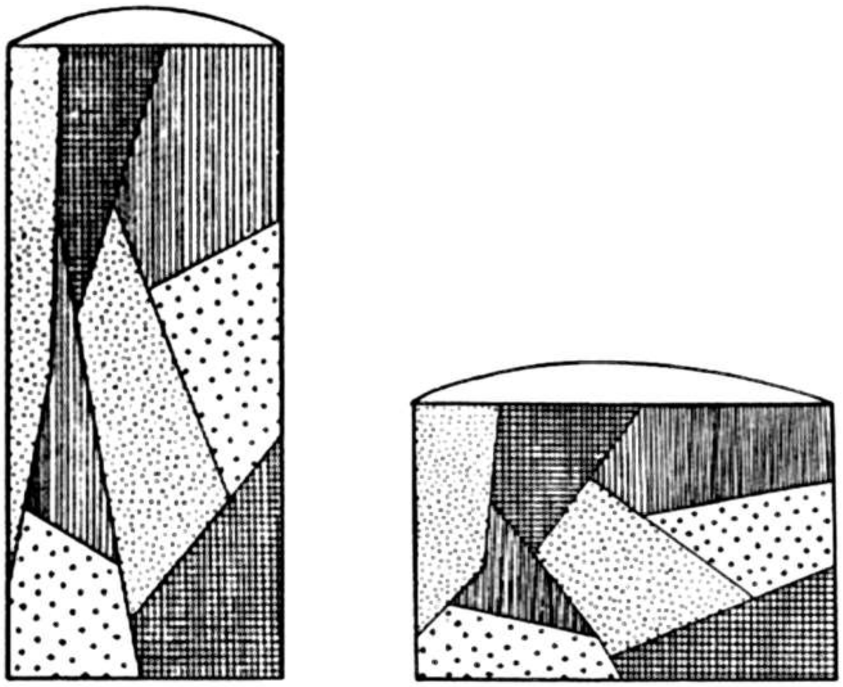


plastic spin from polar decomposition

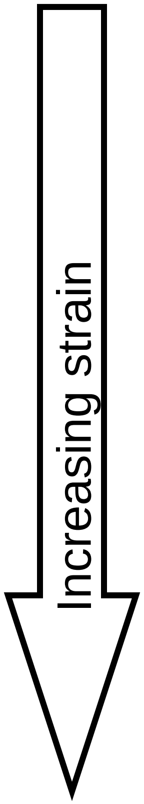
$$\dot{\omega}_{ij}^{K} = W_{ij}^{K} = \frac{1}{2}\left(\dot{u}_{i,j}^{\mathrm{K}} - \dot{u}_{j,i}^{\mathrm{K}} \right) = \sum_{s=1}^{N} m_{ij}^{\mathrm{asym},s} \dot{\gamma}^{s}$$



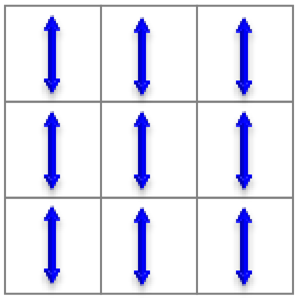
The Taylor Model

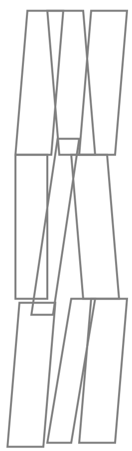


The Taylor Model – comparison to Sachs model



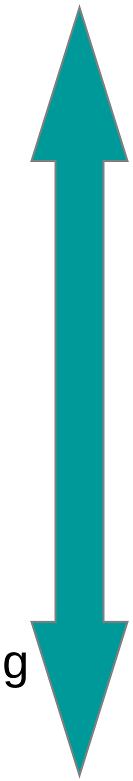
External Stress



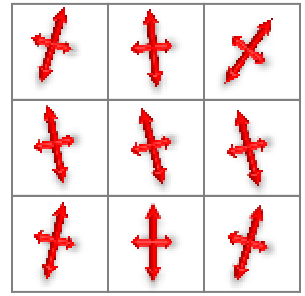


Small arrows indicate identical stress state in each grain

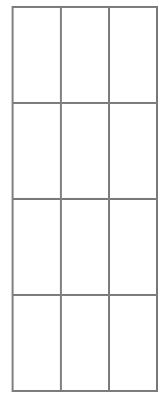
Each grain deforms according to which single slip system is active



External Strain



Small arrows indicate variable stress state in each grain



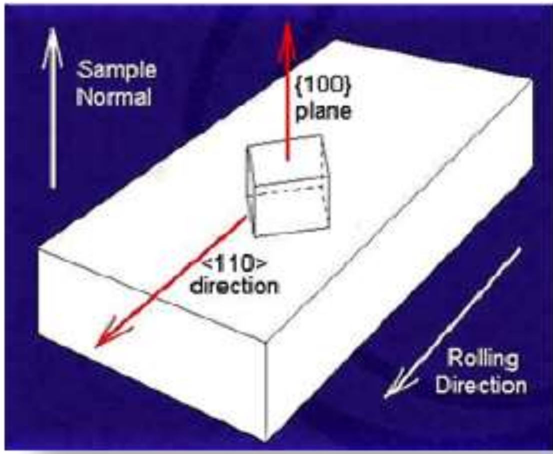
Multiple slip (with 5 or more systems) in each grain satisfies the externally imposed strain, *D*

The Taylor Model – comparison to Sachs model

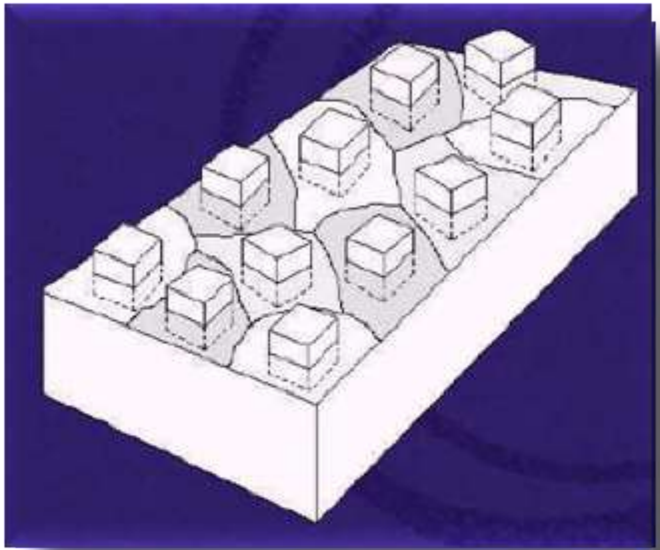
$$\begin{bmatrix} D_2 \\ D_3 \\ D_4 \\ D_5 \\ D_6 \end{bmatrix} = \begin{bmatrix} m_{22}^{(1)} & m_{22}^{(2)} & m_{22}^{(3)} & m_{22}^{(4)} & m_{22}^{(5)} \\ m_{33}^{(1)} & m_{33}^{(2)} & m_{33}^{(3)} & m_{33}^{(4)} & m_{33}^{(5)} \\ (m_{23}^{(1)} + m_{32}^{(1)}) & (m_{23}^{(2)} + m_{32}^{(2)}) & (m_{23}^{(3)} + m_{32}^{(3)}) & (m_{23}^{(4)} + m_{32}^{(4)}) & (m_{23}^{(5)} + m_{32}^{(5)}) \\ (m_{13}^{(1)} + m_{31}^{(1)}) & (m_{13}^{(2)} + m_{31}^{(2)}) & (m_{13}^{(3)} + m_{31}^{(3)}) & (m_{13}^{(4)} + m_{31}^{(4)}) & (m_{13}^{(5)} + m_{31}^{(5)}) \\ (m_{12}^{(1)} + m_{21}^{(1)}) & (m_{12}^{(2)} + m_{21}^{(2)}) & (m_{12}^{(3)} + m_{21}^{(3)}) & (m_{12}^{(4)} + m_{21}^{(4)}) & (m_{12}^{(5)} + m_{21}^{(5)}) \end{bmatrix} \begin{bmatrix} d\gamma_1 \\ d\gamma_2 \\ d\gamma_3 \\ d\gamma_4 \\ d\gamma_5 \end{bmatrix}$$

$$\begin{bmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \\ \tau_4 \\ \tau_5 \end{bmatrix} = \begin{bmatrix} m_{11}^{(1)} & m_{22}^{(1)} & m_{33}^{(1)} & (m_{23}^{(1)} + m_{32}^{(1)}) & (m_{13}^{(1)} + m_{31}^{(1)}) & (m_{12}^{(1)} + m_{21}^{(1)}) \\ m_{11}^{(2)} & m_{22}^{(2)} & m_{33}^{(2)} & (m_{23}^{(2)} + m_{32}^{(2)}) & (m_{13}^{(2)} + m_{31}^{(2)}) & (m_{12}^{(2)} + m_{21}^{(2)}) \\ m_{11}^{(3)} & m_{22}^{(3)} & m_{33}^{(3)} & (m_{23}^{(3)} + m_{32}^{(3)}) & (m_{13}^{(3)} + m_{31}^{(3)}) & (m_{12}^{(3)} + m_{21}^{(3)}) \\ m_{11}^{(4)} & m_{22}^{(4)} & m_{33}^{(4)} & (m_{23}^{(4)} + m_{32}^{(4)}) & (m_{13}^{(4)} + m_{31}^{(4)}) & (m_{12}^{(4)} + m_{21}^{(4)}) \\ m_{11}^{(5)} & m_{22}^{(5)} & m_{33}^{(5)} & (m_{23}^{(5)} + m_{32}^{(5)}) & (m_{13}^{(5)} + m_{31}^{(5)}) & (m_{12}^{(5)} + m_{21}^{(5)}) \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix}$$

Crystal rotations under heterogeneous constraints



Grains in polycrystals do NOT experience the same boundary conditions.

