Microstructure Mechanics
Crystal Mechanics

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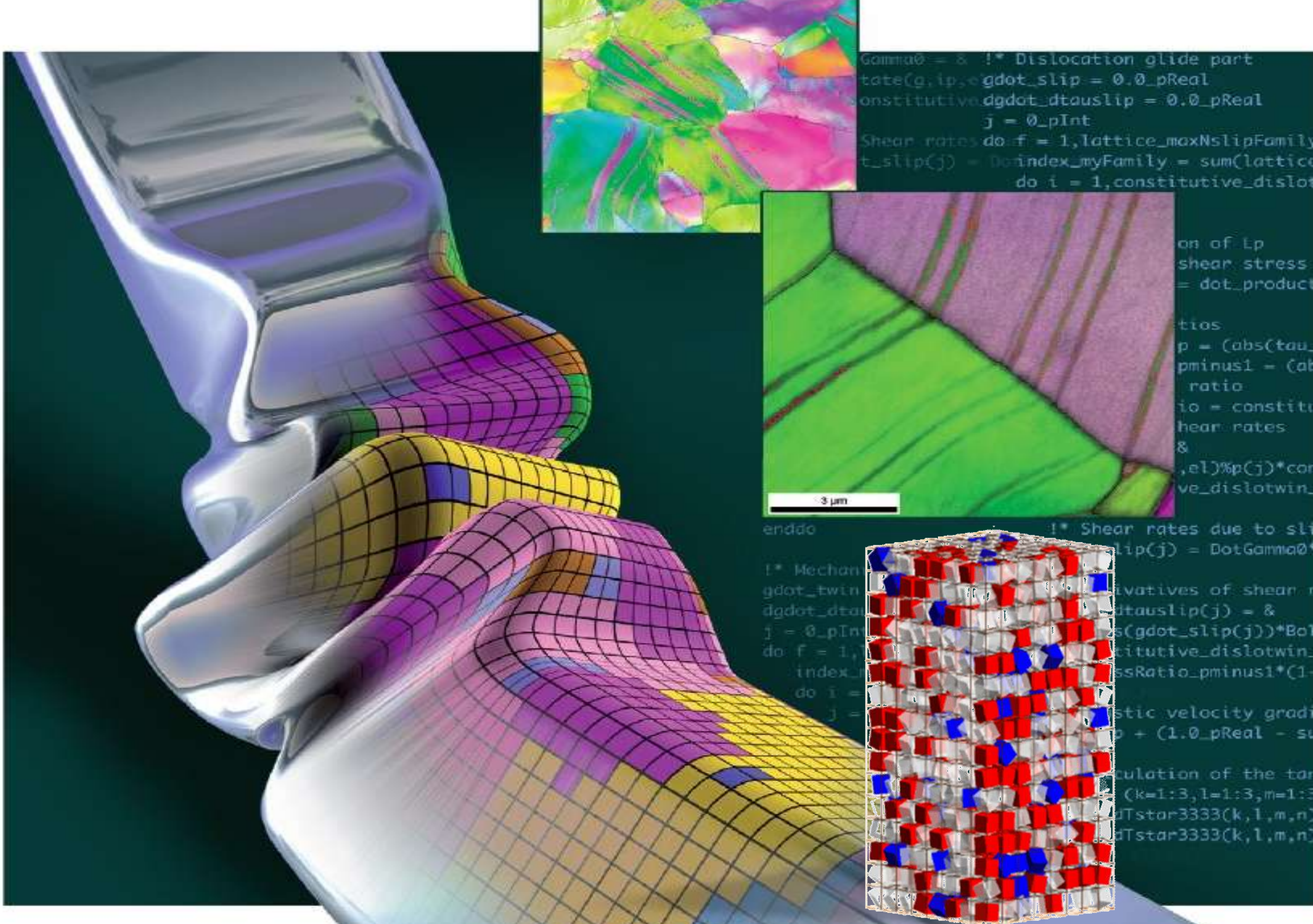
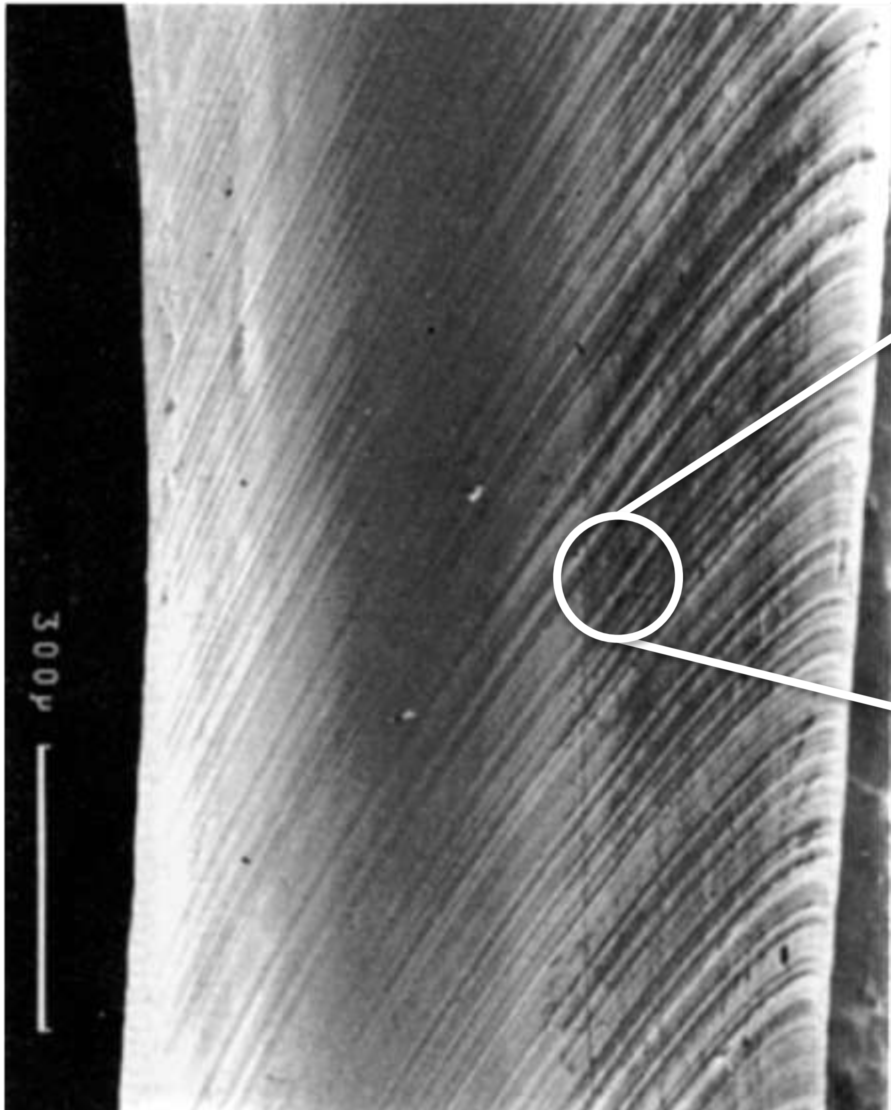


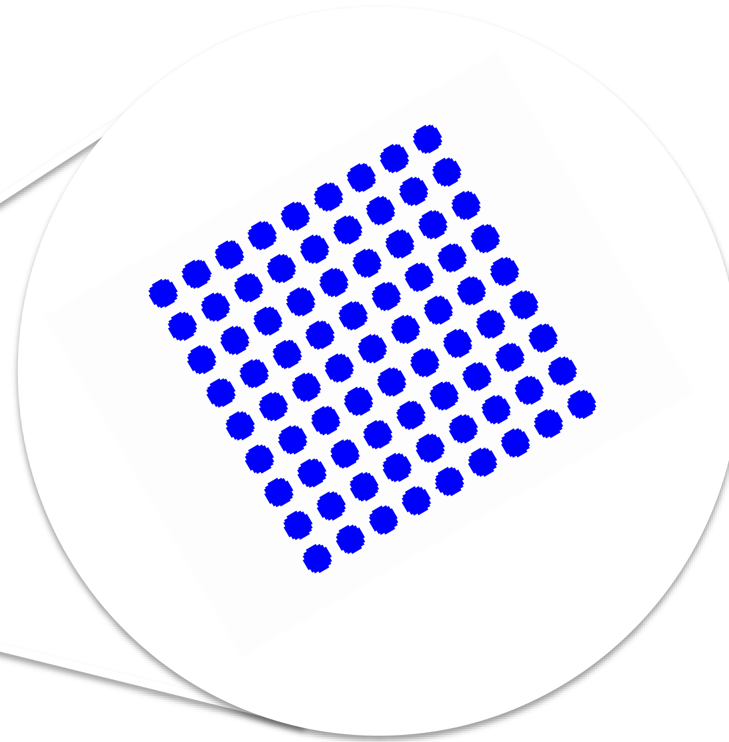
Roters, Eisenlohr, Bieler, Raabe: Crystal Plasticity Finite Element Methods in Materials Science and Engineering, Wiley-VCH

Overview

- Displacements and rotations in crystals
- Single crystal yield surface
- Taylor model for the mechanics of polycrystals
- Examples

