Crystal mechanics and anisotropy

problem formulation

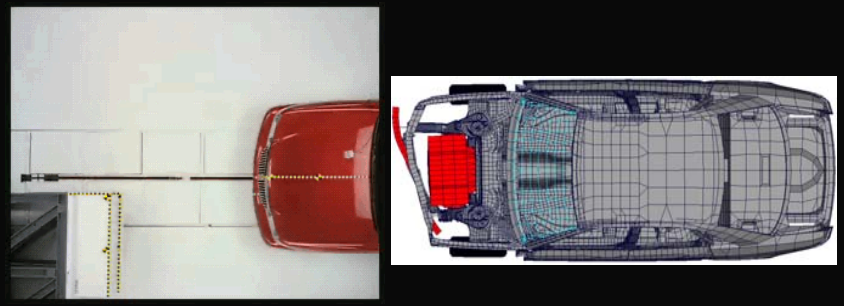
Motivation: Basics of crystal mechanics

Reason #1: basics: connection between (simple) kinematics and (complex) dislocation mechanics; crystal mechanics beyond the single crystal; boundary condition treatment in larger crystal aggregates, homogenization at small scales

Reason #2: small-scale experiments cannot be interpreted without quantitative theoretical mechanics treatment

Motivation: Engineering, Crystal Mechanics

mechanical metalllurgy 2000 B.C.



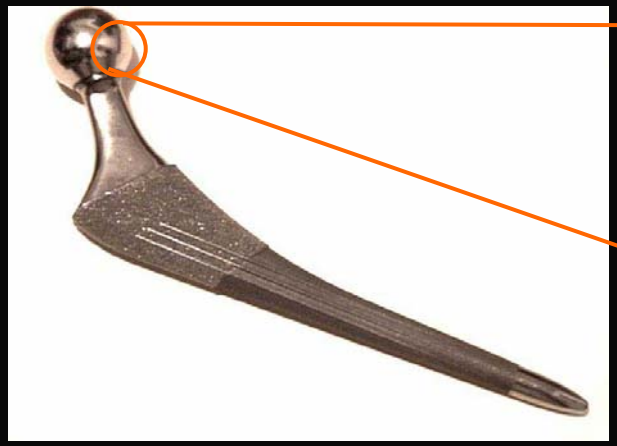
mechanical metalllurgy 2000 A.D.

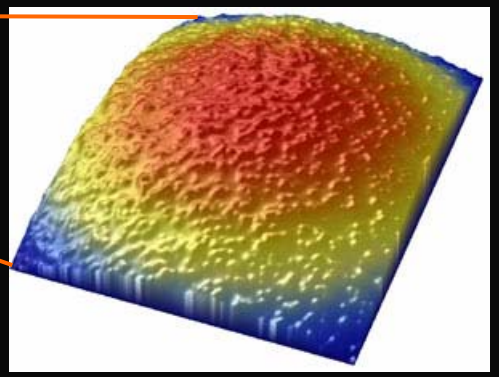
Reason #3: understand macromechanics in terms of micromechanics
(2 essential examples given)

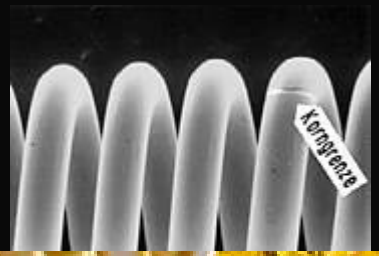
beer can 1820 A.D.

beer can 2000 A.D.

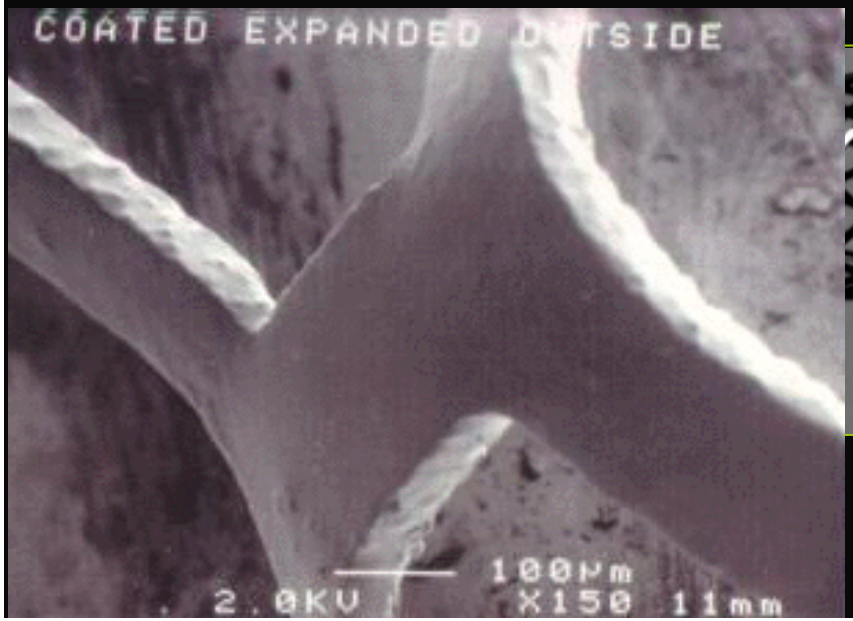
Motivation: Crystal Mechanics at Small Scales

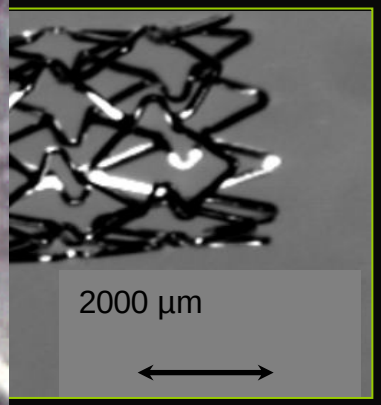


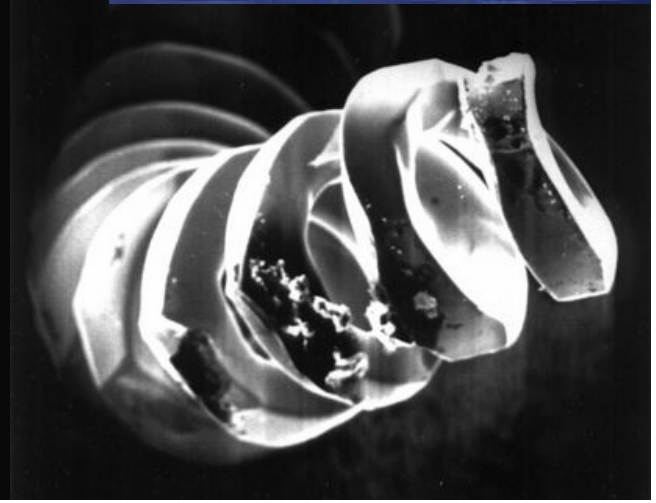




Reason #4: micromechanics as product property: surface, direct grain anisotropy, damage,…







Motivation: Basics of crystal mechanics

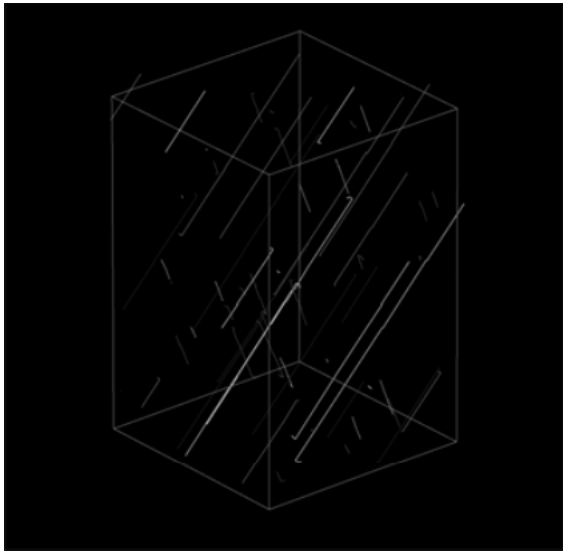
Reason #1: basics: connection between (simple) kinematics and (complex) dislocation mechanics; crystal mechanics beyond the single crystal; boundary condition treatment in larger crystal aggregates, homogenization at small scales

Reason #2: small-scale experiments cannot be interpreted without quantitative theoretical mechanics treatment

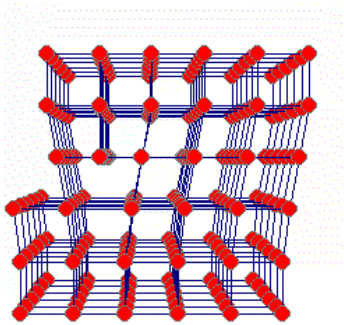
Overview

connection between crystal orientation and lattice defect mechanics (here: dislocations)

Motivation: Fundamentals of crystal mechanics

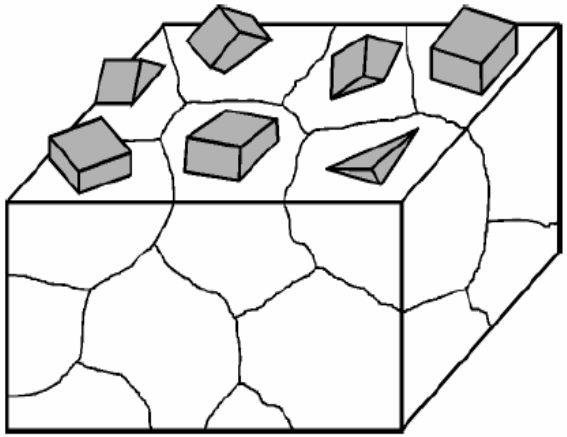


parallel loops

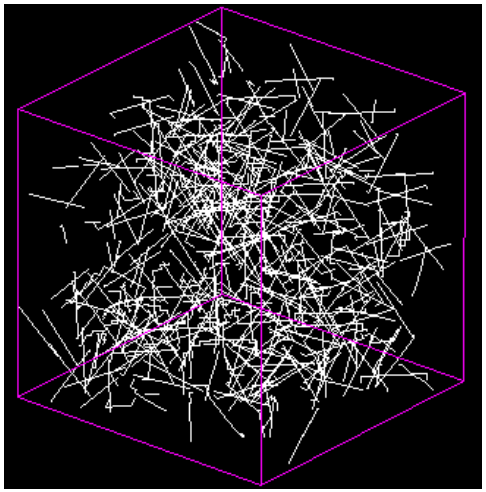


one dislocation

mesoscopic boundary conditions
(grain / orientation neighborhood)