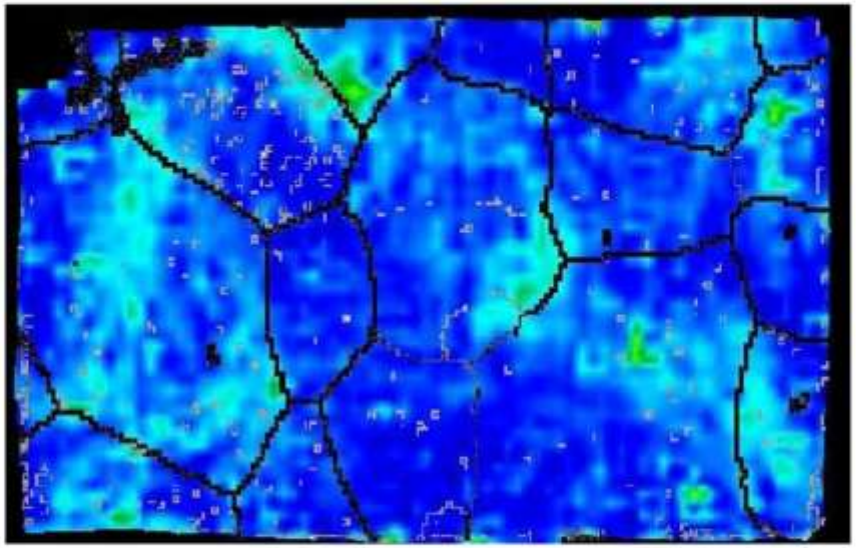


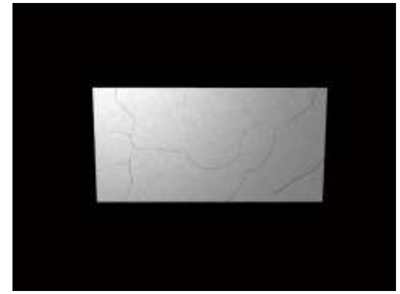
Differentiate between GLOBAL bounday conditions (tool, process) and the LOCAL (micromechanical) boundary conditions. The latter are influenced by grain-to-grain interactions and local inhomogeneity.

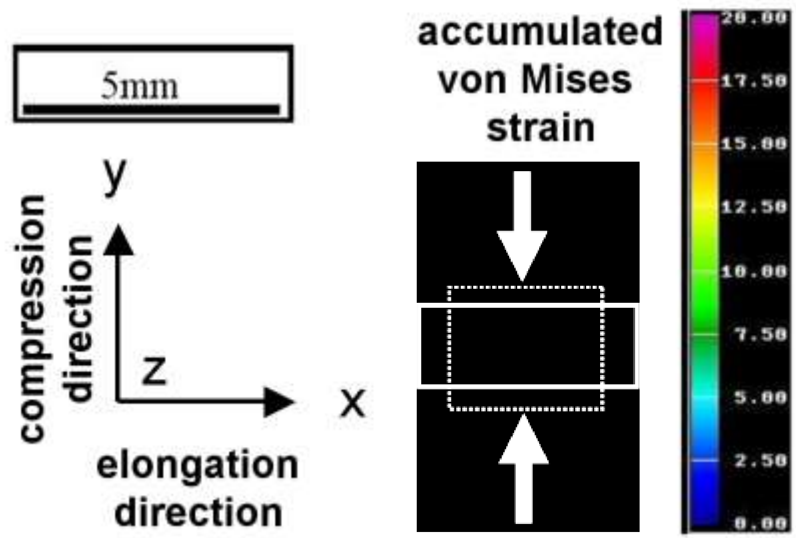
Raabe et al. Acta Mat. 49 (2001)

- Examples

3%

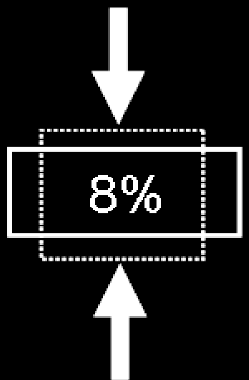


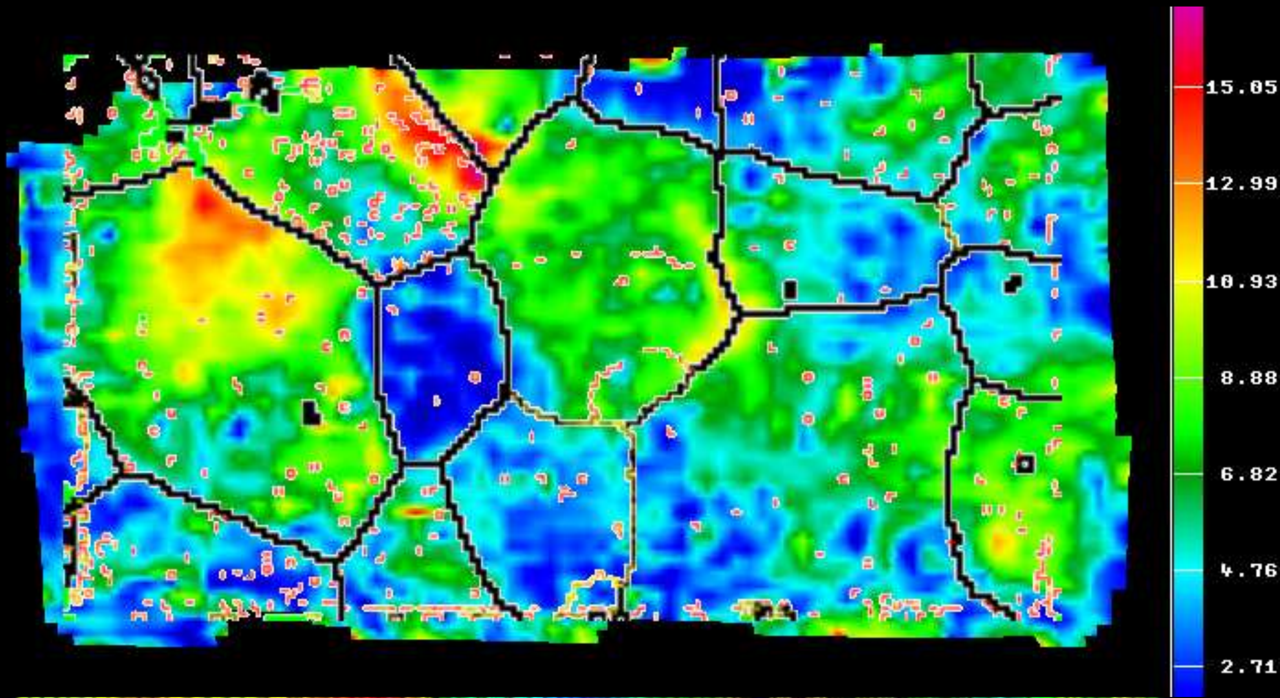




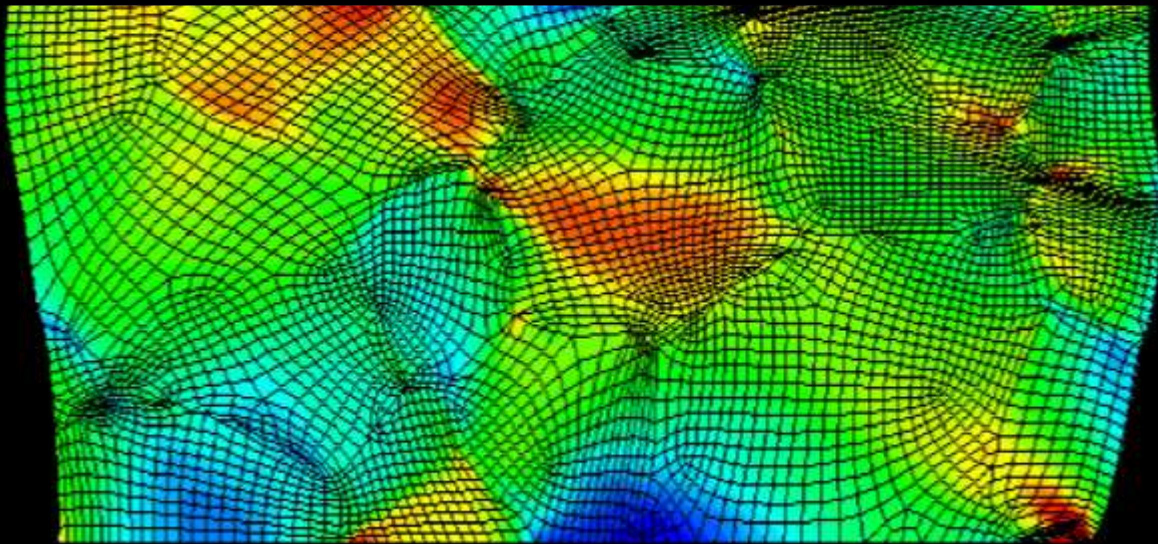
Raabe et al. Acta Mater. 49 (2001) 3433

Crystal Mechanics FEM, grain scale mechanics (2D)