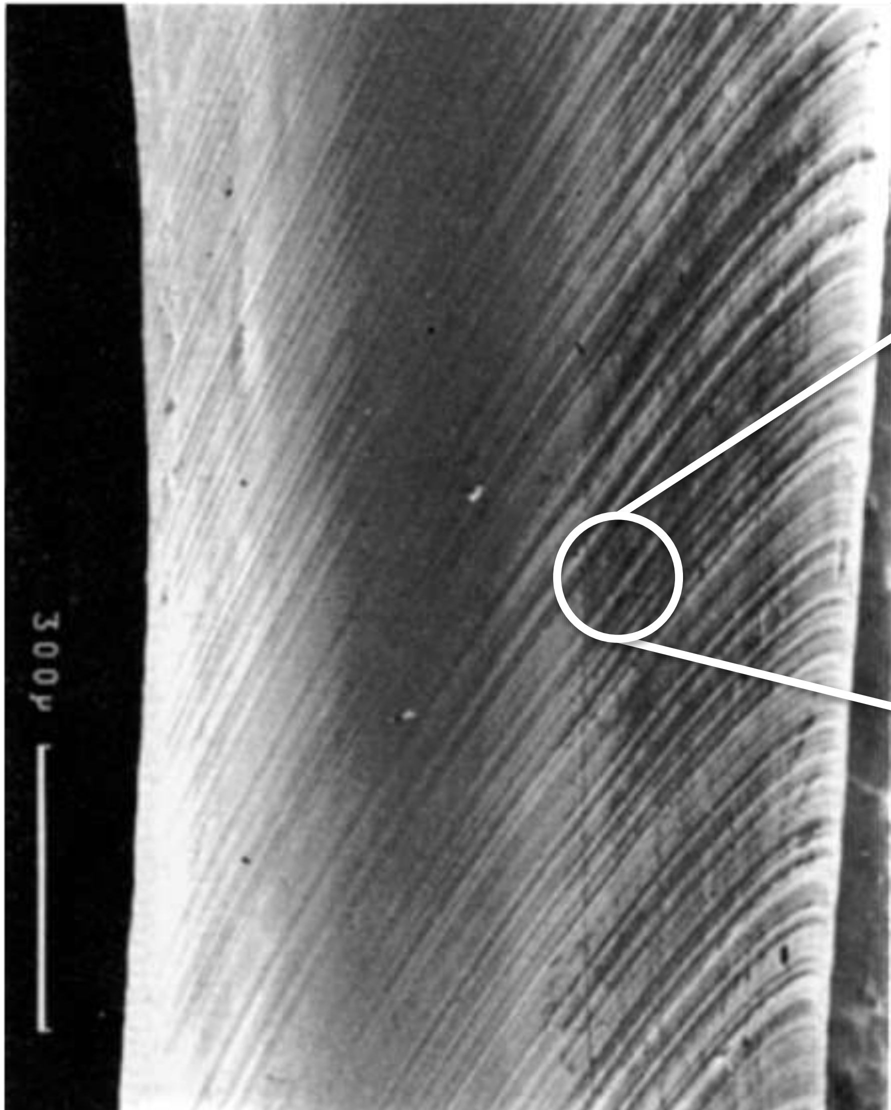


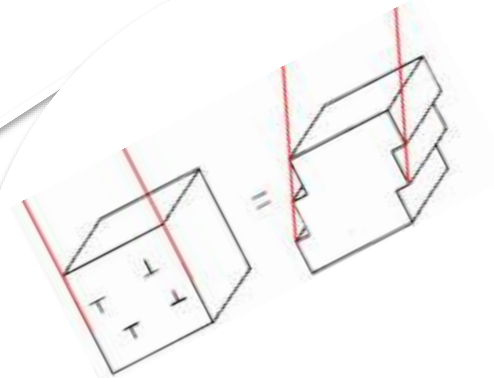
single slip in a single crystal



plastic anisotropy

Plastic deformation of a single crystal by dislocation slip





$$\dot{\gamma} = \frac{\mathrm{d}\gamma}{\mathrm{d}t} = n\frac{\mathrm{d}x}{X}\frac{b}{Z}\frac{1}{\mathrm{d}t} = \rho_{\mathrm{m}} b v$$

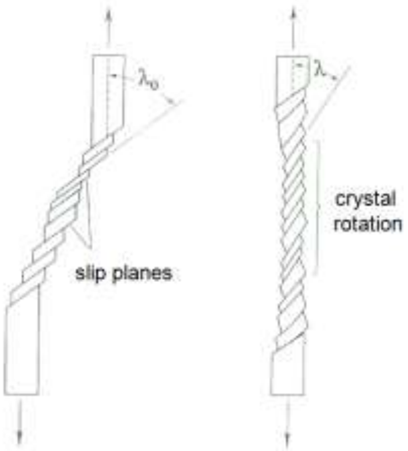
Boundary condition: determines lab frame constraints

Constraints lead to specific crystal rotations

Non-symmetric dislocation shear leads to rotation

Symmetric-shear can lead to shape change without rotation

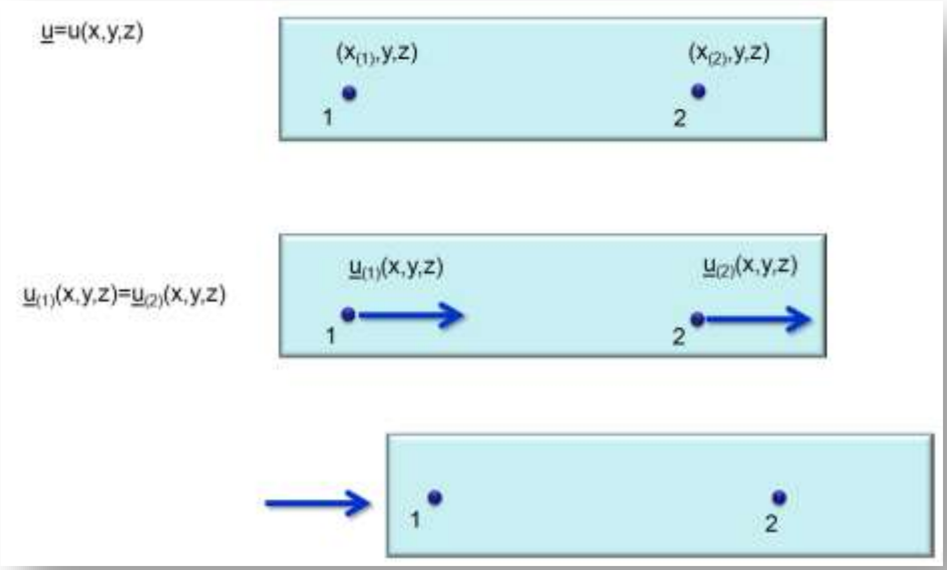
Change in local constraints leads to heterogeneity

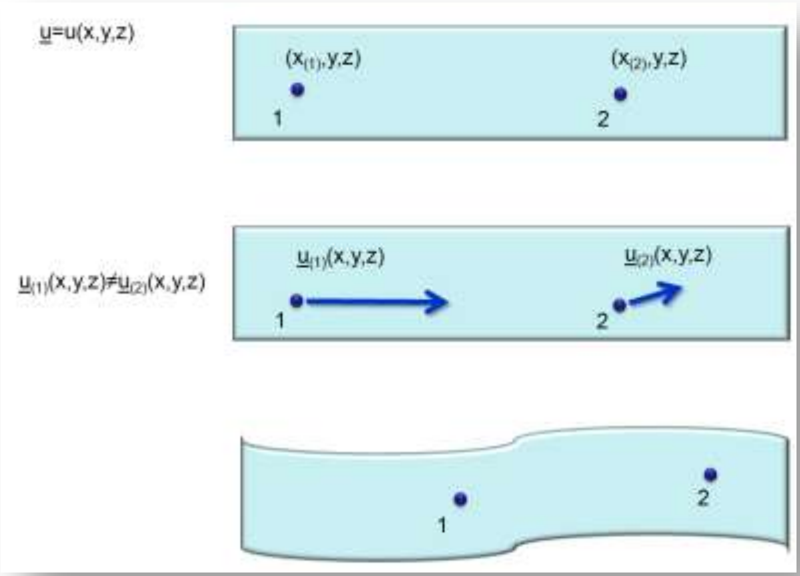


Roters et al. Acta Mater.58 (2010)

strain rates and displacement gradients in crystals

$$\dot{\varepsilon}_{ij}^{K} = D_{ij}^{K} = \frac{1}{2}\left(\dot{u}_{i,j}^{\mathrm{K}} + \dot{u}_{j,i}^{\mathrm{K}}\right) = \sum_{s=1}^{N} m_{ij}^{\mathrm{sym},s}\dot{\gamma}^{s} \qquad \text{mit} \qquad m_{ij}^{\mathrm{sym}} = m_{ji}^{\mathrm{sym}} = \frac{1}{2}\left(n_i b_j + n_j b_i\right)$$