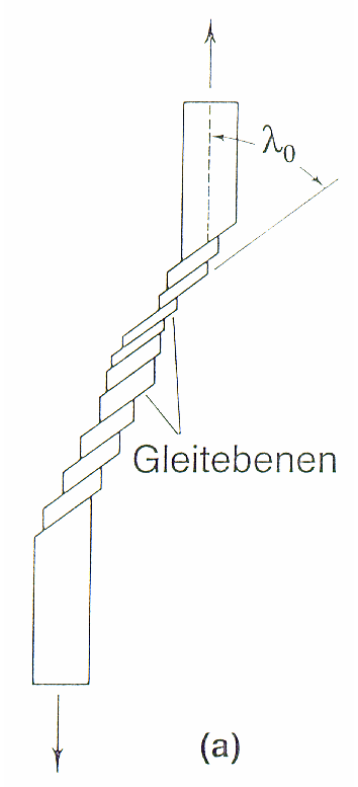
reactions



spin (orientation change)

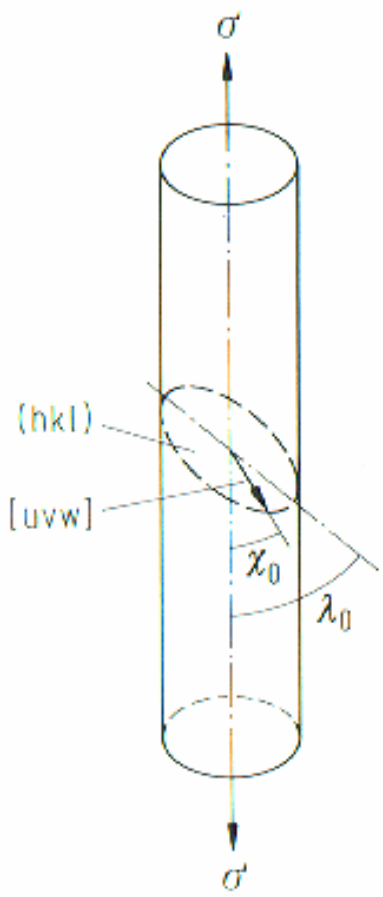
Motivation: Fundamentals of crystal mechanics

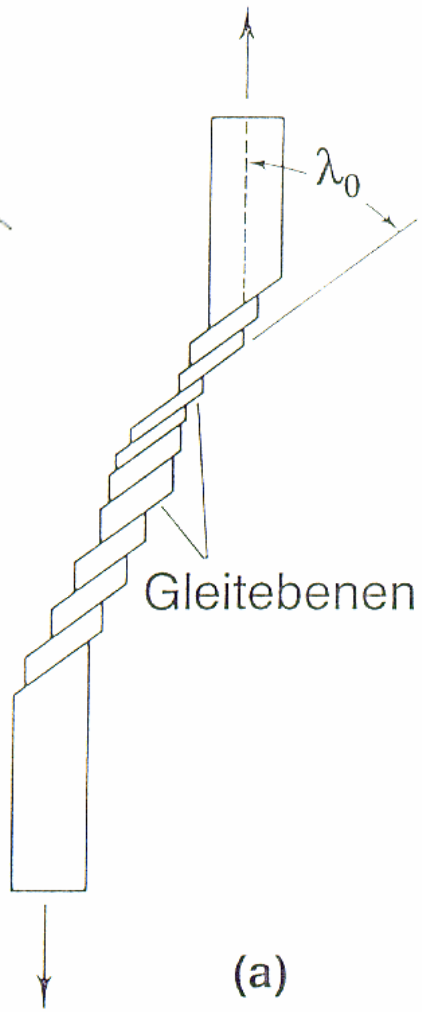
<u>kinematics</u>:
strain (symmetric part of plasticity)



<u>kinematics</u>:
rotation / texture (antisymmetric part of plasticity)

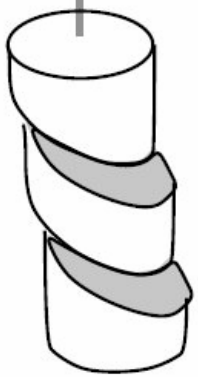
single crystal level





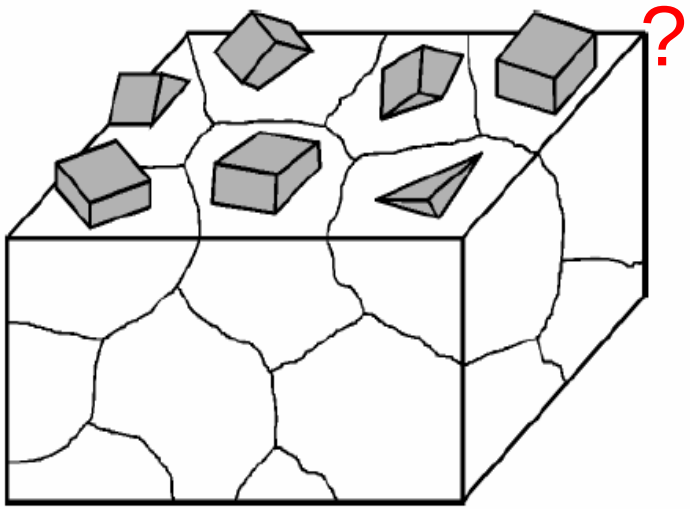
Plastically stretched zinc single crystal.

Adapted from Fig. 7.9, *Callister 6e.* (Fig. 7.9 is from C.F. Elam, *The Distortion of Metal Crystals*, Oxford University Press, London, 1935.)