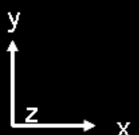




Experiment
(DIC, EBSD)
v Mises strain

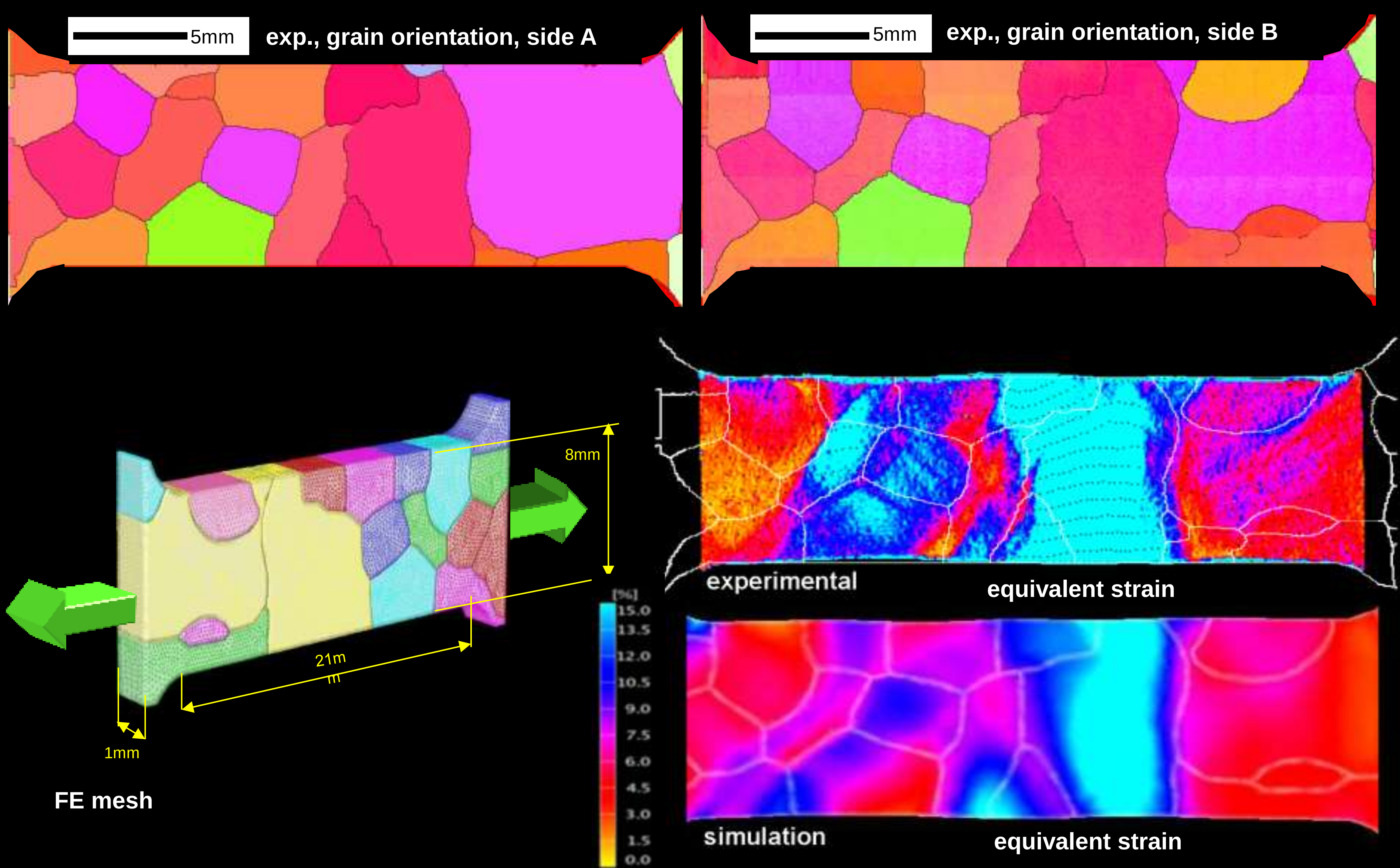


Simulation
(CP-FEM)
v Mises strain



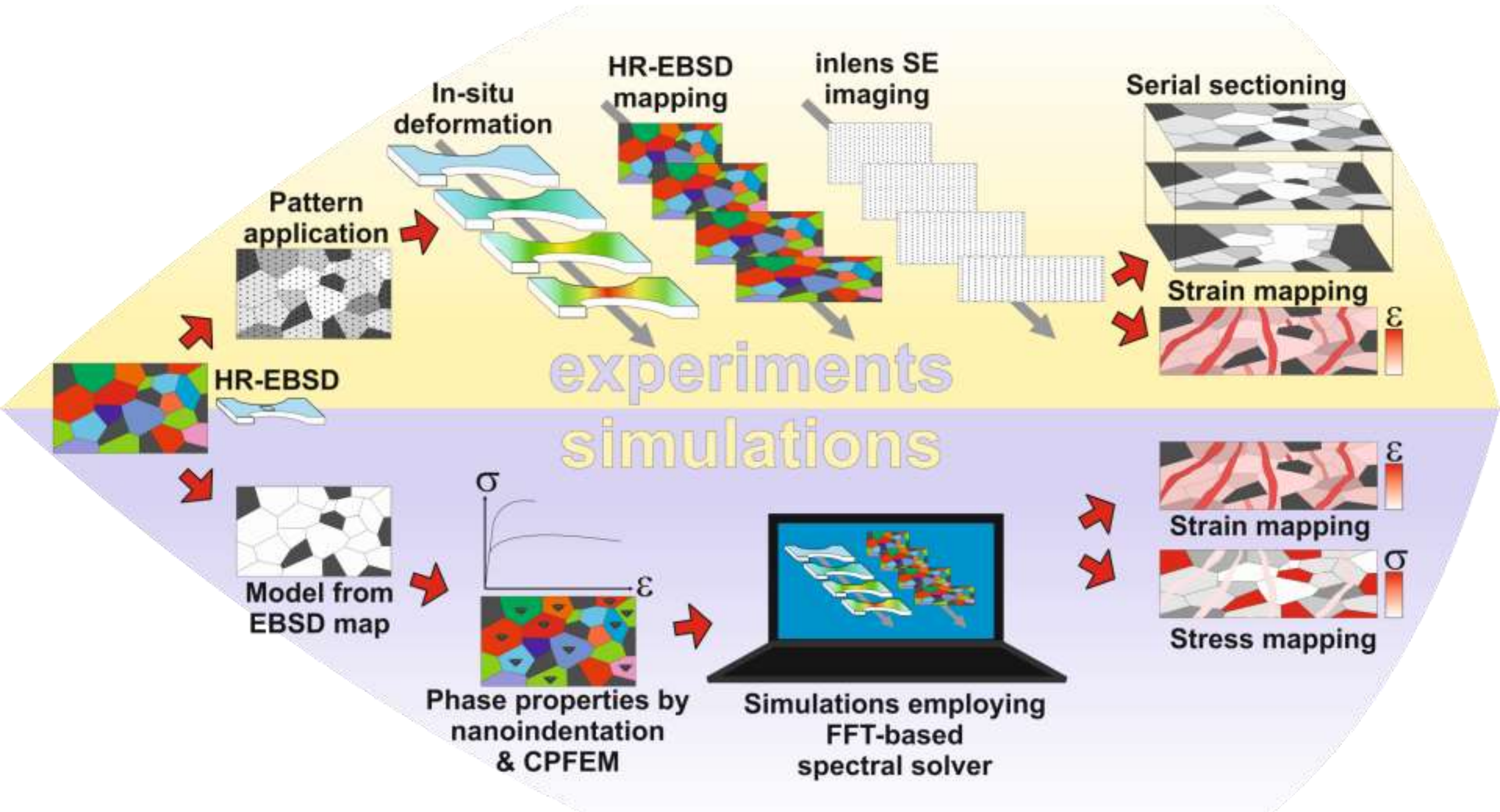
Sachtleber, Zhao, Raabe: Mater. Sc. Engin. A 336 (2002) 81

Crystal plasticity FEM, grain scale mechanics (3D Al)

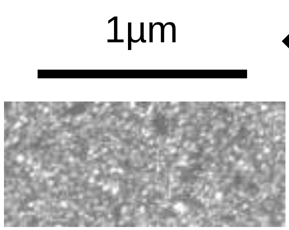


Zhao, Rameshwaran, Radovitzky, Cuitino, Roters, Raabe : Intern. J. Plast. 24 (2008)

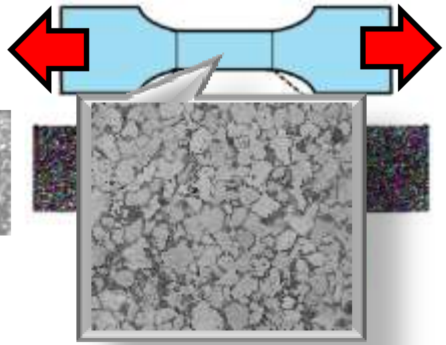
ICME: Integrated Computational Materials Engineering