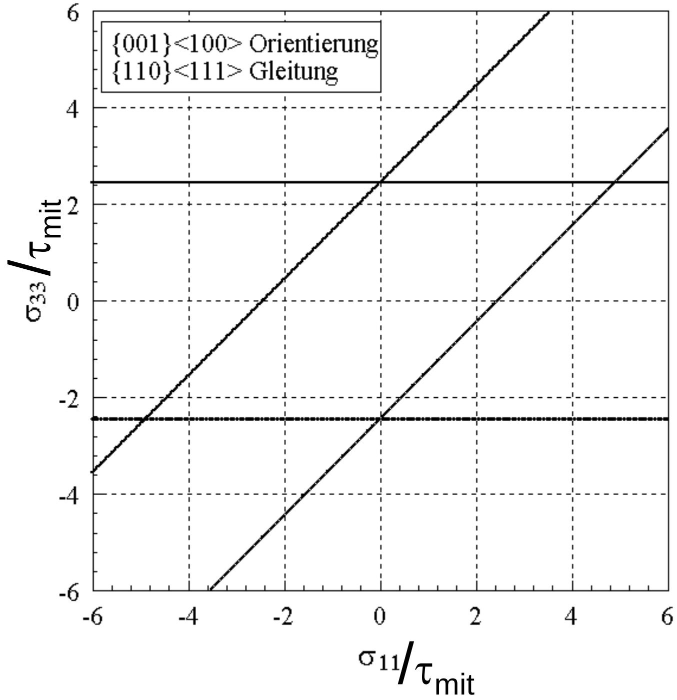


slip system s

$n_i^s \, , b_i^s$

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

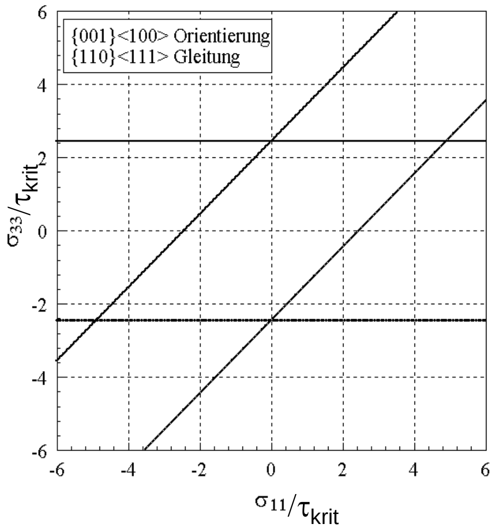
symmetric part $m_{kl}^{sym,s} = \frac{1}{2}\left(a_{ki}^c n_i^s \, a_{lj}^c b_j^s + a_{lj}^c n_j^s \, a_{ki}^c b_i^s\right)$

yield surface
(active systems)

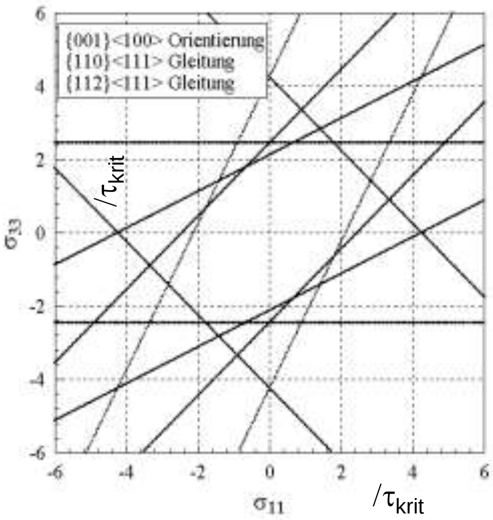
$$m_{kl}^{sym,s=aktiv}\sigma_{kl} = \sigma_{aufg}^s = \tau_{krit,(+)}^{s=aktiv}$$
$$m_{kl}^{sym,s=aktiv}\sigma_{kl} = \sigma_{aufg}^s = \tau_{krit,(-)}^{s=aktiv}$$

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

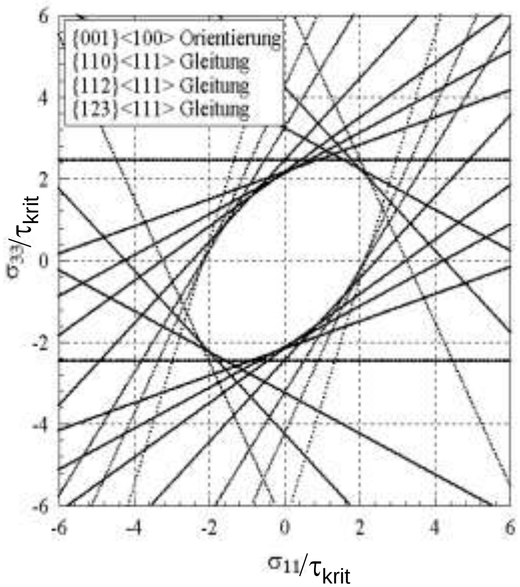
Single crystal plasticity: constructing the yield surface



FCC, BCC
12 systems
section



BCC
24 systems
section



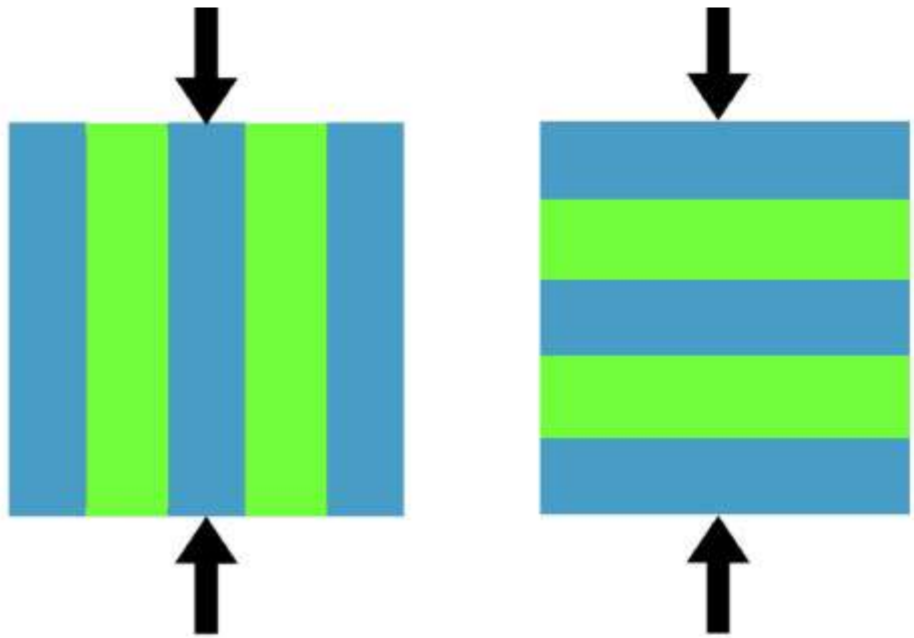
BCC
48 systems
section

YIELD SURFACE, BCC

SINGLE CRYSTAL, BCC, (001)[100]

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

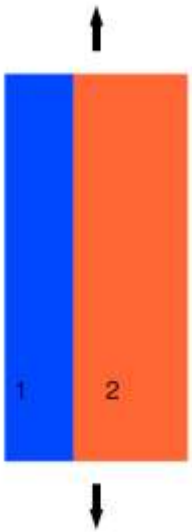
Iso-stress and iso-strain



Isostrain	Isostress
$\varepsilon = \varepsilon_s = \varepsilon_d$	$\varepsilon = \varepsilon_s + \varepsilon_d$
$\sigma = \sigma_s + \sigma_d$	$\sigma = \sigma_s = \sigma_d$
Displacement continuity across layers	Stress continuity across layers

Iso-stress and iso-strain

Bounding Case - Isostrain



$$\epsilon_1 = \epsilon_2 = \epsilon_{tot}$$

$$\sigma_1 = E_1 \epsilon_1 = E_1 \epsilon_{tot} \quad ; \quad \sigma_2 = E_2 \epsilon_2 = E_2 \epsilon_{tot}$$

$$P_1 = A_1 \sigma_1 = A_1 E_1 \epsilon_{tot} \quad ; \quad P_2 = A_2 \sigma_2 = A_2 E_2 \epsilon_{tot}$$

$$P_{tot} = P_1 + P_2 = \epsilon_{tot} (A_1 E_1 + A_2 E_2)$$

$$\sigma_{tot} = \frac{P_{tot}}{A_1 + A_2} = \epsilon_{tot} \left(\frac{A_1}{A_1 + A_2} E_1 + \frac{A_2}{A_1 + A_2} E_2 \right)$$

$$\sigma_{tot} = (f_1 E_1 + f_2 E_2) \epsilon_{tot}$$

$$\boxed{E_{tot} = f_1 E_1 + f_2 E_2}$$

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

$$\sigma_1 = \sigma_2 = \sigma_{tot}$$

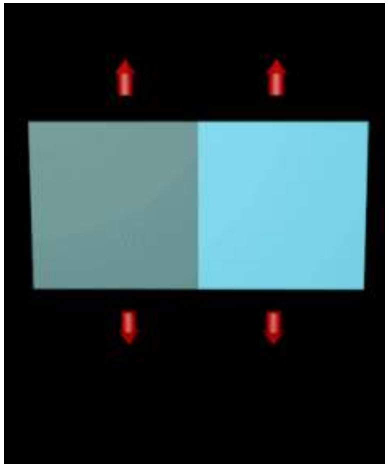
$$\sigma_1 = E_1 \epsilon_1 \quad ; \quad \sigma_2 = E_2 \epsilon_2$$

$$\epsilon_{tot} = f_1 \epsilon_1 + f_2 \epsilon_2 = f_1 \frac{\sigma_{tot}}{E_1} + f_2 \frac{\sigma_{tot}}{E_2}$$