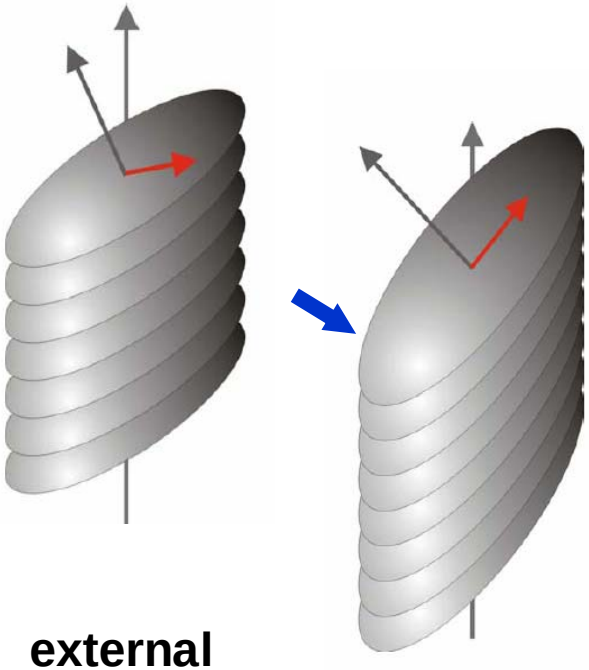


Adapted from Fig. 7.8, *Callister 6e.*

strain is the symmetric part of the displacement gradient

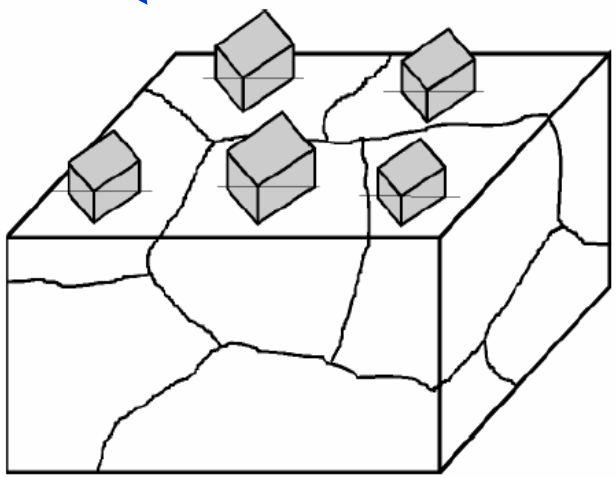


internal boundary conditions



external boundary conditions

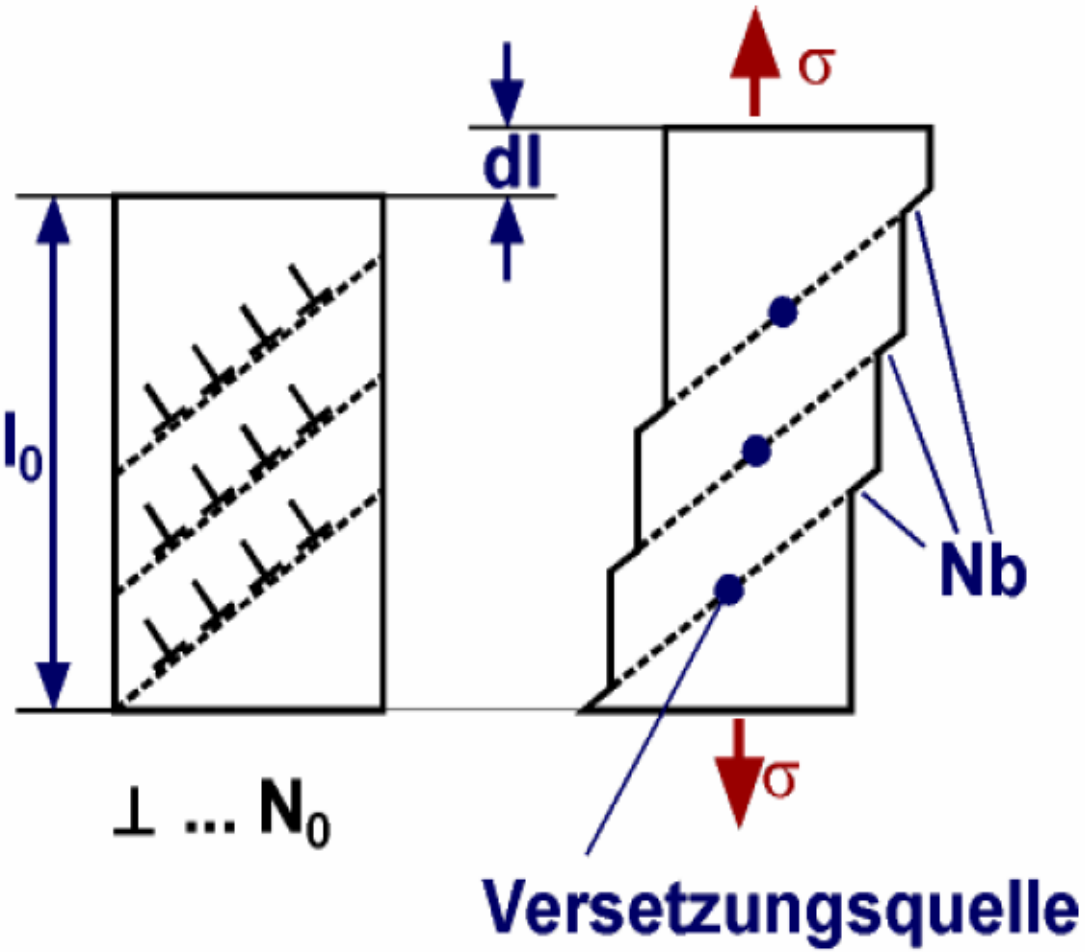
?



rotation (texture) is the antisymmetric part of the displacement gradient

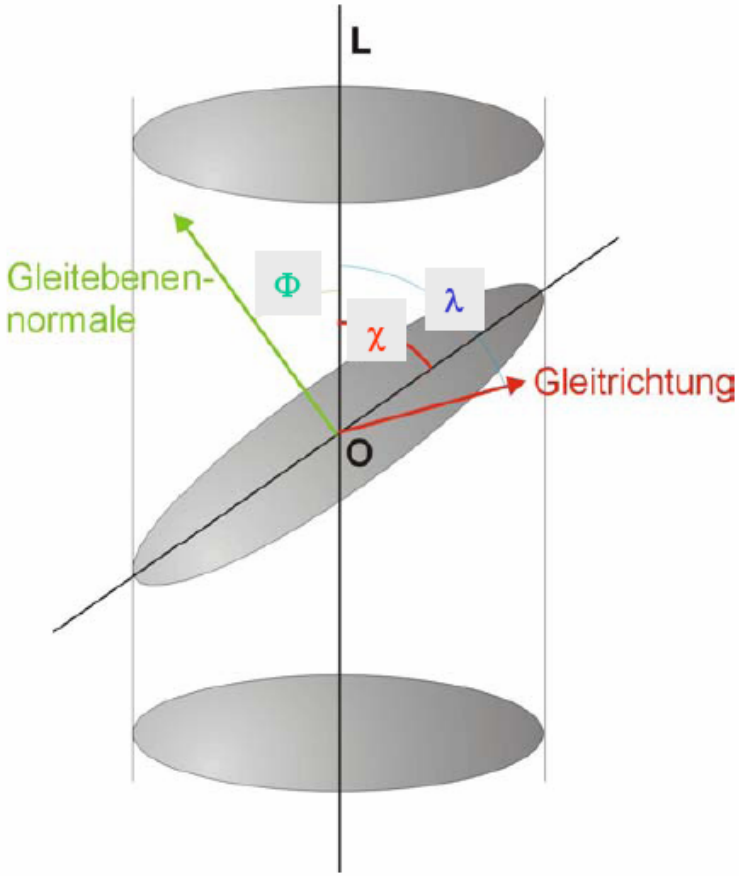
Crystal mechanics and anisotropy

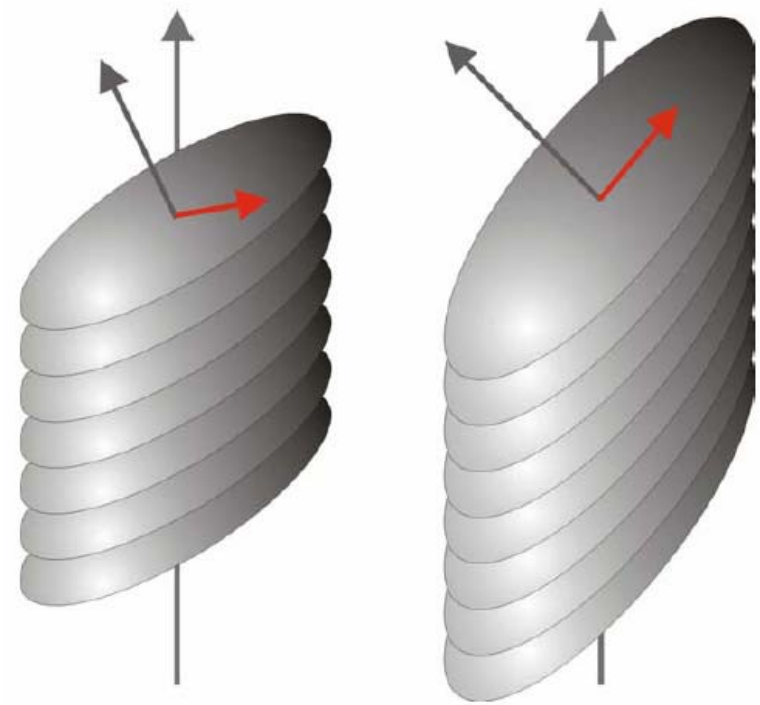
single crystal level



Anisotropy of plasticity

single crystal plasticity



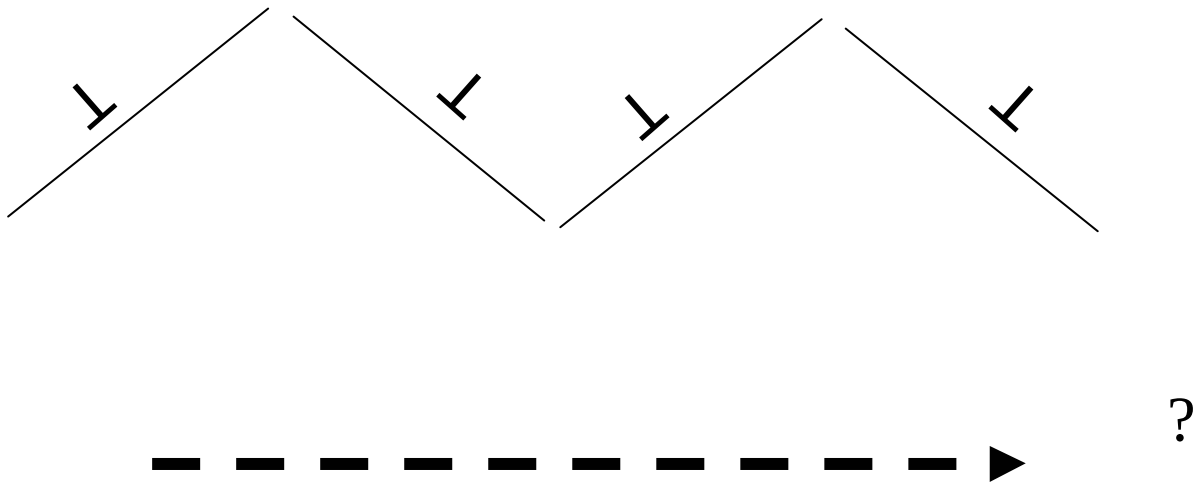


Anisotropy of plasticity

single crystal level

strain rates and displacement gradients in crystals

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



single crystal level

strain rates and displacement gradients in crystals

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

plastic spin from polar decomposition

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

example

$$\mathbf{n} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\end{pmatrix},\ \mathbf{b} = \begin{pmatrix}0\\0\\1\end{pmatrix},\ \mathbf{L} = \frac{\dot{\gamma}}{\sqrt{2}}\begin{pmatrix}0&0&1\\0&0&1\\0&0&0\end{pmatrix},\ \mathbf{D} = \frac{\dot{\gamma}}{2\sqrt{2}}\begin{pmatrix}0&0&1\\0&0&1\\1&1&0\end{pmatrix},\ \mathbf{W} = \frac{\dot{\gamma}}{2\sqrt{2}}\begin{pmatrix}0&0&1\\0&0&1\\-1&-1&0\end{pmatrix}$$