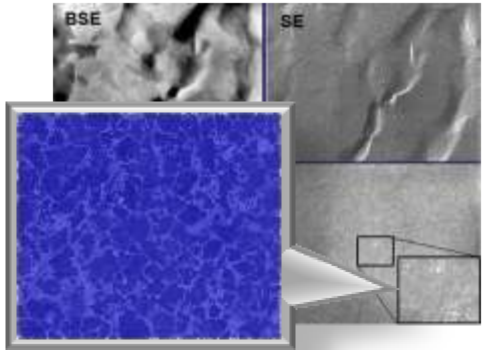
ICME applied to dual phase steel



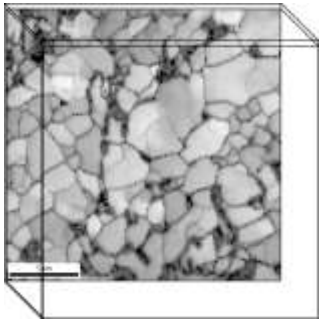
SiO_2 pattern



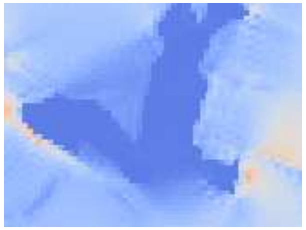
Deformation



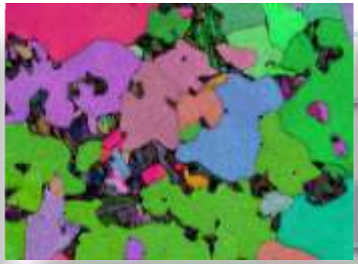
Imaging & DIC



Sectioning



Strain map

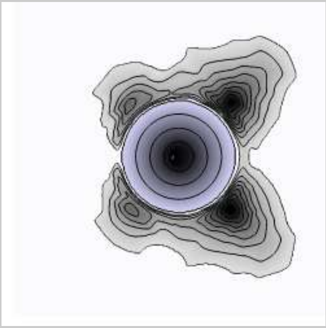


Experiments

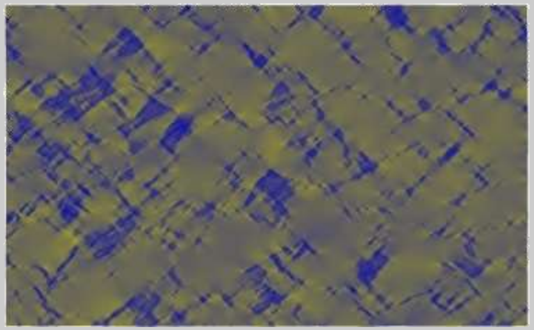
Simulations

Digital model

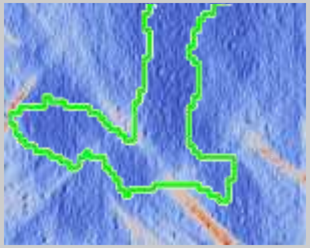
Indents



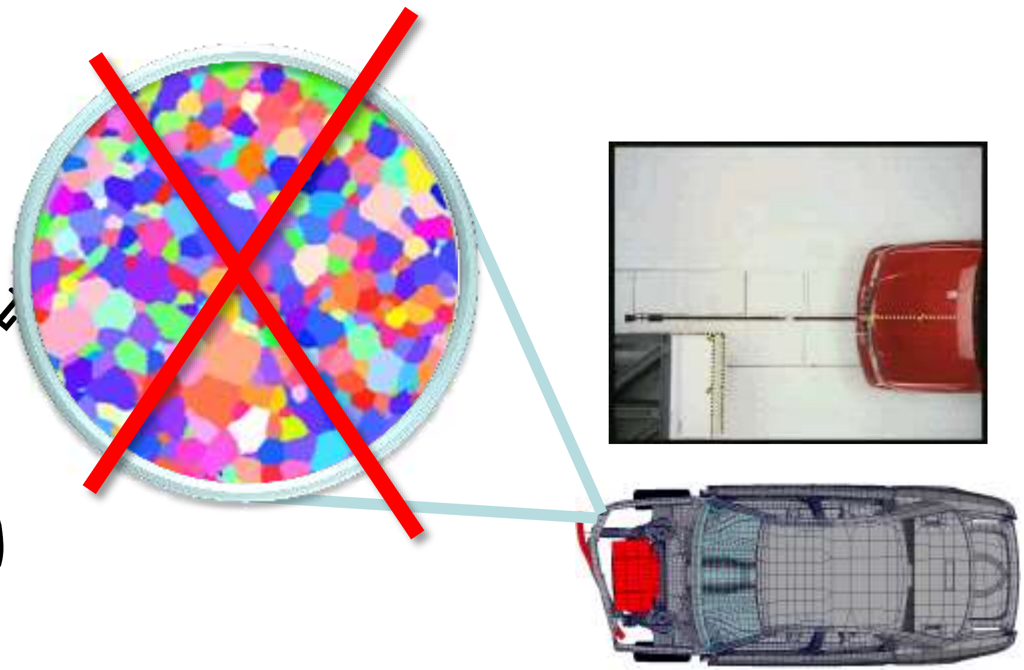