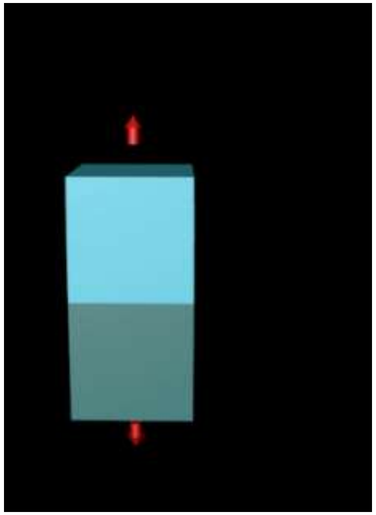
$$\boxed{E = \frac{\sigma_{tot}}{\epsilon_{tot}} = \frac{1}{\frac{f_1}{\epsilon_1} + \frac{f_2}{\epsilon_2}} = \frac{E_1 E_2}{f_1 E_2 + f_2 E_1}}$$

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):

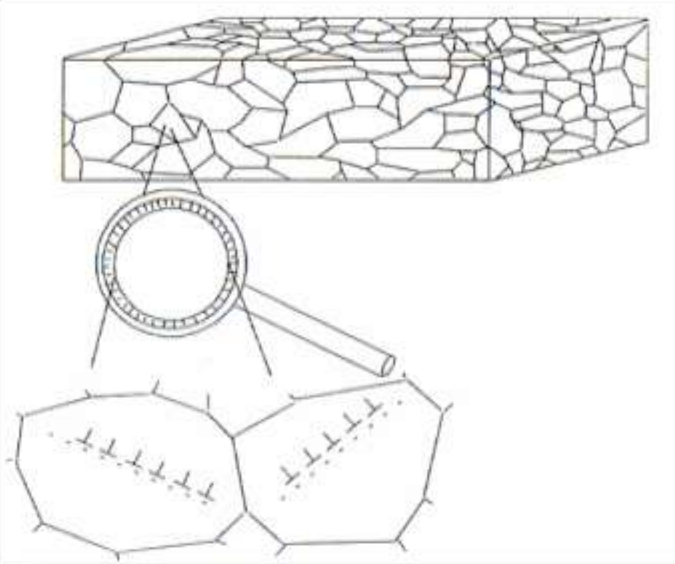
- All grains with aggregate or polycrystal experience the same state of stress;
- Equilibrium condition across the grain boundaries satisfied;
- Compatibility conditions between the grains violated, thus, finite strains will lead to gaps and overlaps between grains;
- Generally most successful for single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

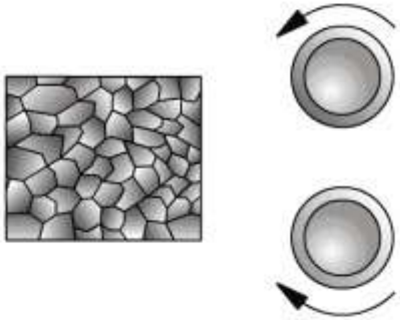
Taylor Model (this lecture):

- 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.

Polycrystal model

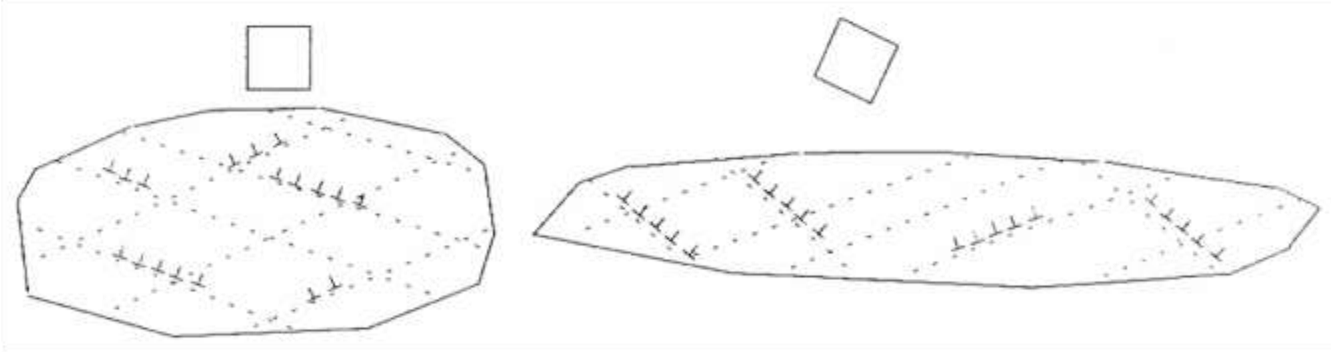
- **Taylor model for the mechanics of polycrystals**