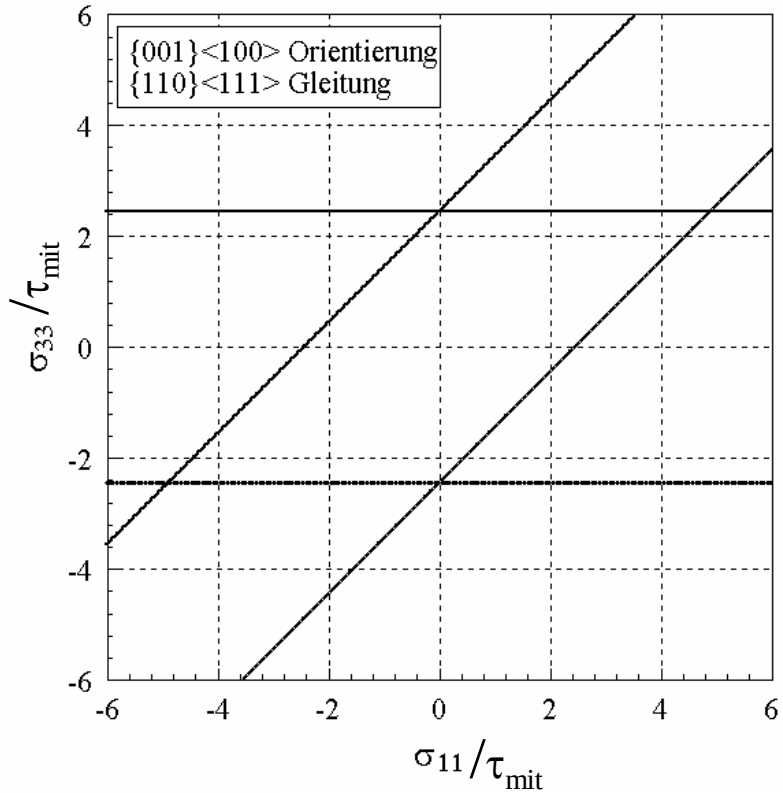
single crystal level

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

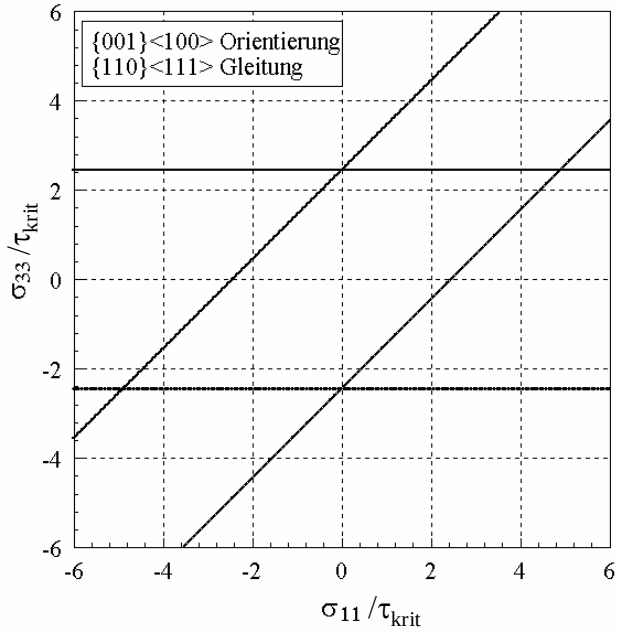
symmetric part $$m_{kl}^{sym,s} = \frac{1}{2}\left(a_{ki}^c \, n_i^s \; a_{lj}^c \, b_j^s + a_{lj}^c \, n_j^s \; a_{ki}^c \, b_i^s\right)$$

yield surface
(active systems)

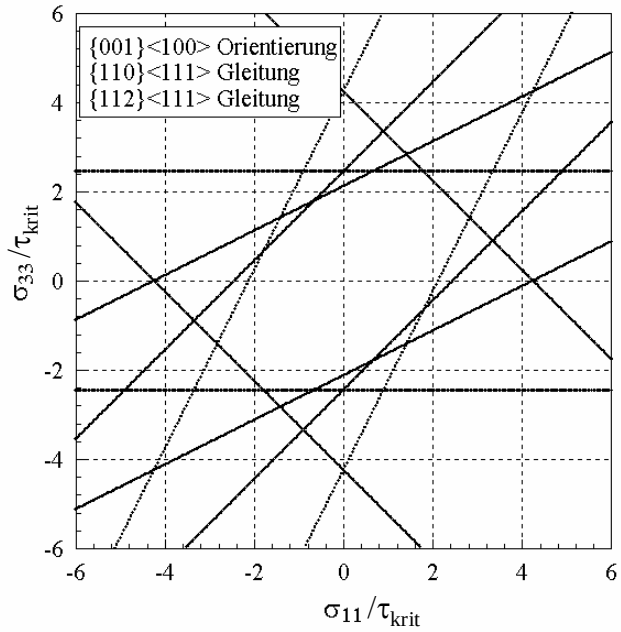
$$m_{kl}^{sym,s=aktiv} \sigma_{kl} = \sigma_{aufg}^s = \tau_{krit,(+)}^{s=aktiv}$$

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

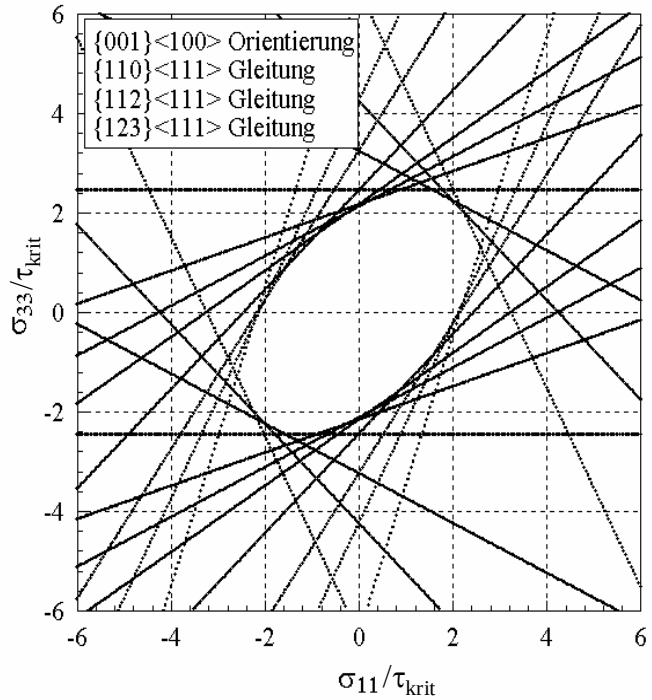
(non-active systems) $$m_{kl}^{sym,s=inaktiv} \sigma_{kl} = \sigma_{aufg}^s < \tau_{krit,(\pm)}^{s=inaktiv}$$