Spectral solver



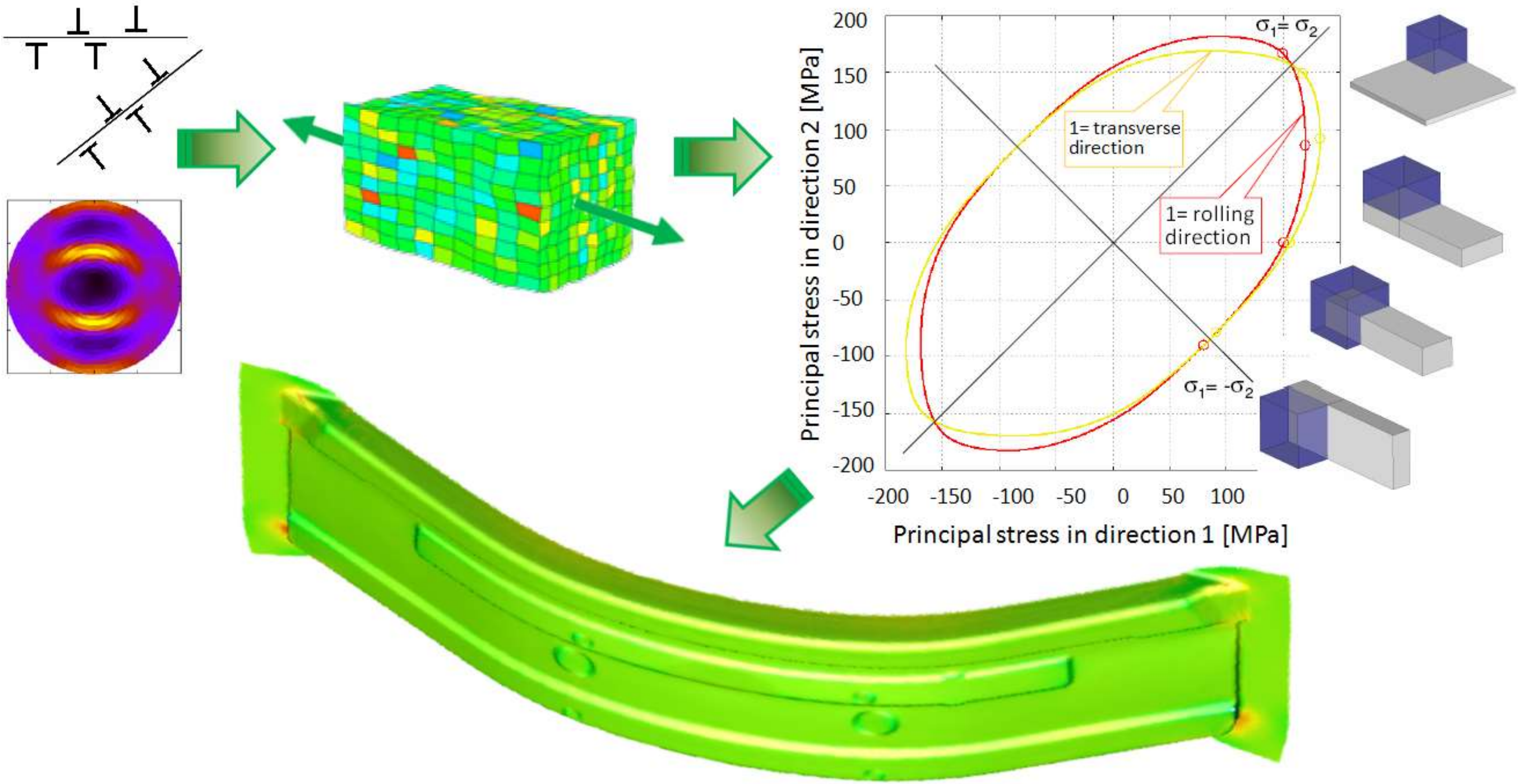
Strain map & stress map



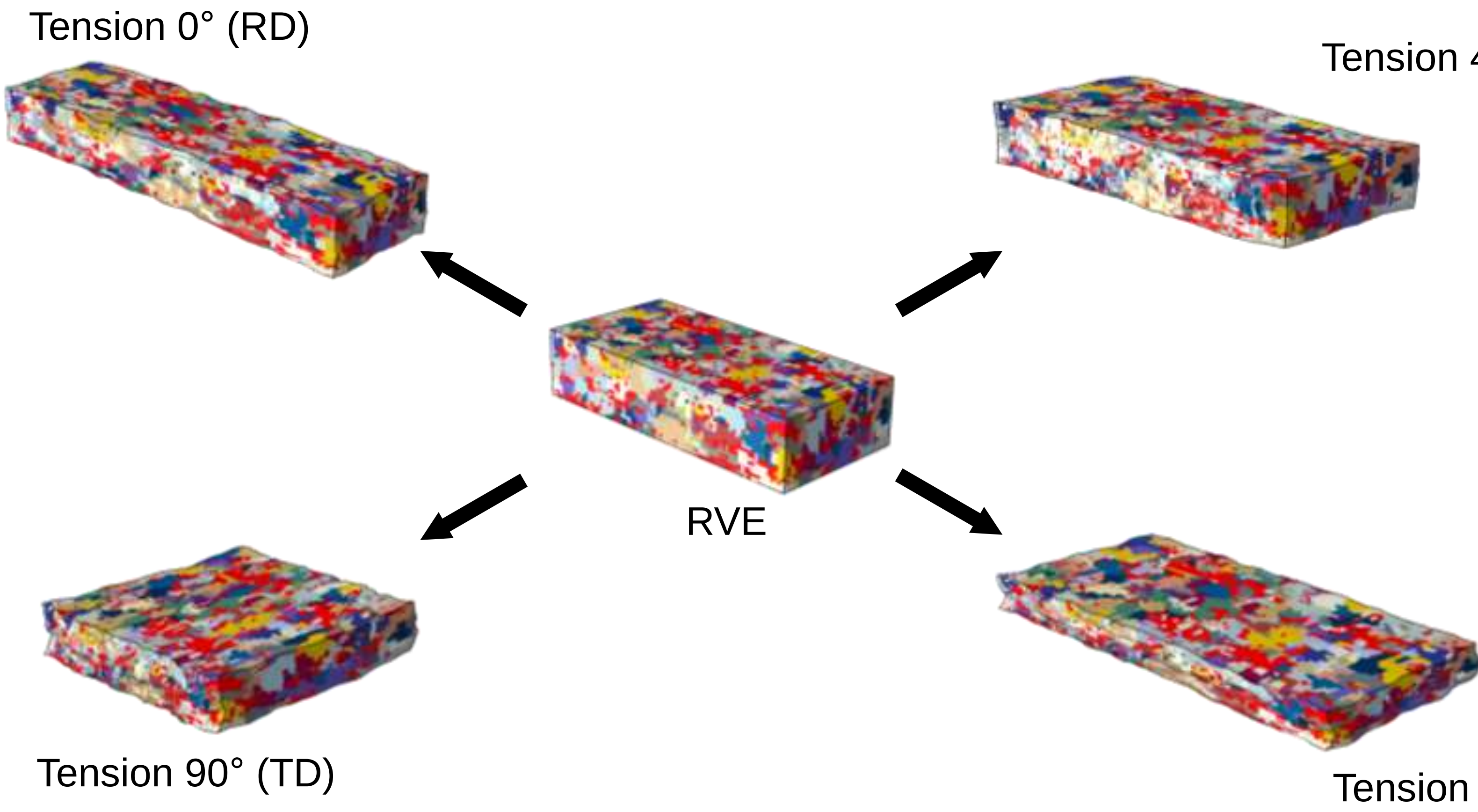
too many
grains



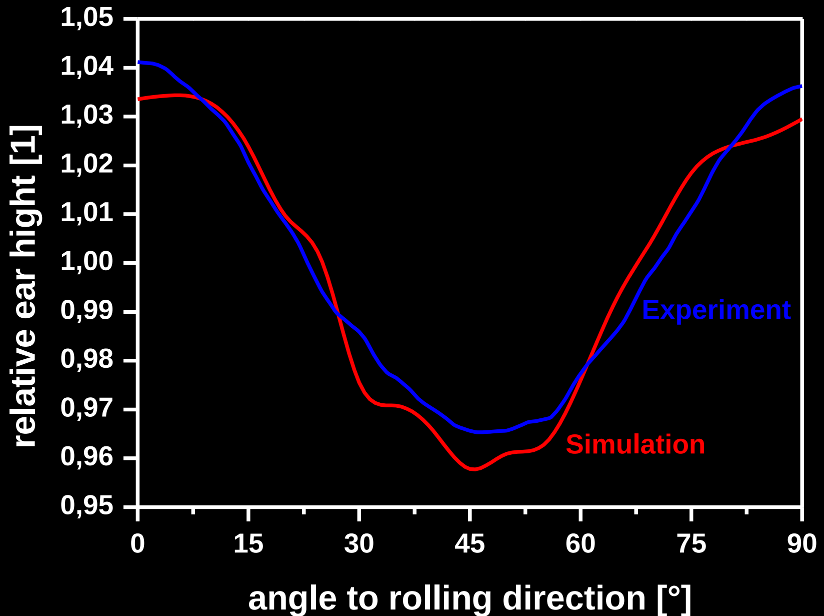
Numerical Laboratory: From CPFEM to yield surface (engineering)

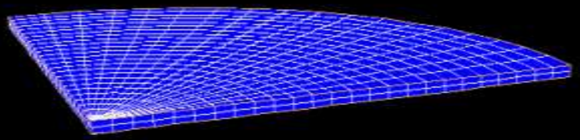


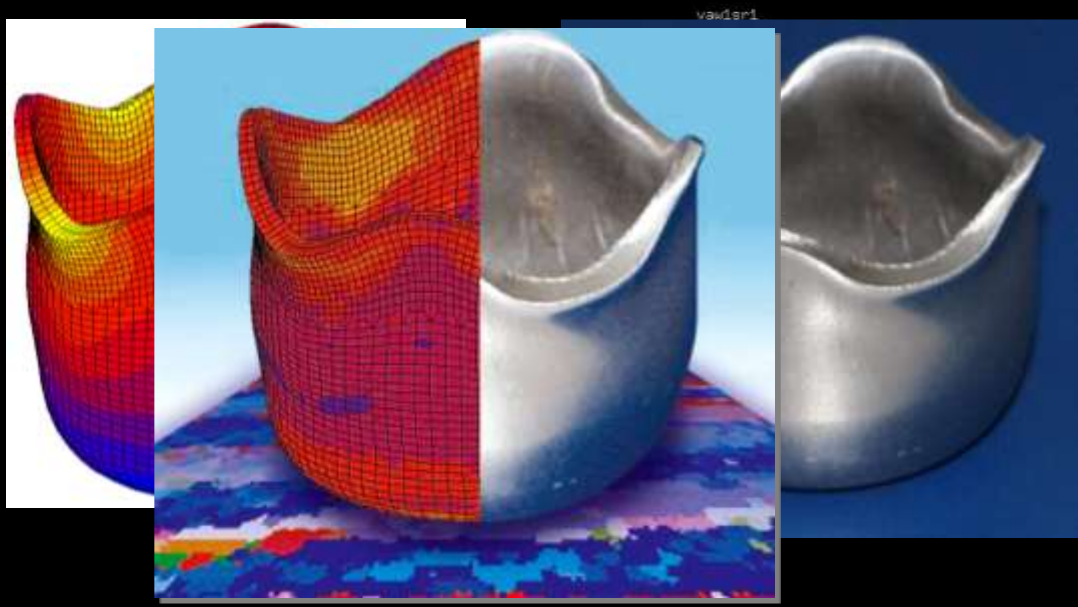
Representative Volume Element



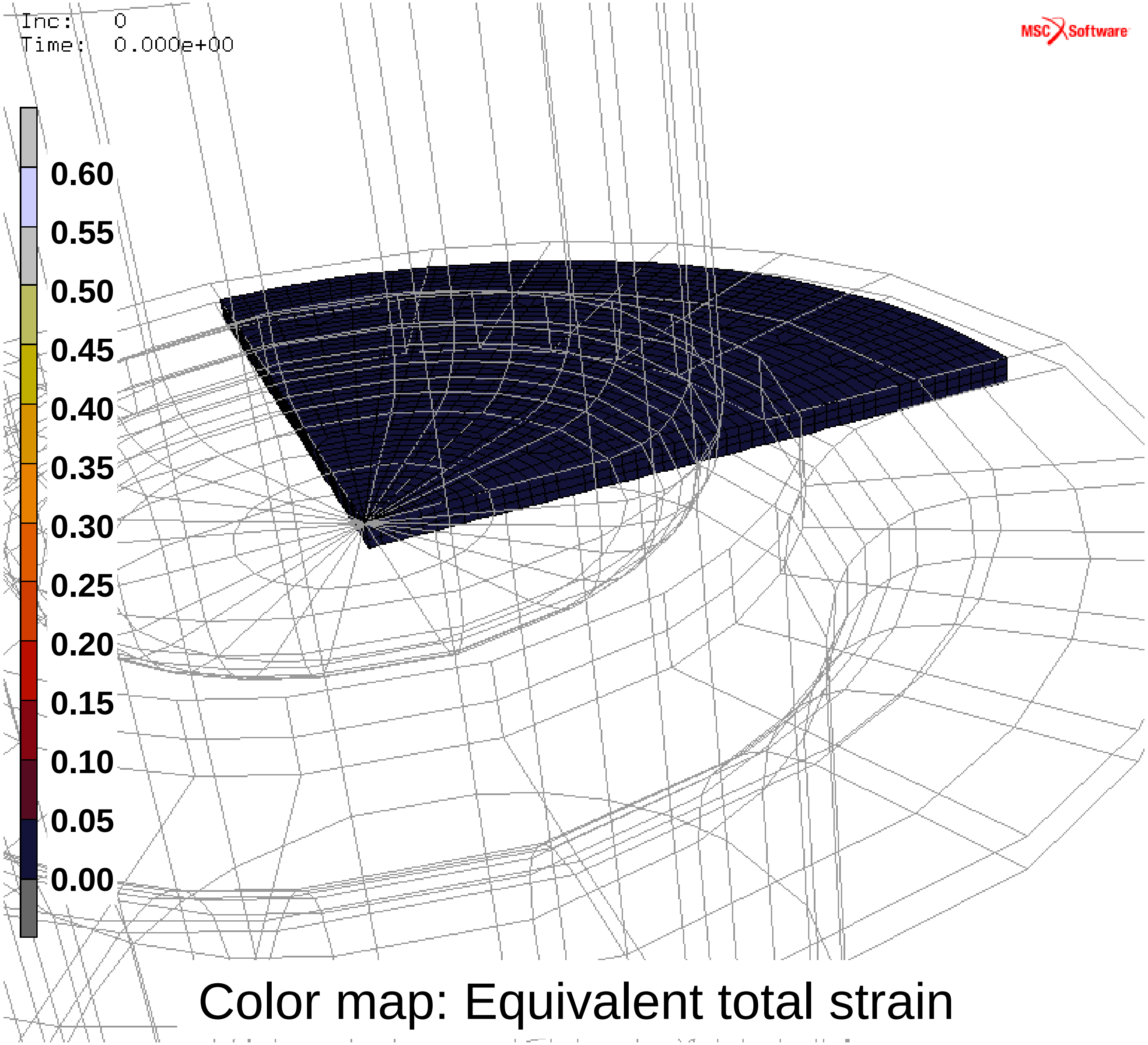
Texture component crystal plasticity FEM for large scale forming