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

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

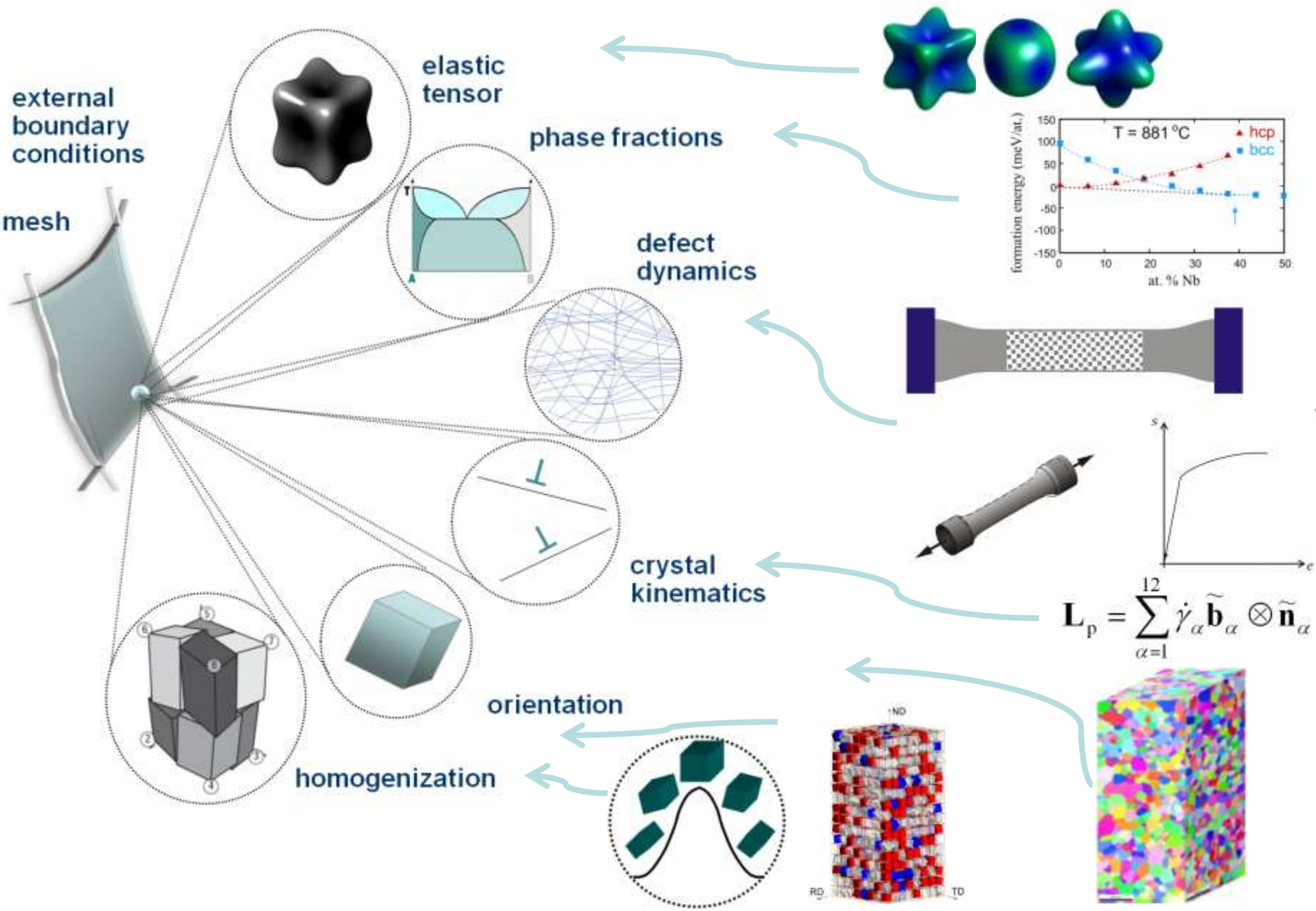


plastic spin from polar decomposition

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

- Examples

Multiscale crystal plasticity FEM



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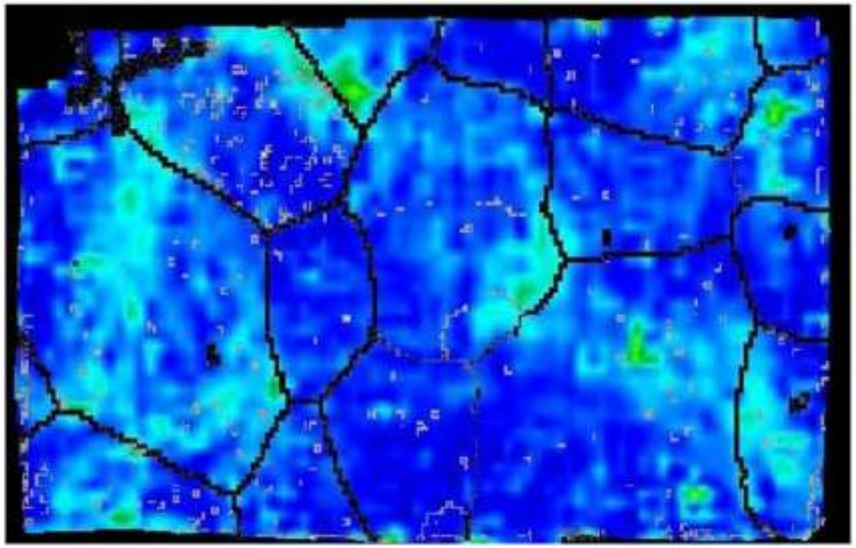
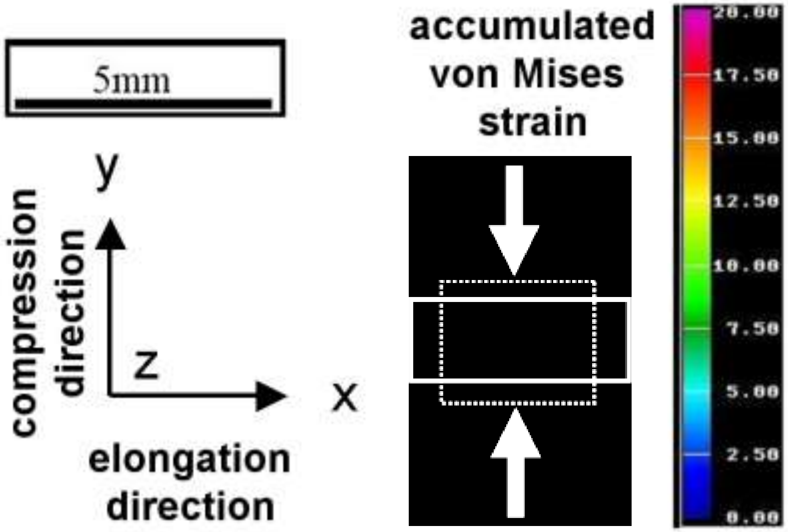
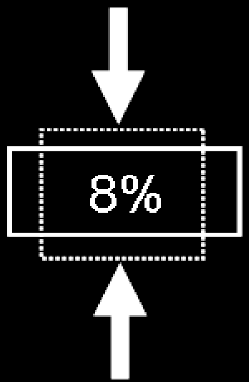


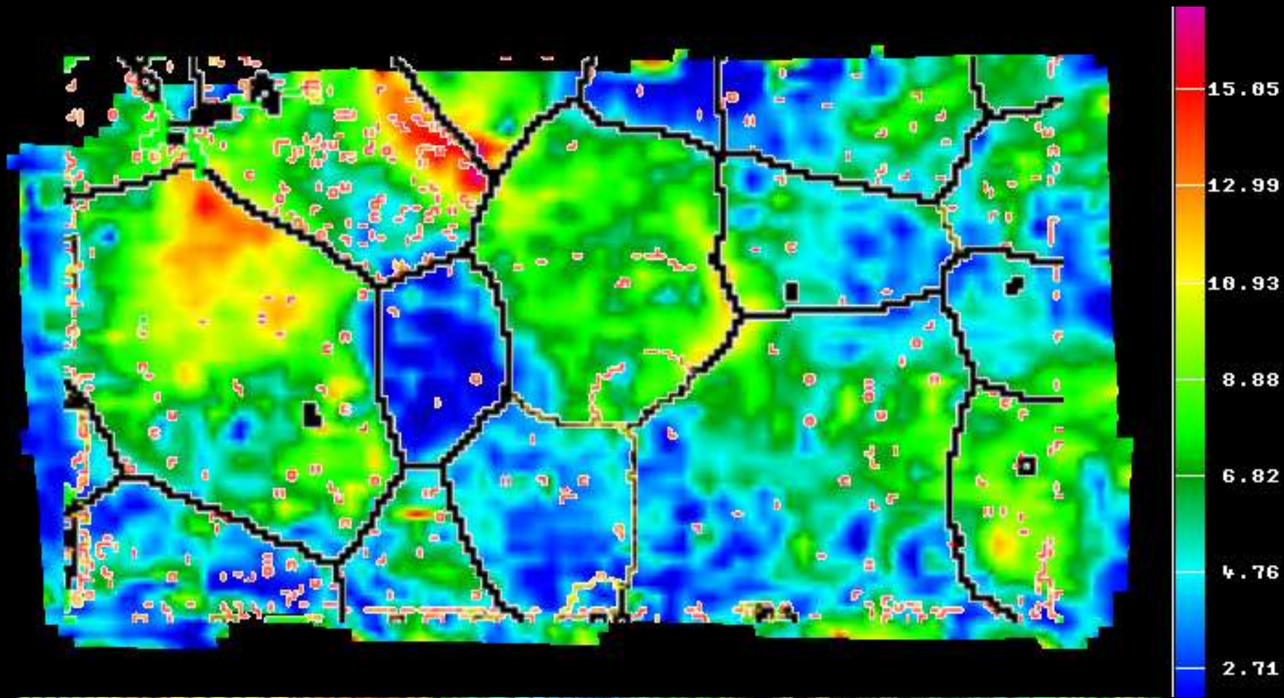


Raabe et al. Acta Mater. 49 (2001) 3433

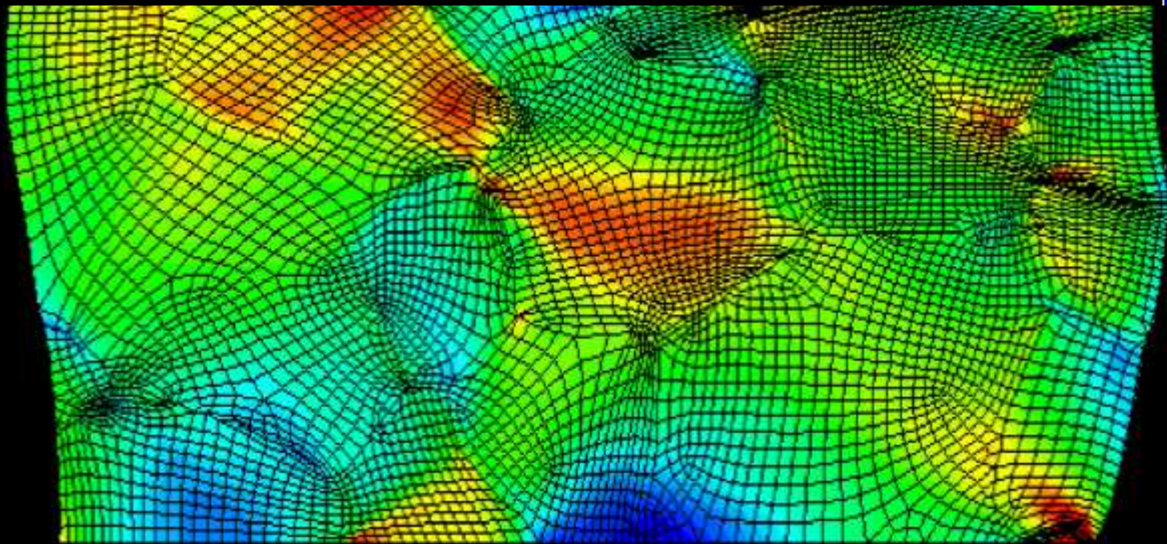
Sachtleber, Zhao, Raabe: Mater. Sc. Engin. A 336 (2002) 81

Crystal Mechanics FEM, grain scale mechanics (2D)