krz, kfz, Schnitt



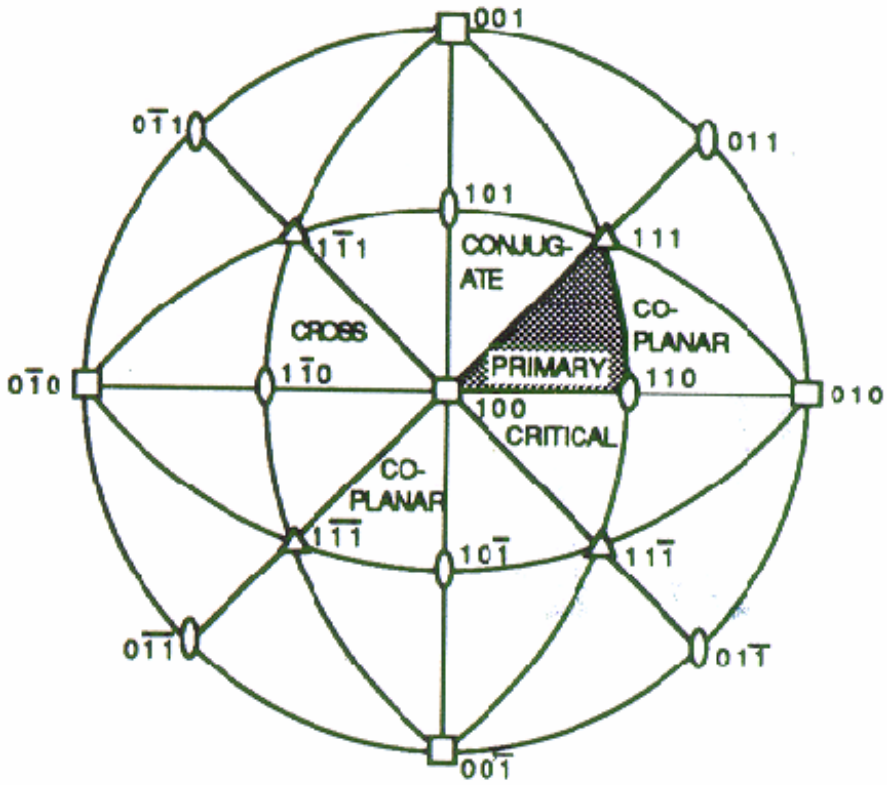
krz, 24 Systeme, Schnitt

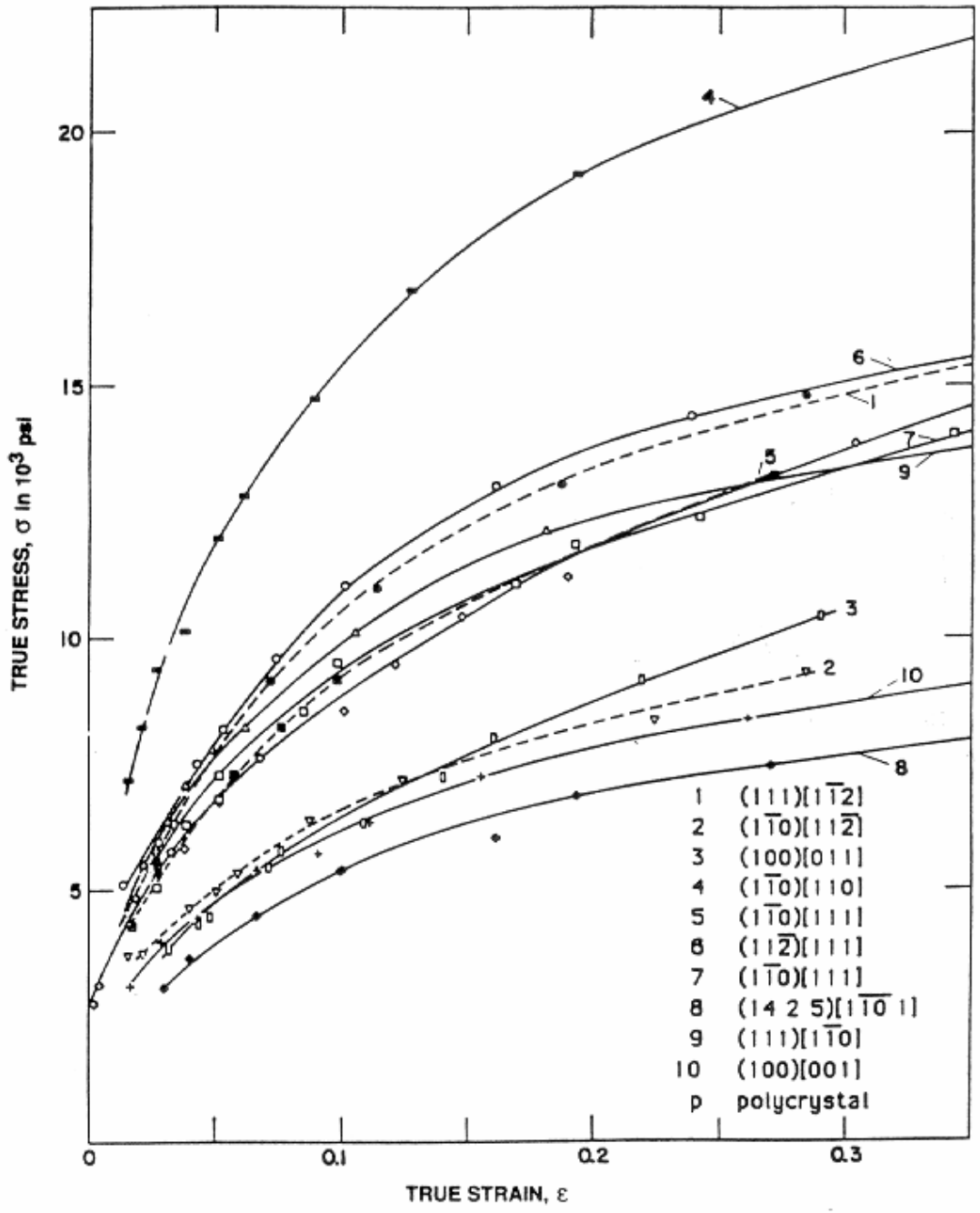


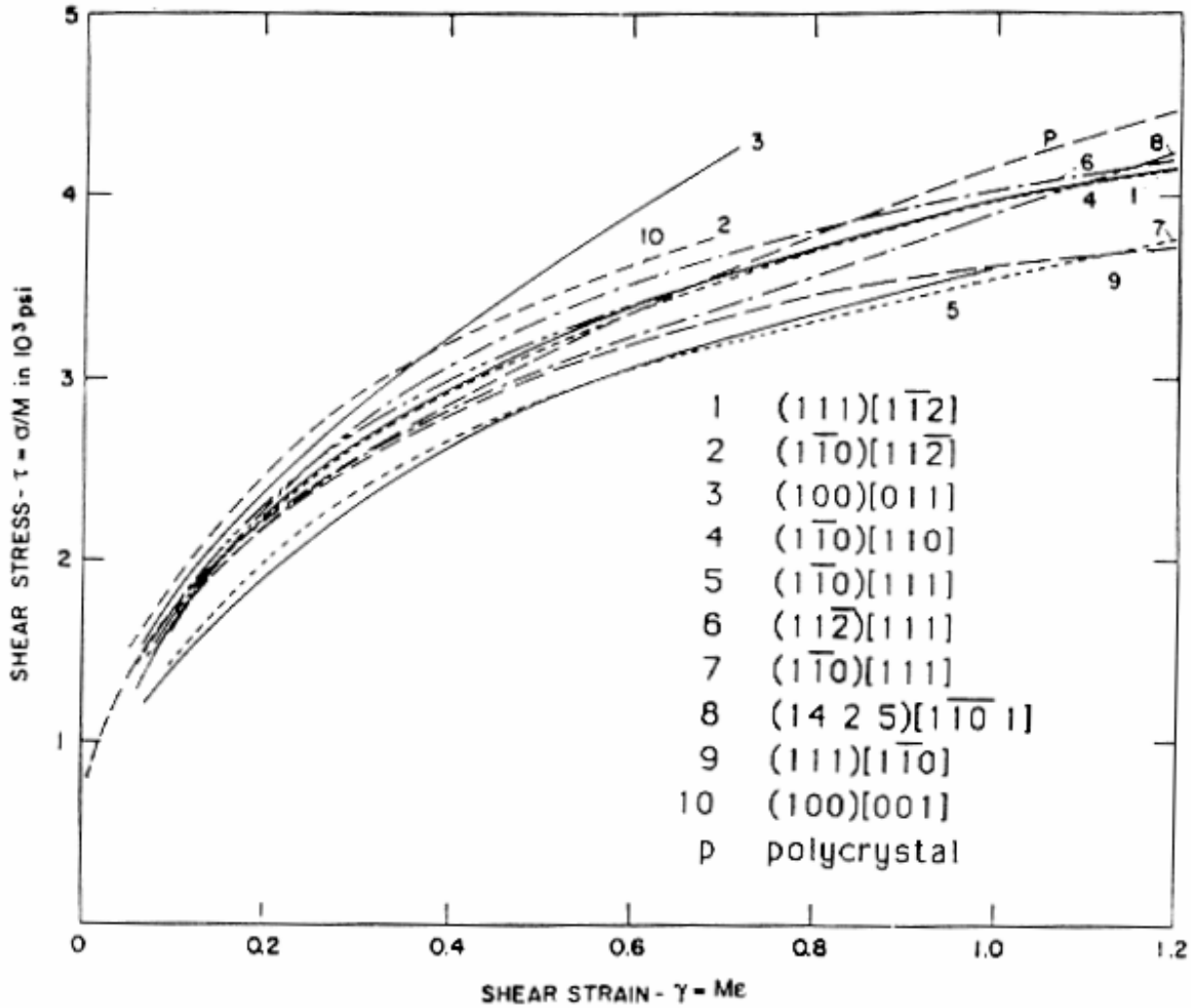
krz, 48 Systeme, Schnitt

yield surface, bcc

single crystal, bcc, (001)[100]

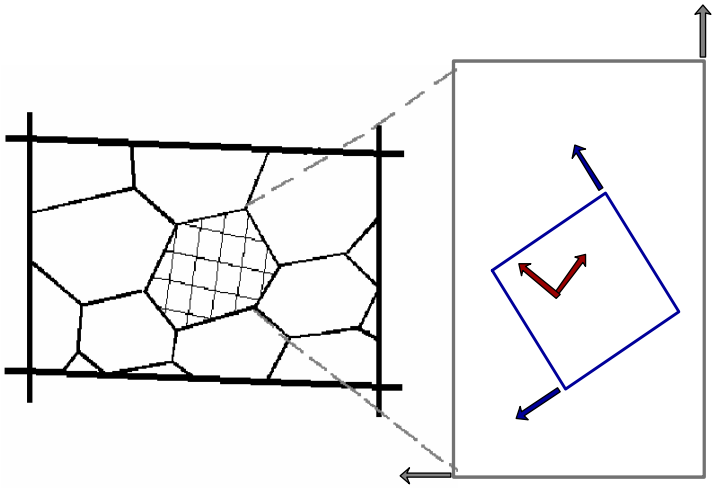

001
0$\bar{1}$1
011
101
1$\bar{1}$1
111
CONJUG-
ATE
CO-
PLANAR
CROSS
PRIMARY
0$\bar{1}$0
1$\bar{1}$0
110
010
100
CRITICAL
CO-
PLANAR
1$\bar{1}\bar{1}$
10$\bar{1}$
11$\bar{1}$
0$\bar{1}\bar{1}$
01$\bar{1}$
00$\bar{1}$


TRUE STRESS, σ in 10^3 psi
TRUE STRAIN, ε
0
0.1
0.2
0.3
5
10
15
20
1 (111)[1$\bar{1}$2]
2 (1$\bar{1}$0)[11$\bar{2}$]
3 (100)[011]
4 (1$\bar{1}$0)[110]
5 (1$\bar{1}$0)[111]
6 (11$\bar{2}$)[111]
7 (1$\bar{1}$0)[111]
8 (14 2 5)[1$\bar{1}$0 1]
9 (111)[1$\bar{1}$0]
10 (100)[001]
p polycrystal


SHEAR STRESS - τ = σ/M in 10³ psi
SHEAR STRAIN - γ = Mε
0
0.2
0.4
0.6
0.8
1.0
1.2
1
2
3
4
5
1 (111)[1$\bar{1}$2]
2 (1$\bar{1}$0)[112$\bar{}$]
3 (100)[011]
4 (1$\bar{1}$0)[110]
5 (1$\bar{1}$0)[111]
6 (112$\bar{}$)[111]
7 (1$\bar{1}$0)[111]
8 (14 2 5)[1$\bar{1}$0 1]
9 (111)[1$\bar{1}$0]
10 (100)[001]
p polycrystal

Crystal mechanics and anisotropy

polycrystal level



slip systems

$\vec{n}\,\vec{b}$

crystal (k,l)

$m_{kl} = n_k b_l$

sample (i,j)