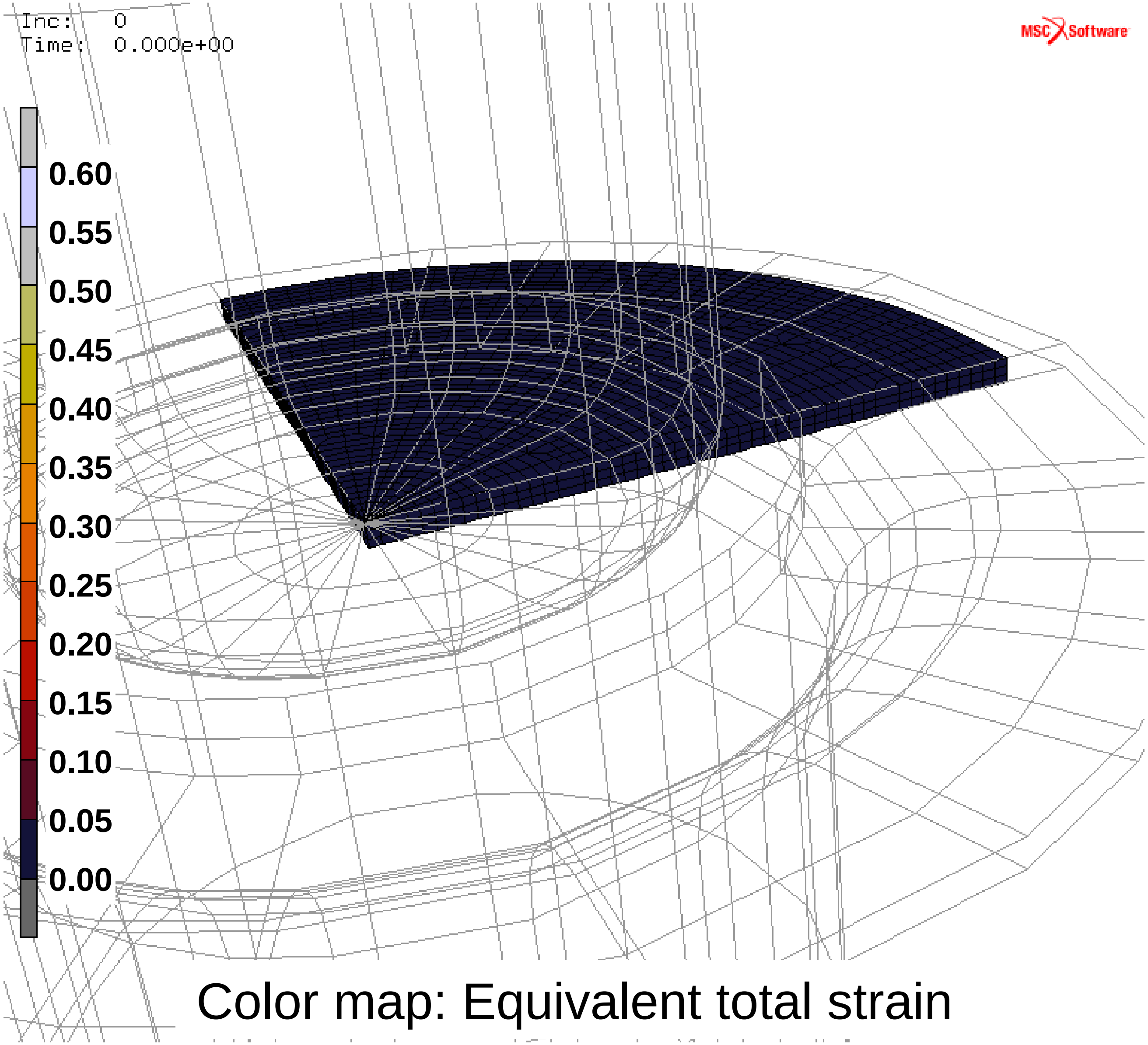
Simulation result: Taylor model



Color map: Equivalent total strain

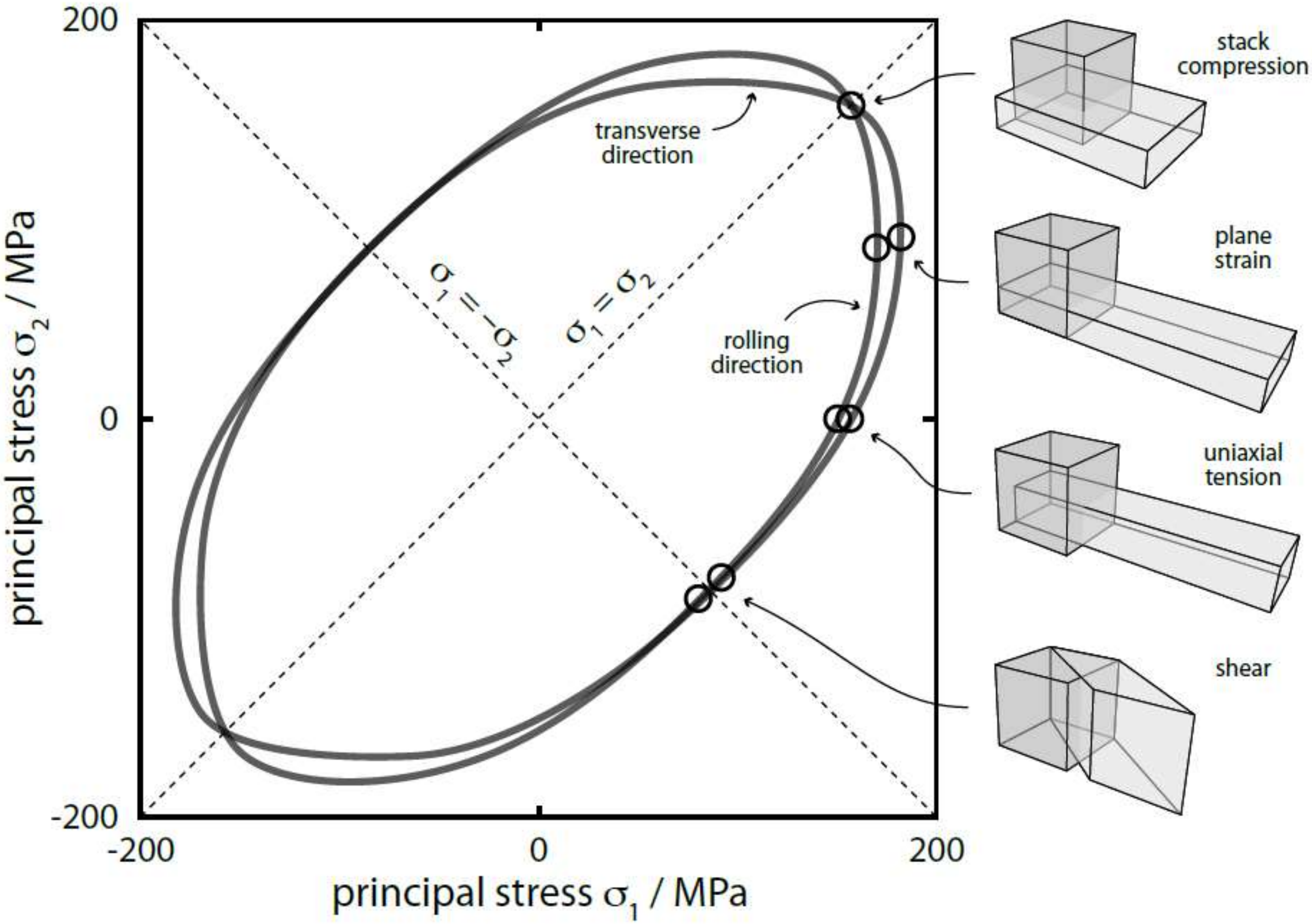
Roters et al. Acta Mater.58 (2010)

Simulation result: RGC scheme



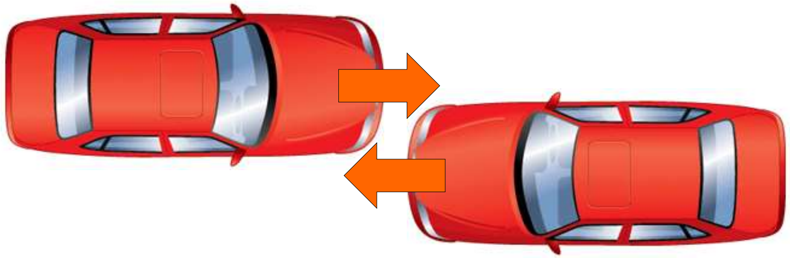
Color map: Equivalent total strain

Roters et al. Acta Mater.58 (2010)

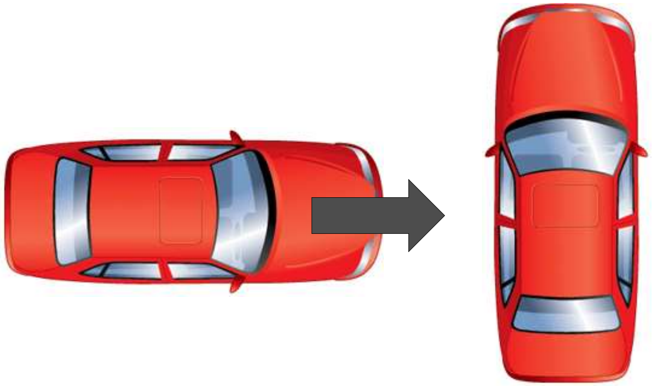

200
0
-200
-200
0
200
principal stress σ1 / MPa
principal stress σ2 / MPa
transverse direction
rolling direction
σ1 = −σ2
σ1 = σ2
stack compression
plane strain
uniaxial tension
shear