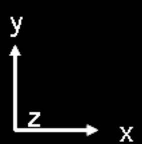




Experiment
(DIC, EBSD)
v Mises strain

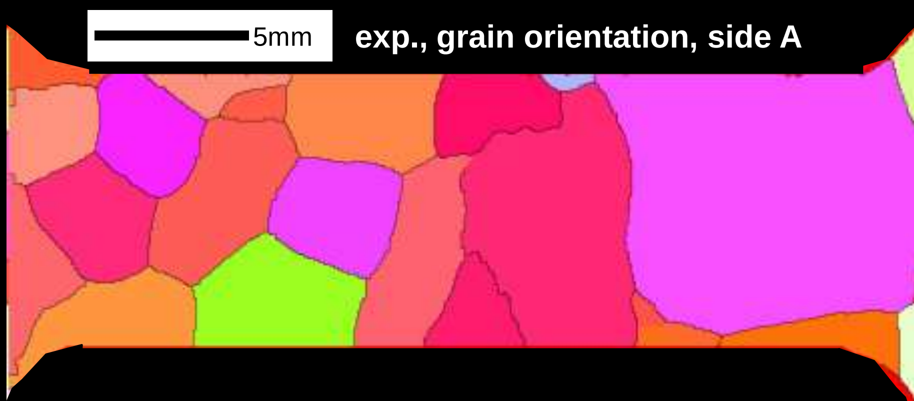


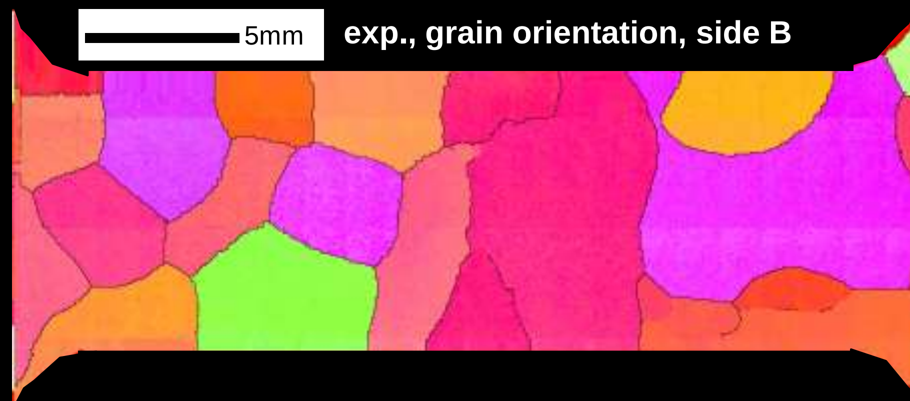
Simulation
(CP-FEM)
v Mises strain

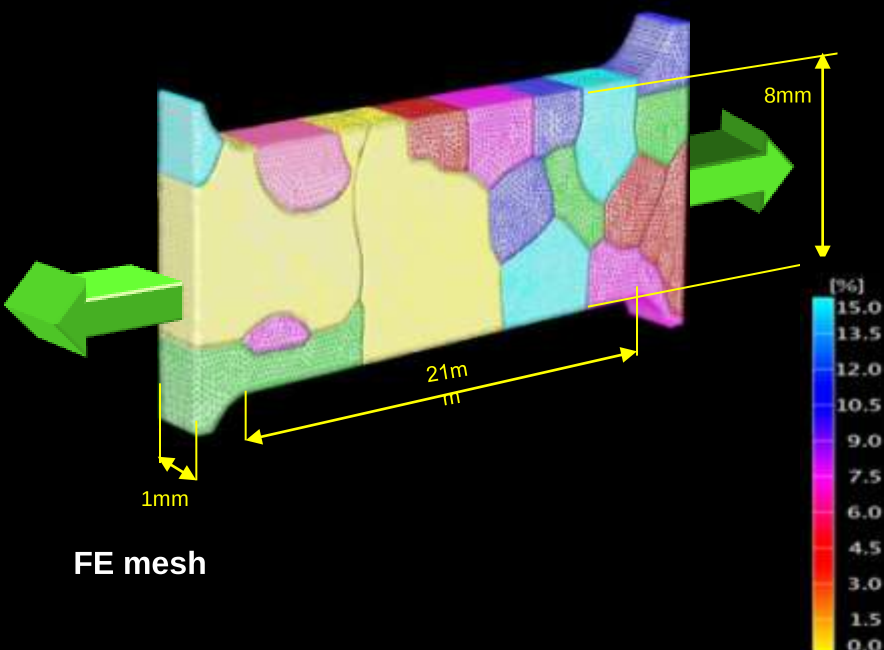


Sachtleber, Zhao, Raabe: Mater. Sc. Engin. A 336 (2002) 81

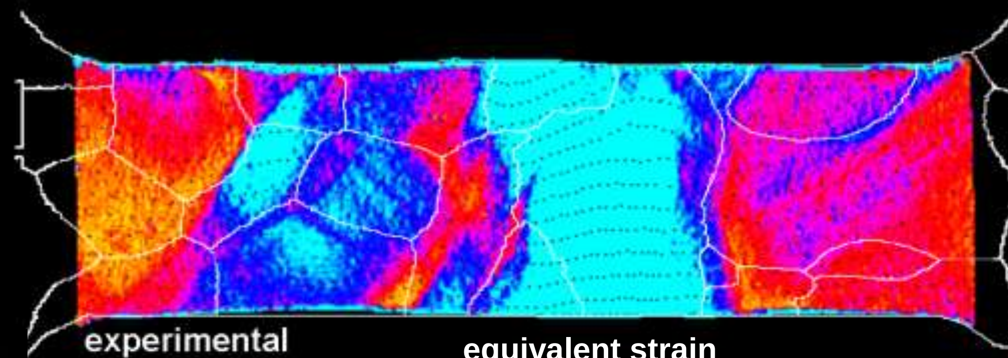
Crystal plasticity FEM, grain scale mechanics (3D Al)