$m_{ij} = a_{ik} n_k \; a_{jl} b_l$

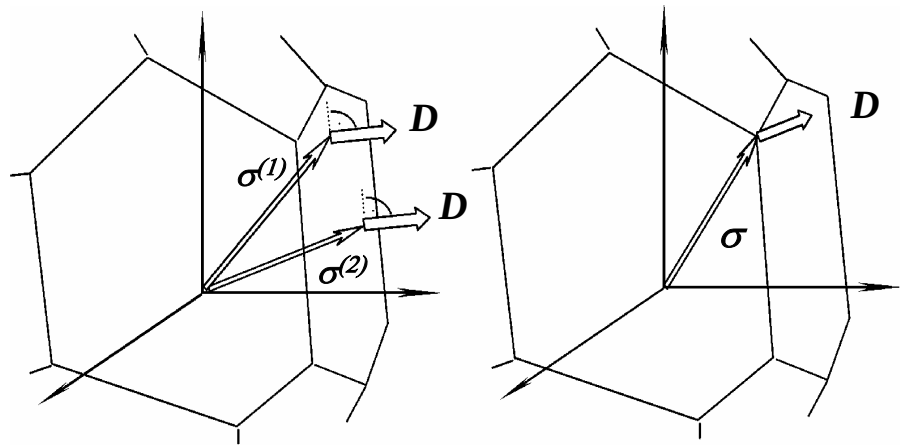
1 grain, 1 system:

kinematics **kinetics**

$$a_{ik} n_k a_{jl} b_l \, \sigma_{ij} = \tau^{crit}$$

1 grain, many systems (stress space)

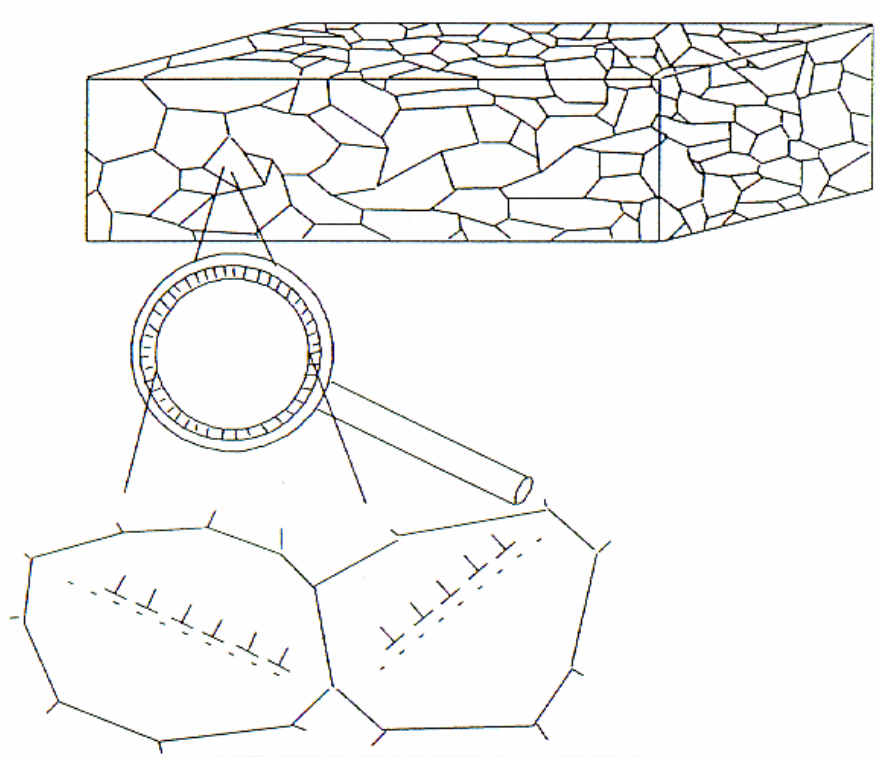
yield surface:
on YS: elastic-plastic flow
below YS: elastic
above YS: does not exist

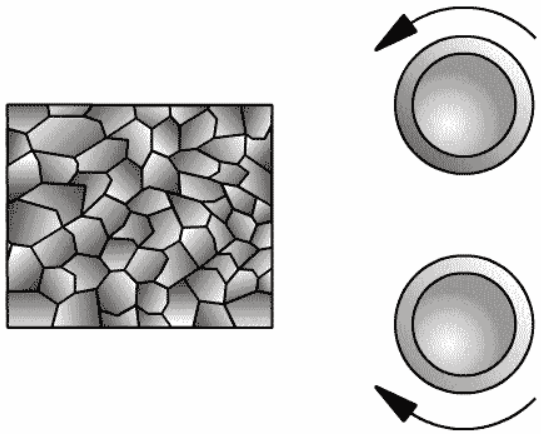


scales

The Taylor Model

- texture
- kinematik hardness (orientation dependent hardness)
- assumption of strain rate homogeneity





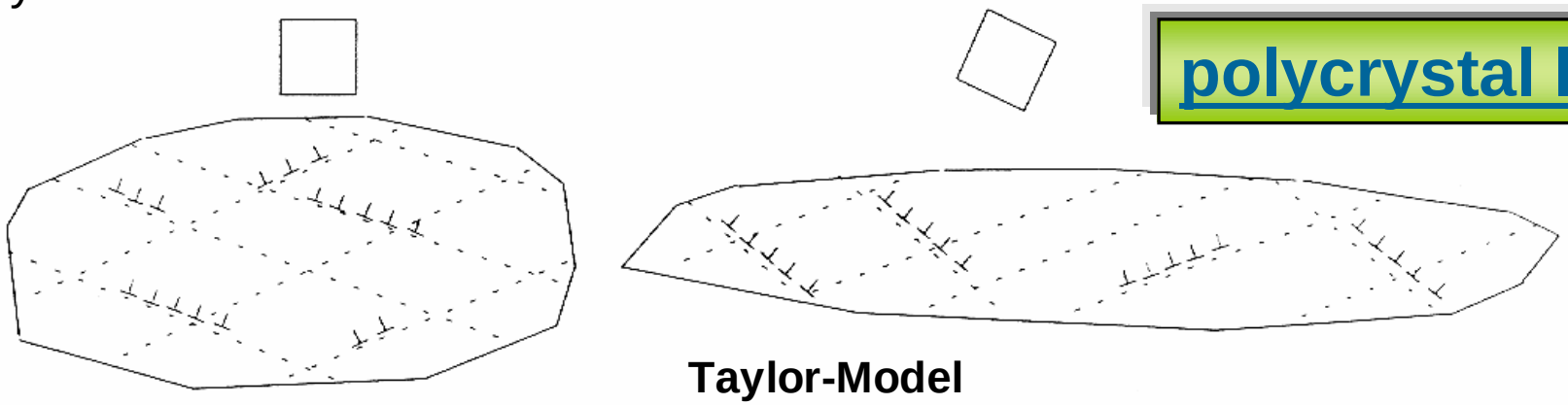
Cold Rolling

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

important anisotropy issues:

crystal interaction, mechanics at grain boundaries,
slip system selection

polycrystal level



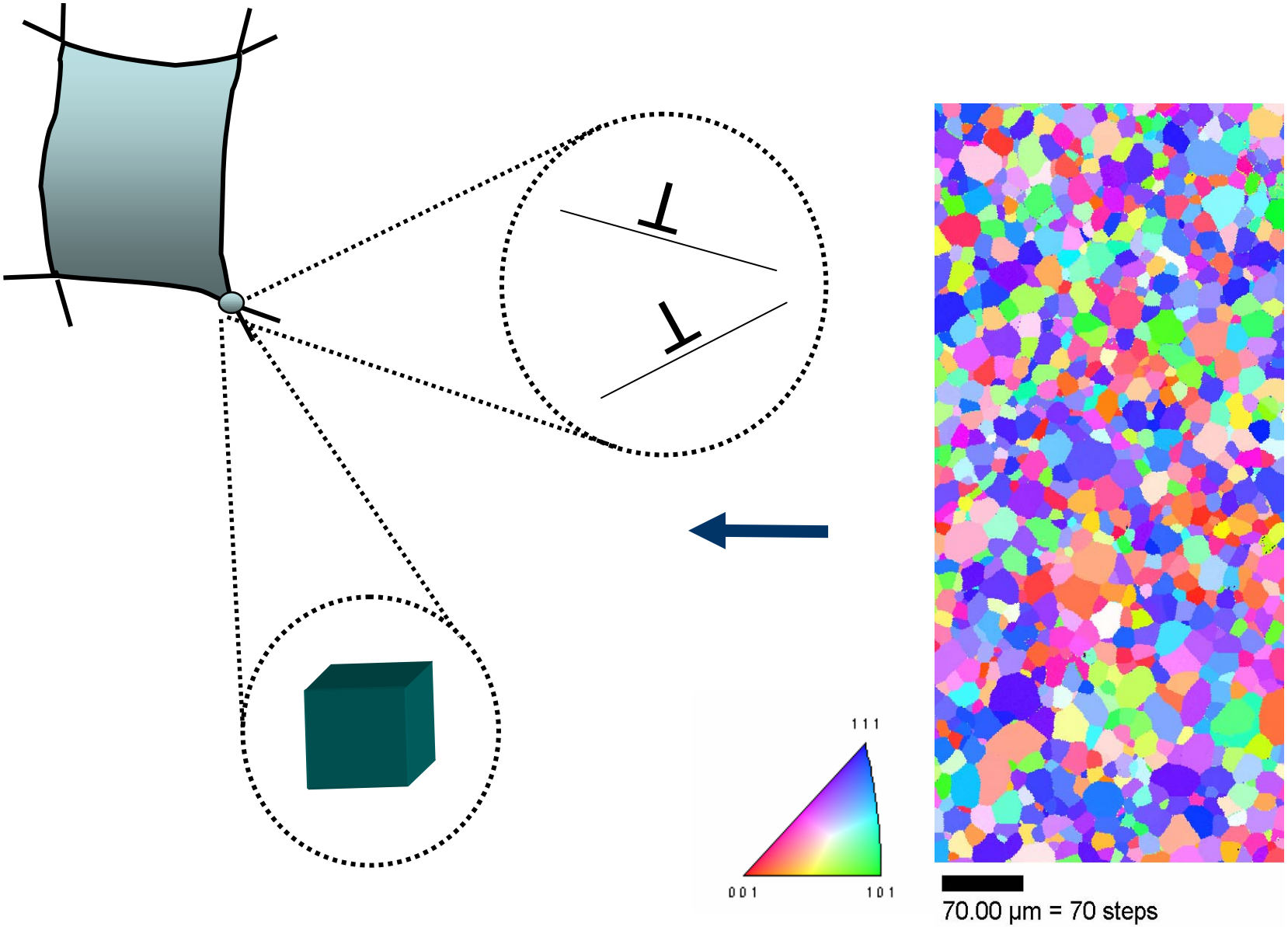
Taylor-Model

Crystal mechanics and FEM

One-to-one mapping of orientations / texture

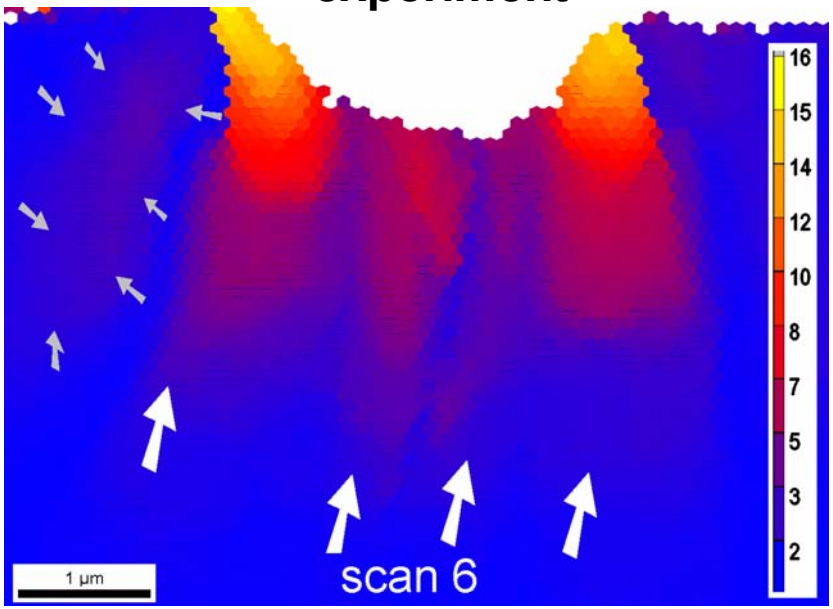
Polycrystals

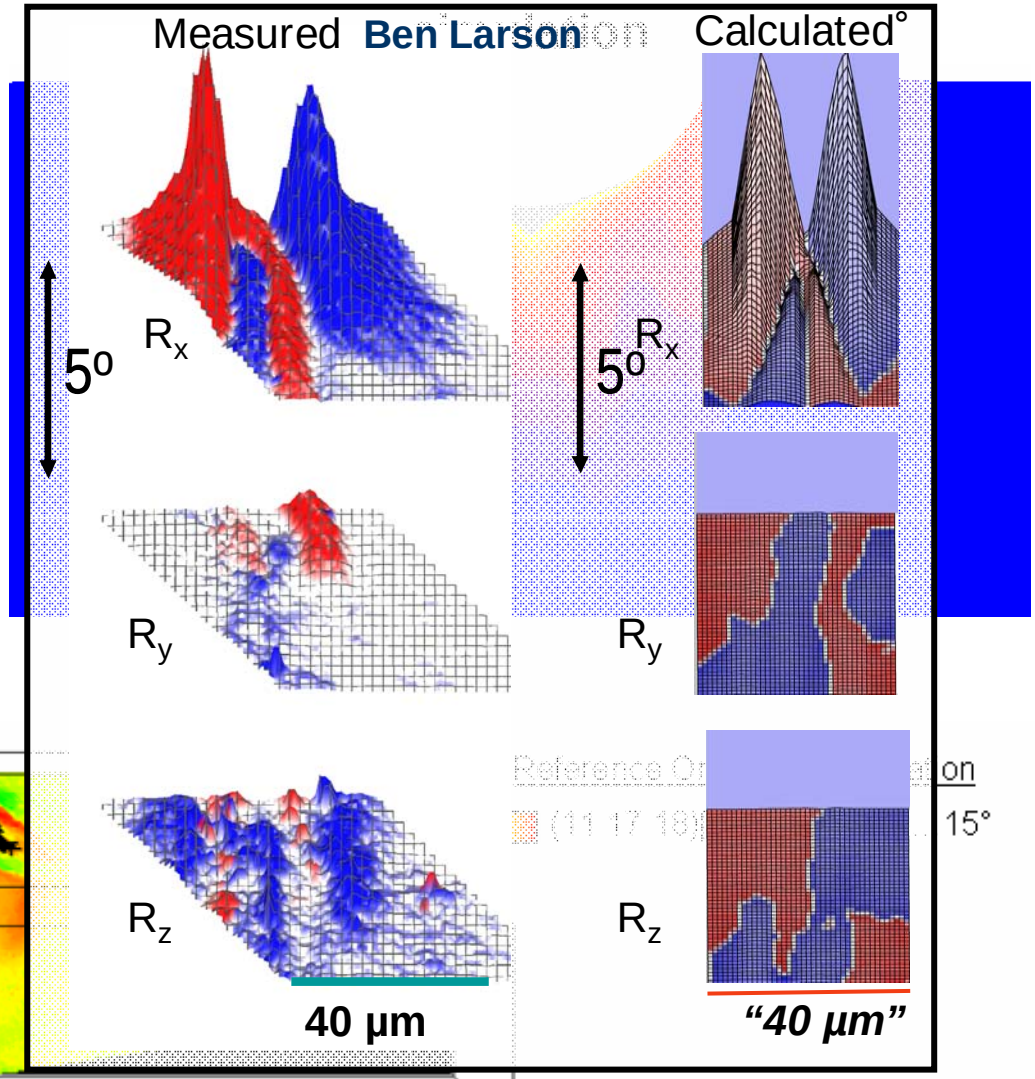
Crystal plasticity finite element method