Component-specific property mix

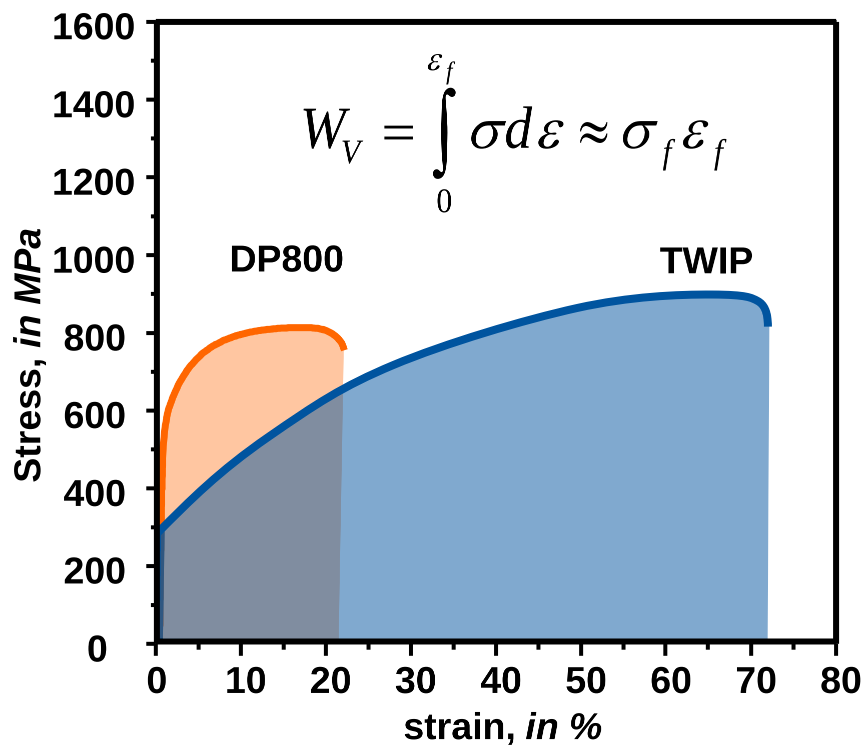
Front crash ⇨ Energy absorption



Side crash ⇨ Strength



Strain rate 800/s: compare TWIP steel to DP800



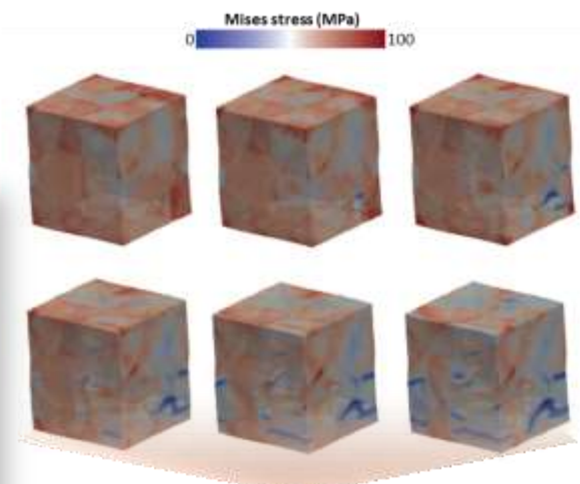
Awareness of impact situation

DAMASK

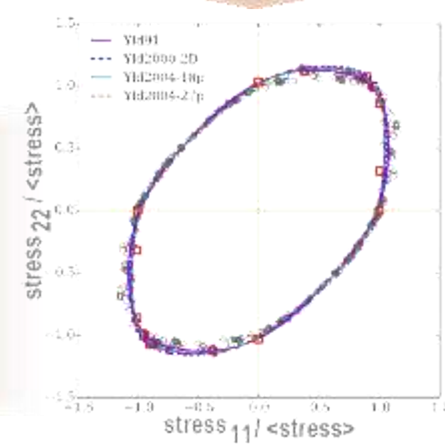
Düsseldorf Advanced Material Simulation Kit

Freeware, GPL 3

Crystal plasticity & phase field:
Mechanics, damage, phase transformation, diffusion

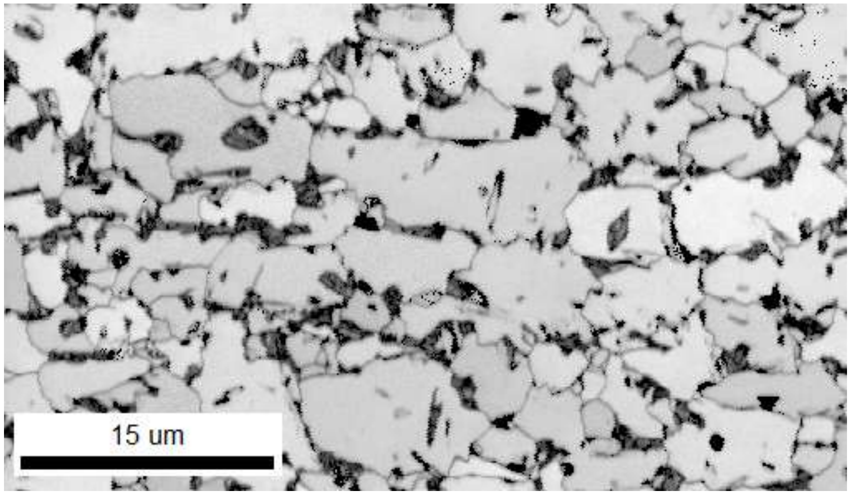


- > 15 years of development
- > 50 man years of expertise
- > 50.000 lines of code
- Pre- and post-processing
- Blends with MSC.Marc and Abaqus
- Standalone (FFT) spectral solver
- Many user groups



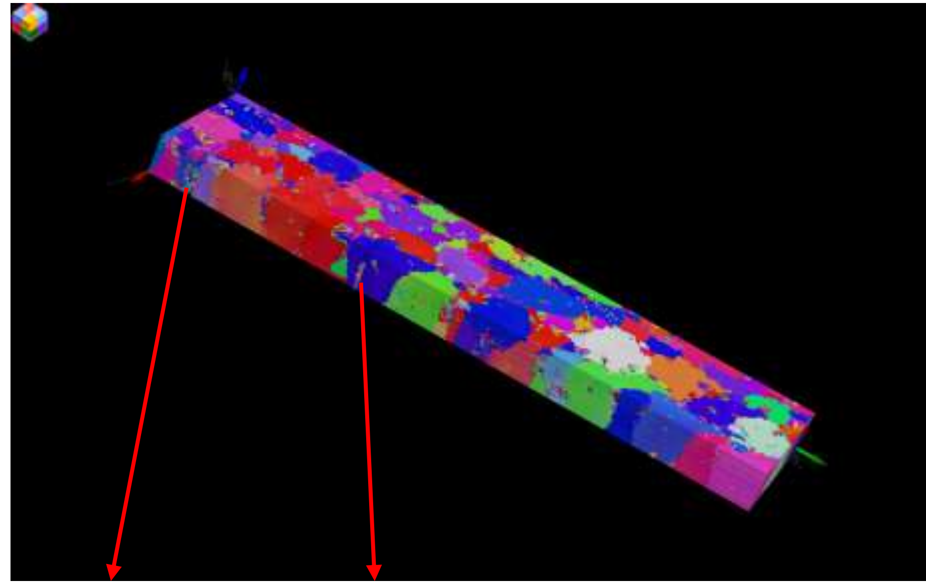
http://DAMASK.mpie.de

Real 3D Microstructure

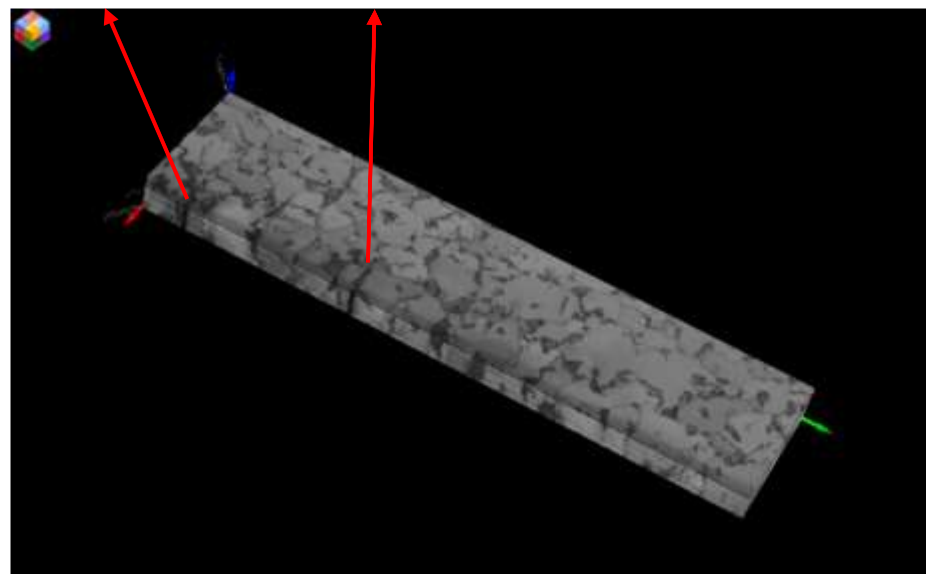


Average grain size: 5 µm
EBSD step size: 0,2 µm
EBSD scan size: 20 × 70 µm
Target polished thickness: 0,15 µm
Total slices number: 22