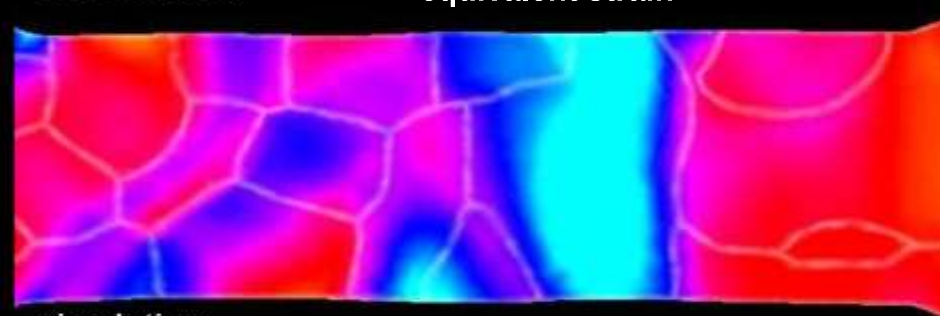




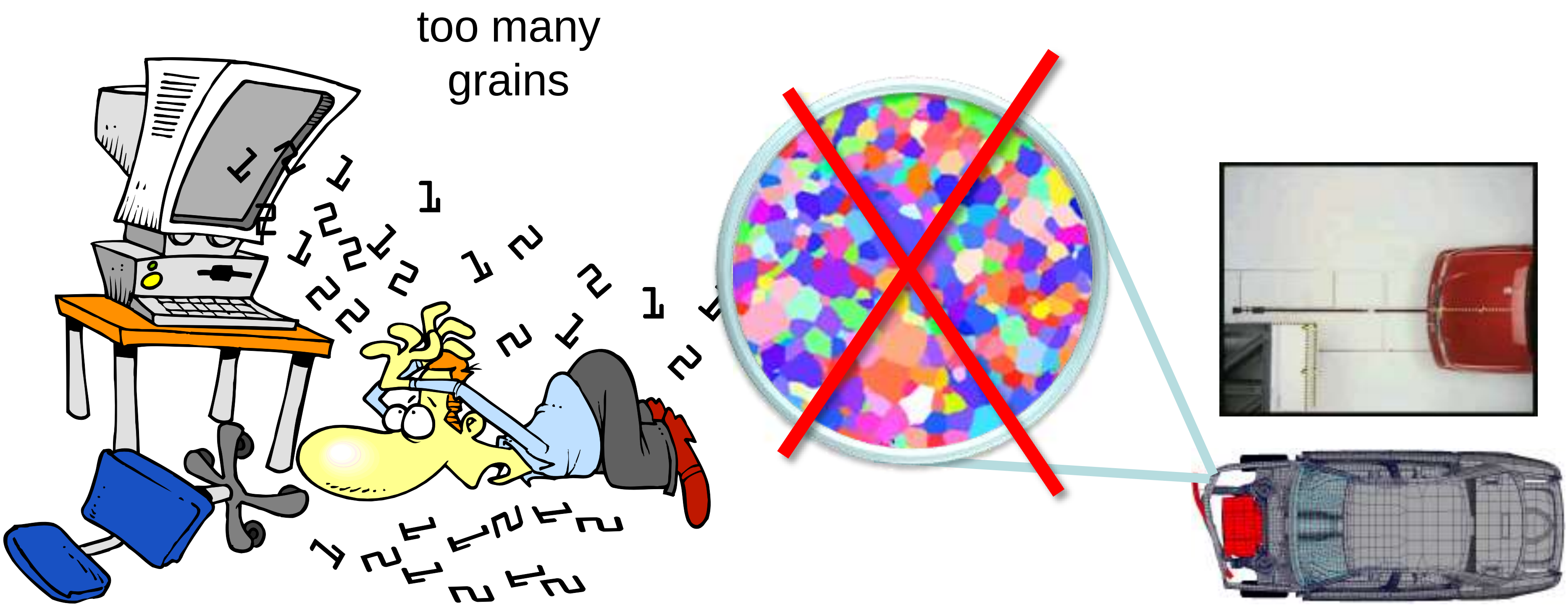


FE mesh

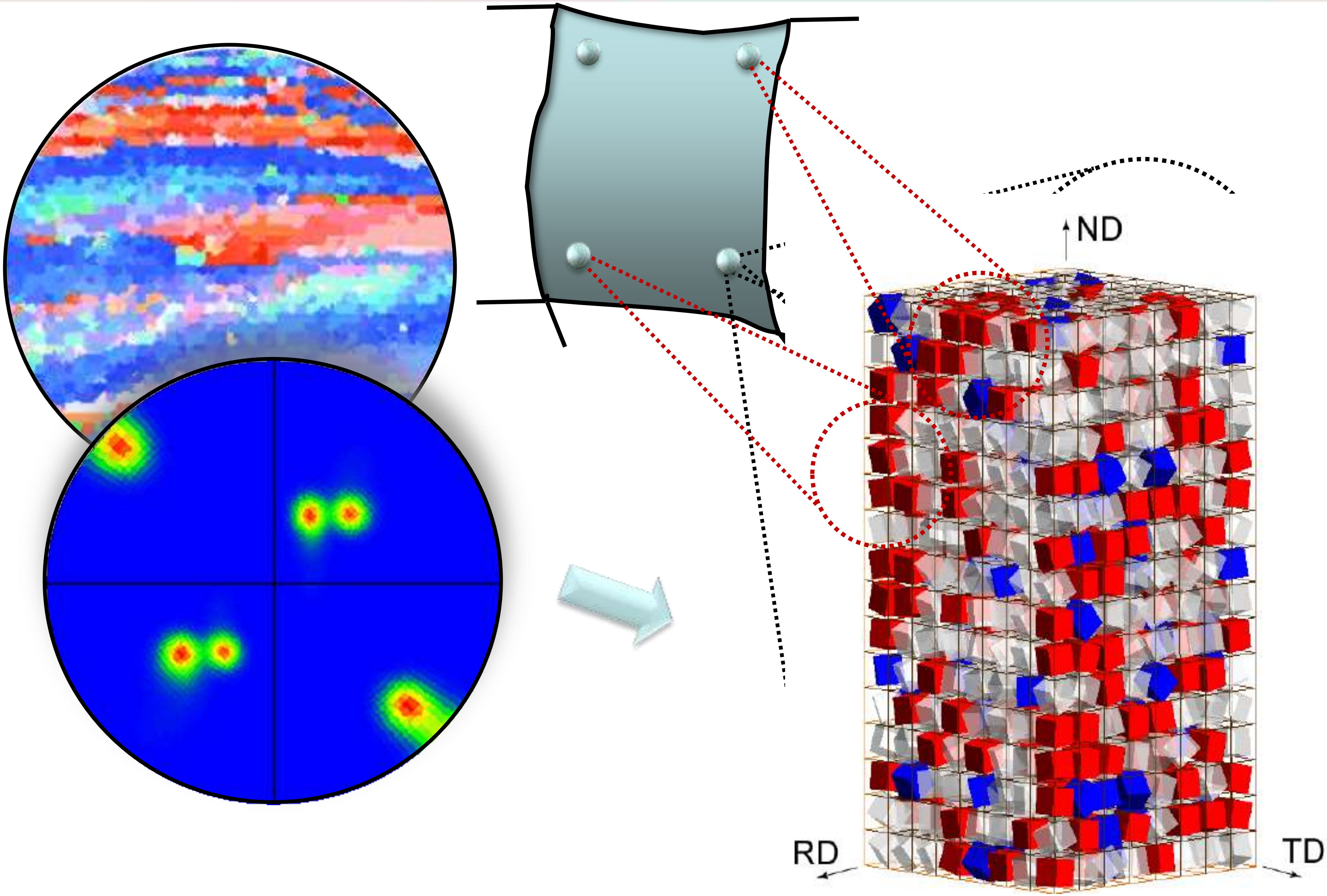




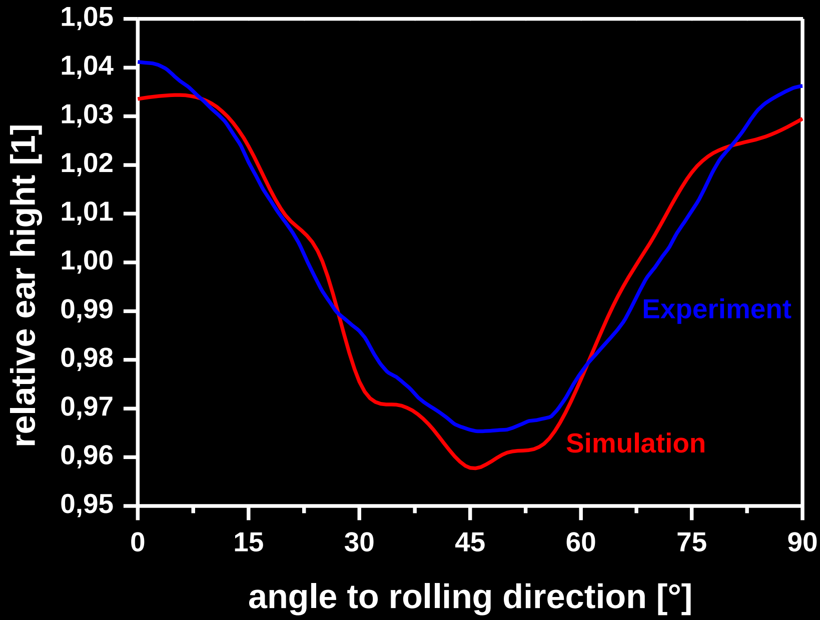
Crystal plasticity FEM for large scale forming predictions

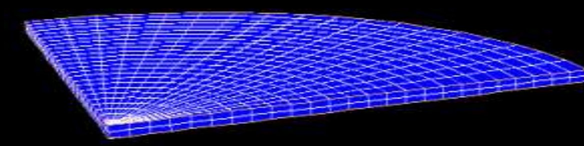


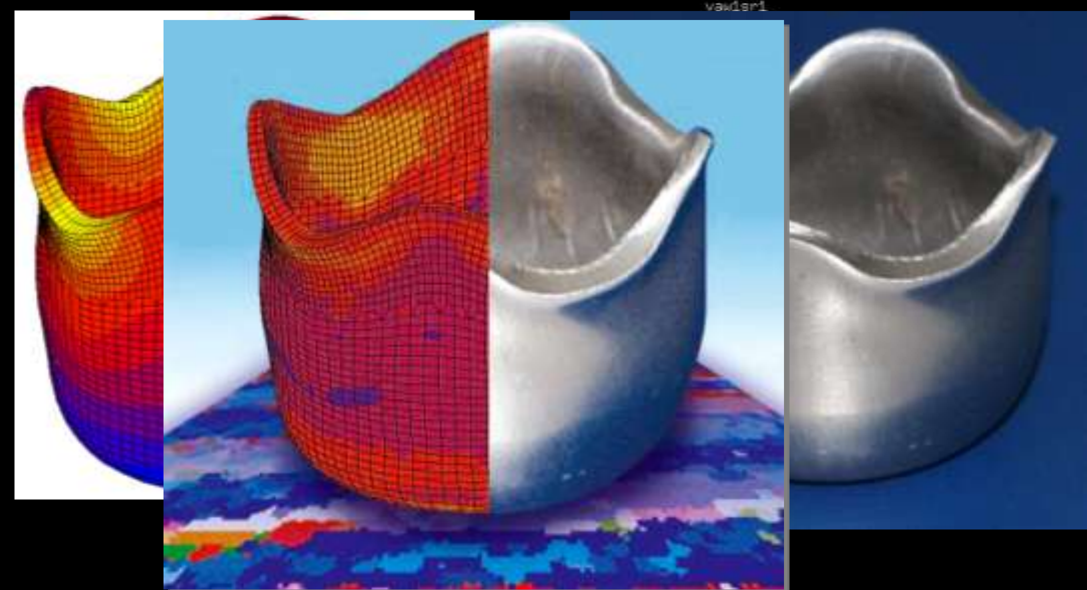
Texture component crystal plasticity FEM for large scale forming