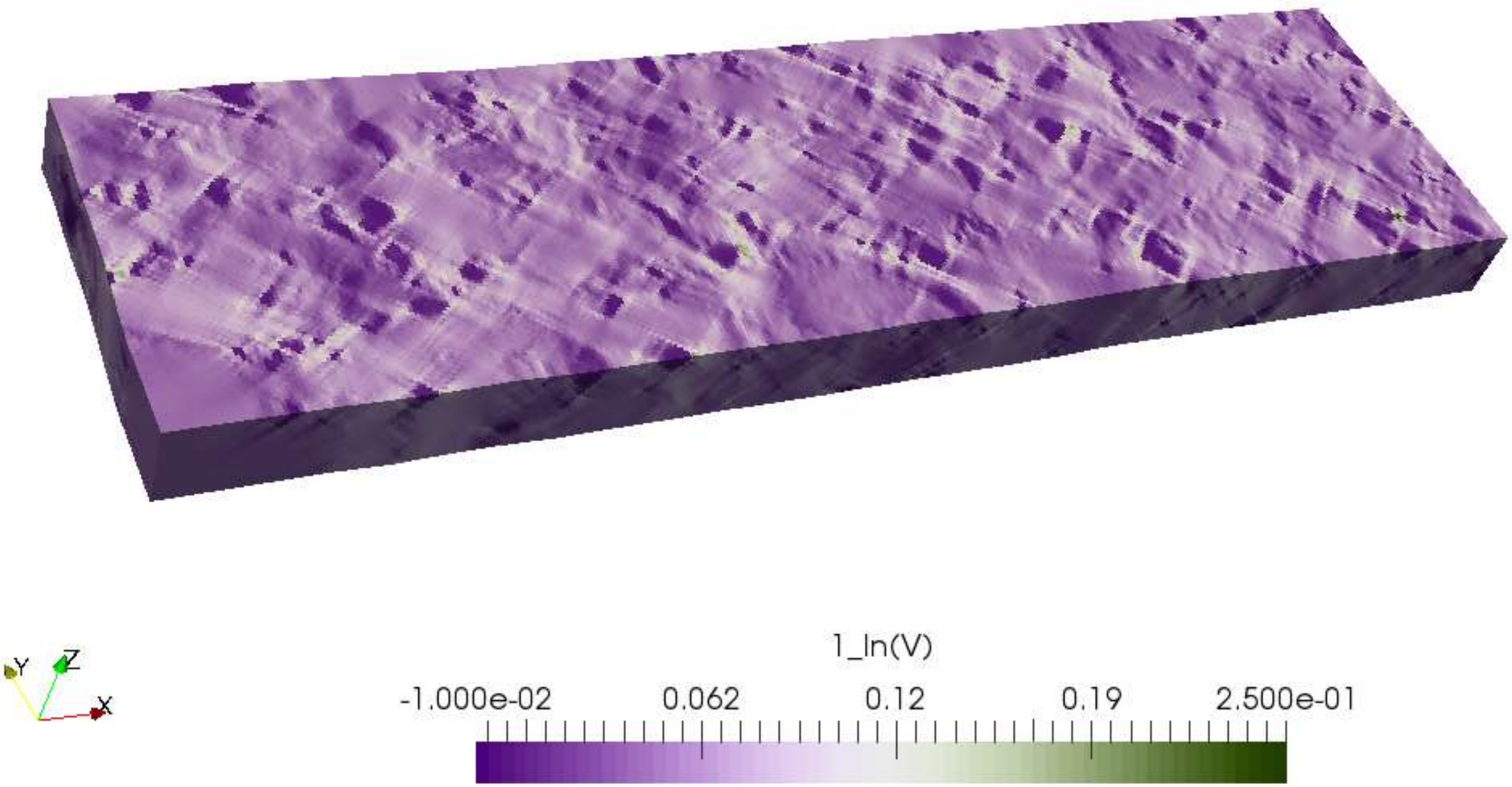
Experiment by Dayong An, MPIE



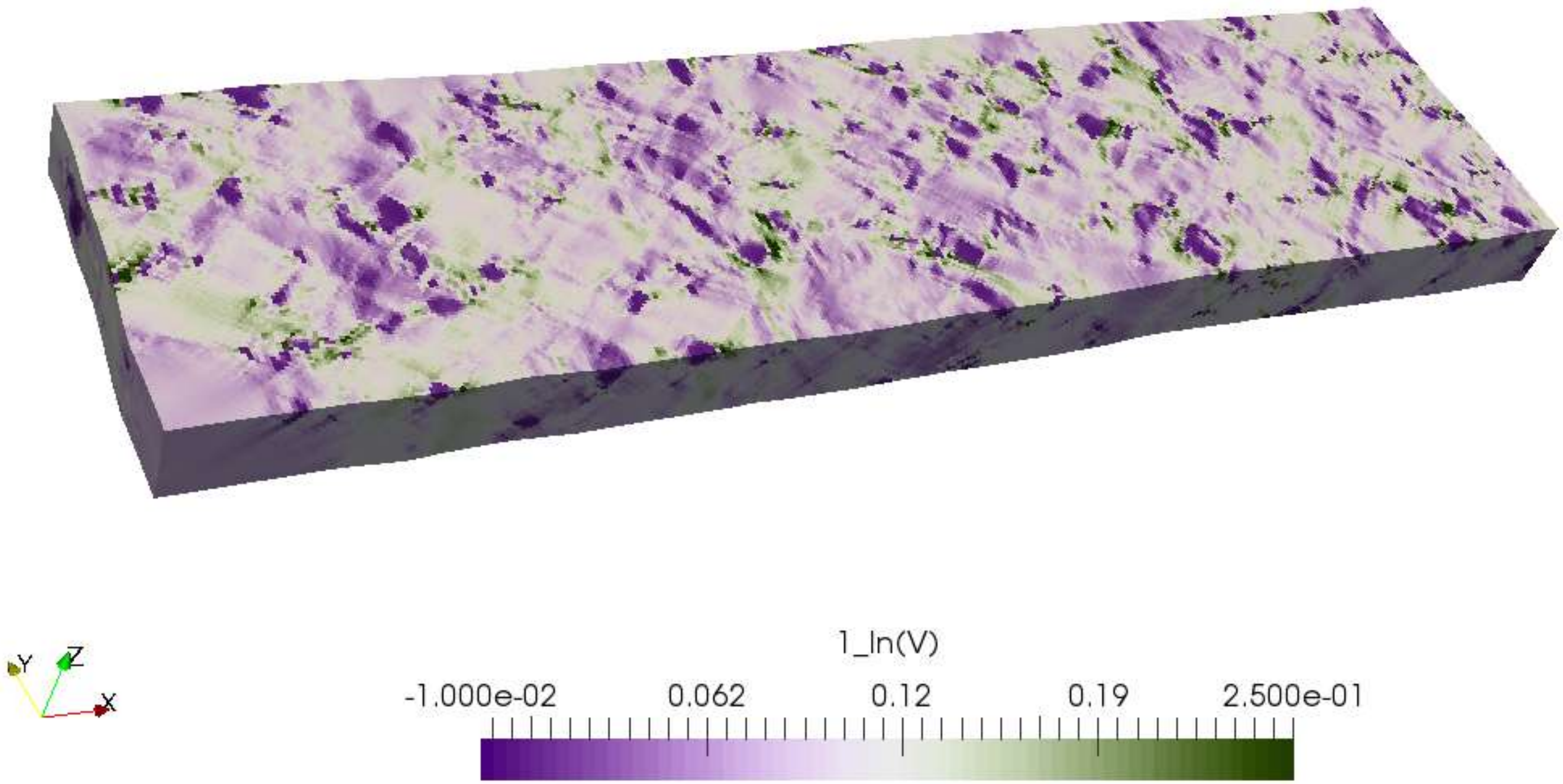
Marker lines act as a realignment reference



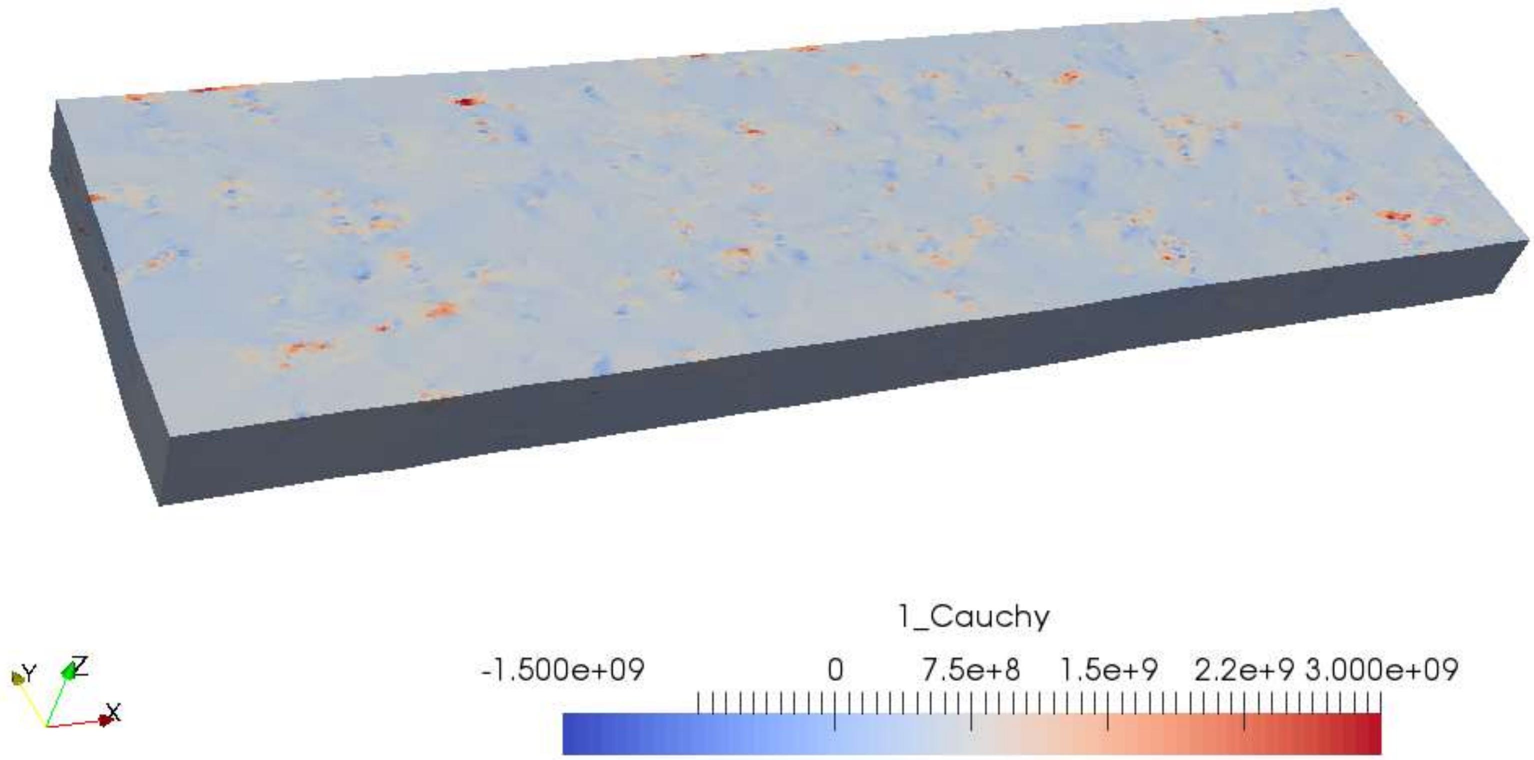
Real 3D Microstructure



Real 3D Microstructure



Real 3D Microstructure



Real 3D Microstructure