Texture component crystal plasticity FEM for large scale forming

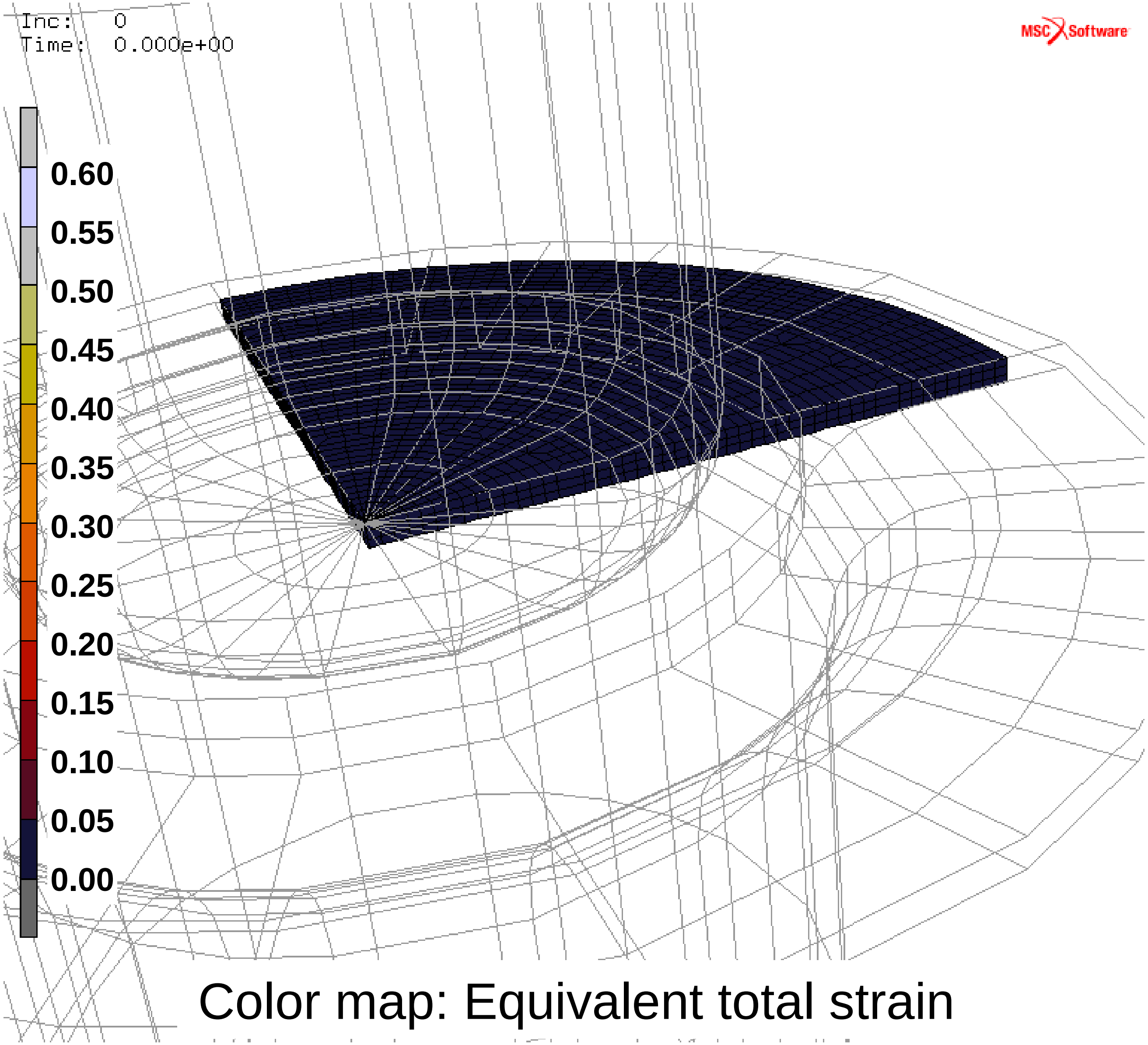






D. Raabe and F. Roters: Intern. J. Plast. 20 (2004) 339

Simulation result: Taylor model



Color map: Equivalent total strain

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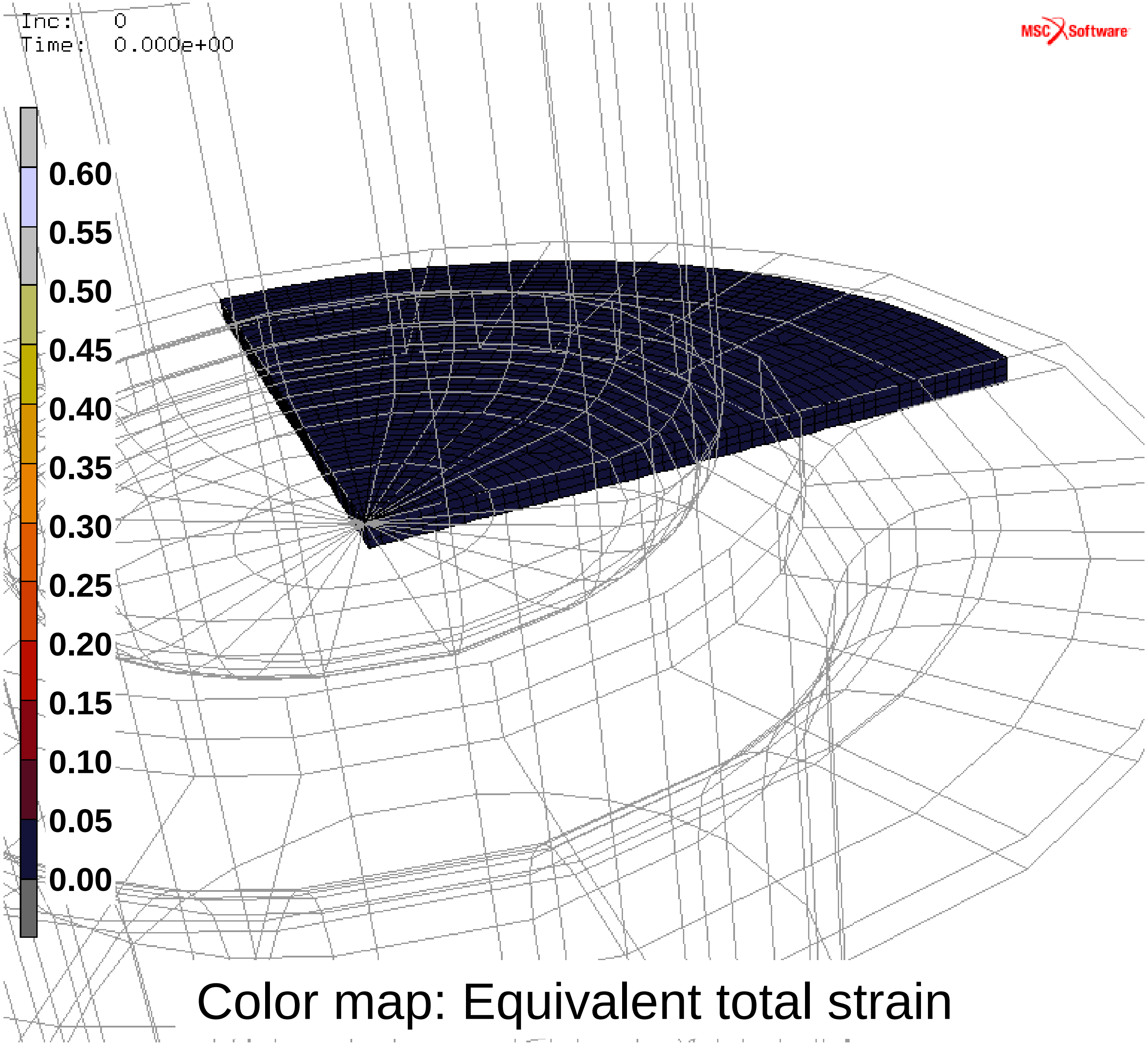
Simulation result: RGC scheme



Color map: Equivalent total strain

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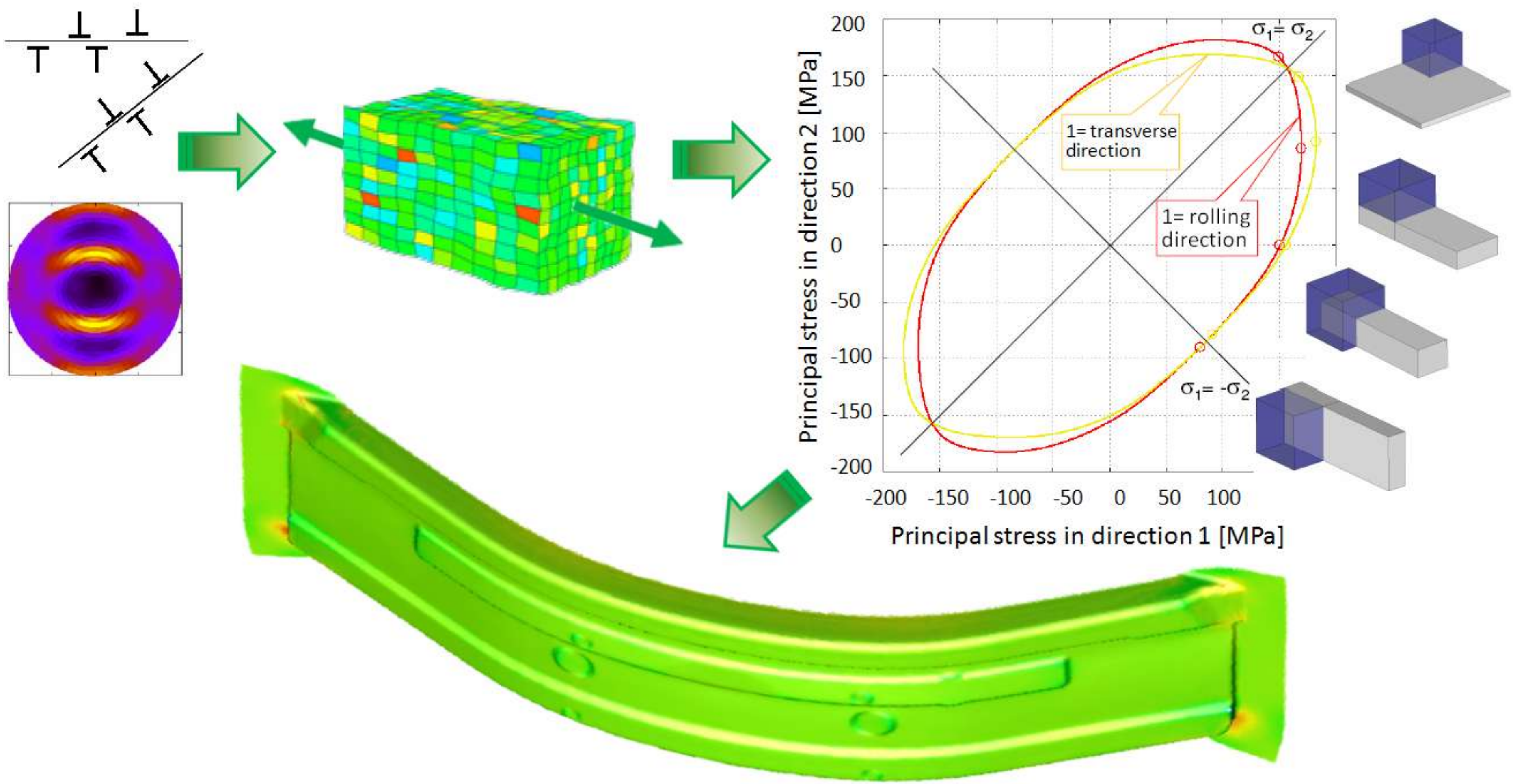
Numerical Laboratory: From CPFEM to yield surface (engineering)



DC04 study with Mercedes, Volkswagen, Audi, Inpro