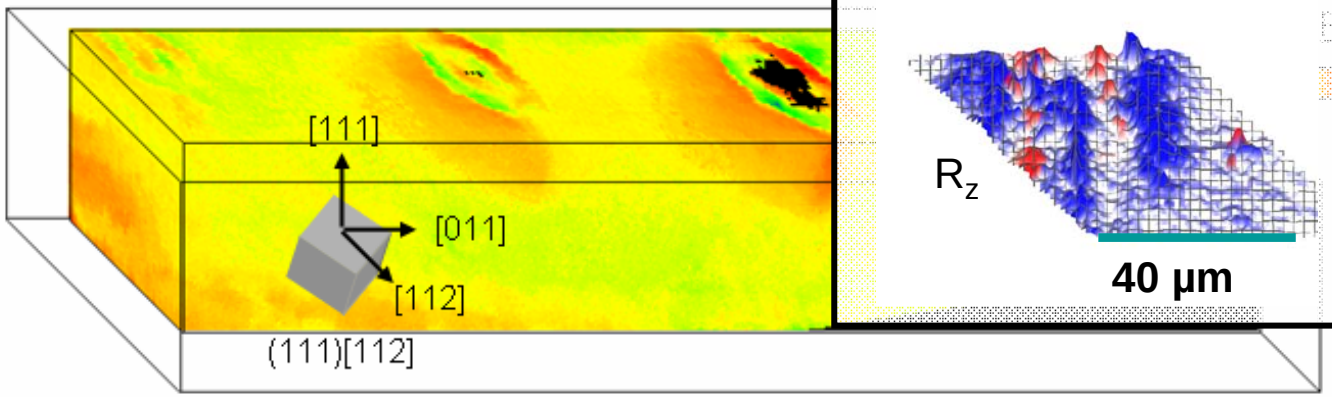


Crystal mechanics FEM, nanoindentation, Cu single crystal

experiment

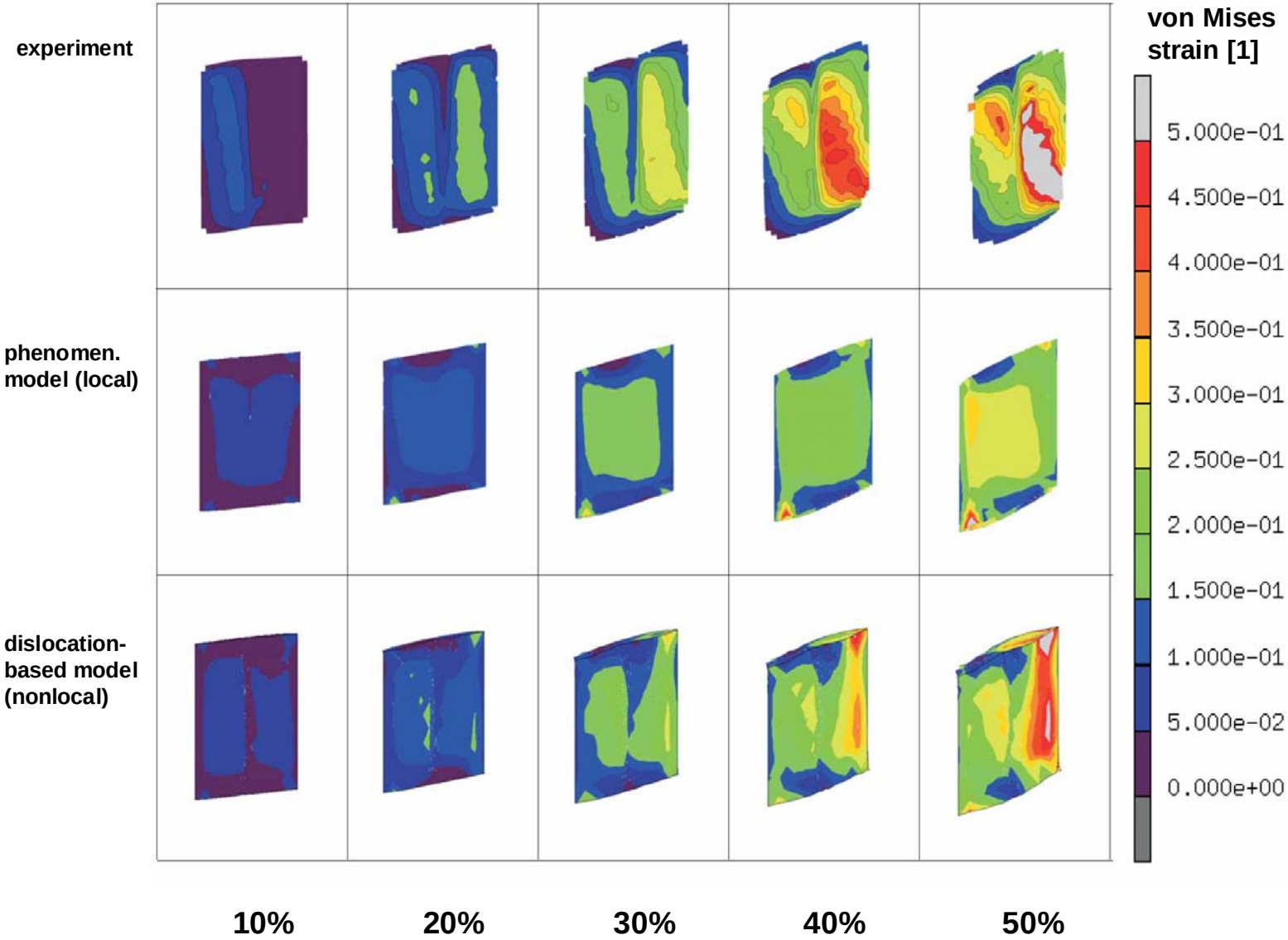




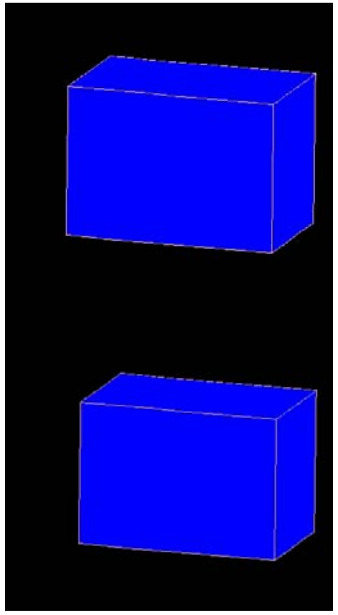


Forces: 4, 6, 8, and 10 µN

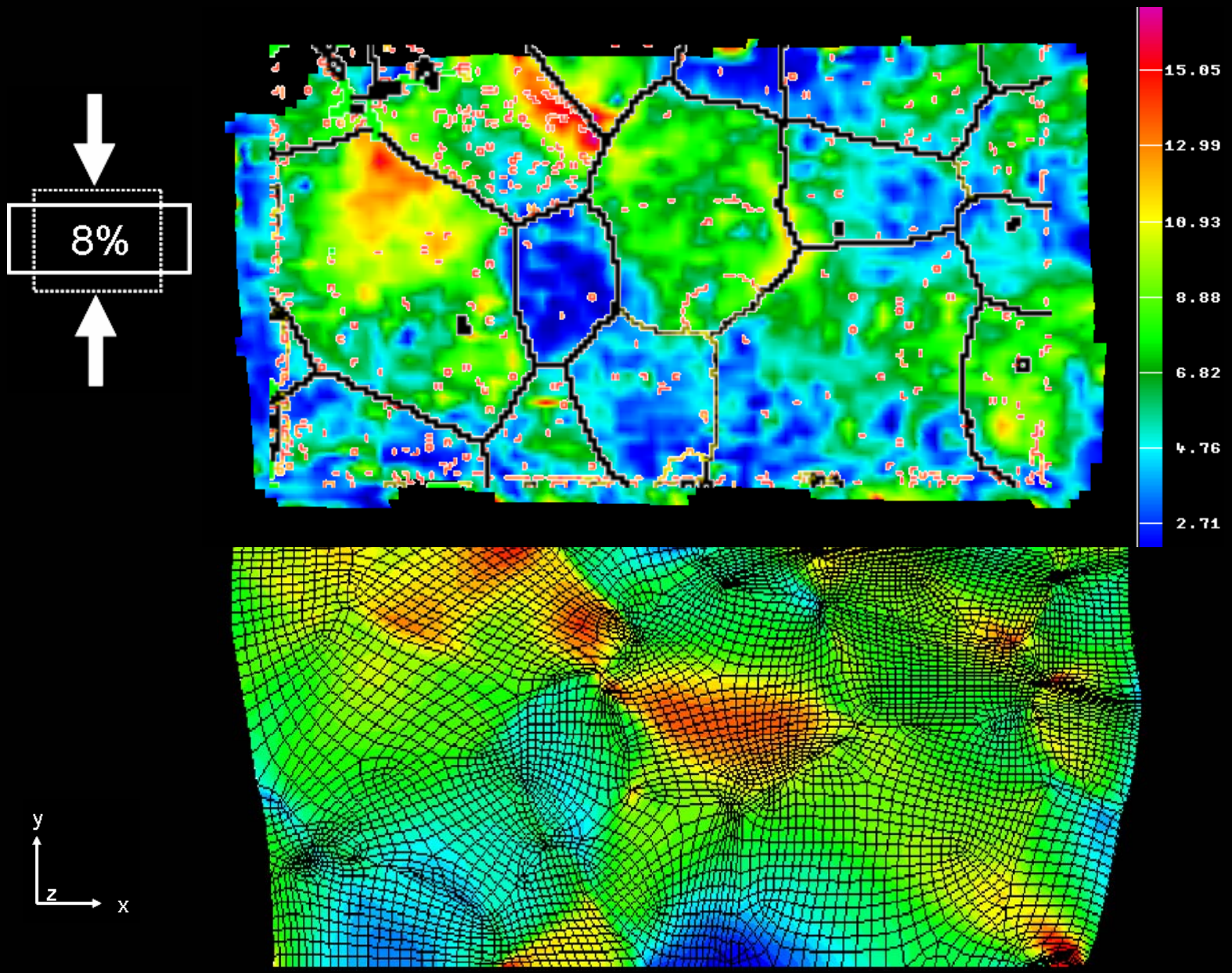
Bicrystals, Al, low angle [112] g.b.



7.4°
v. Mises
Al



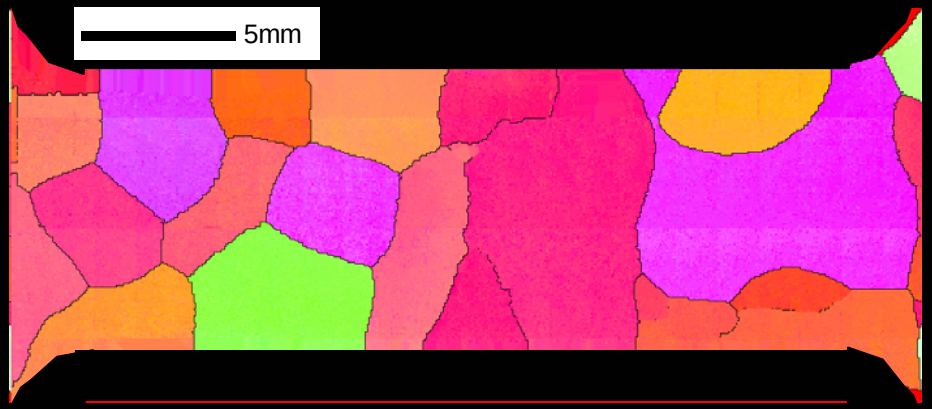
Crystal Mechanics FEM, grain scale mechanics (2D)

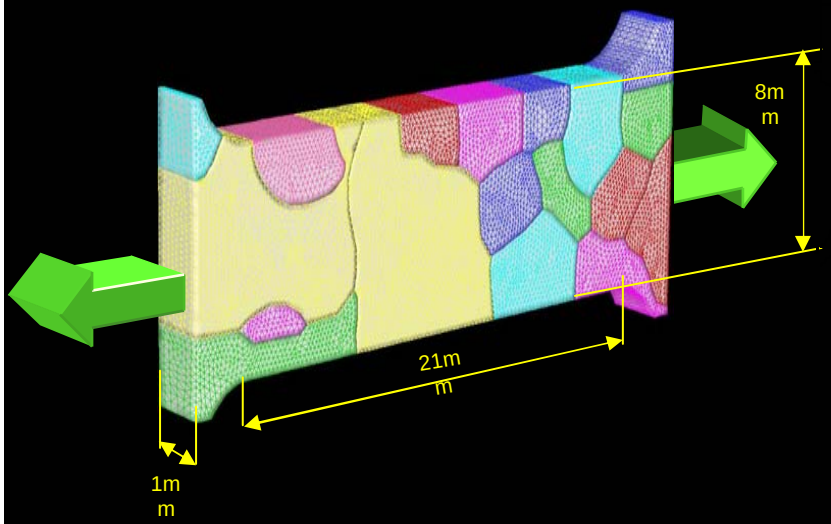


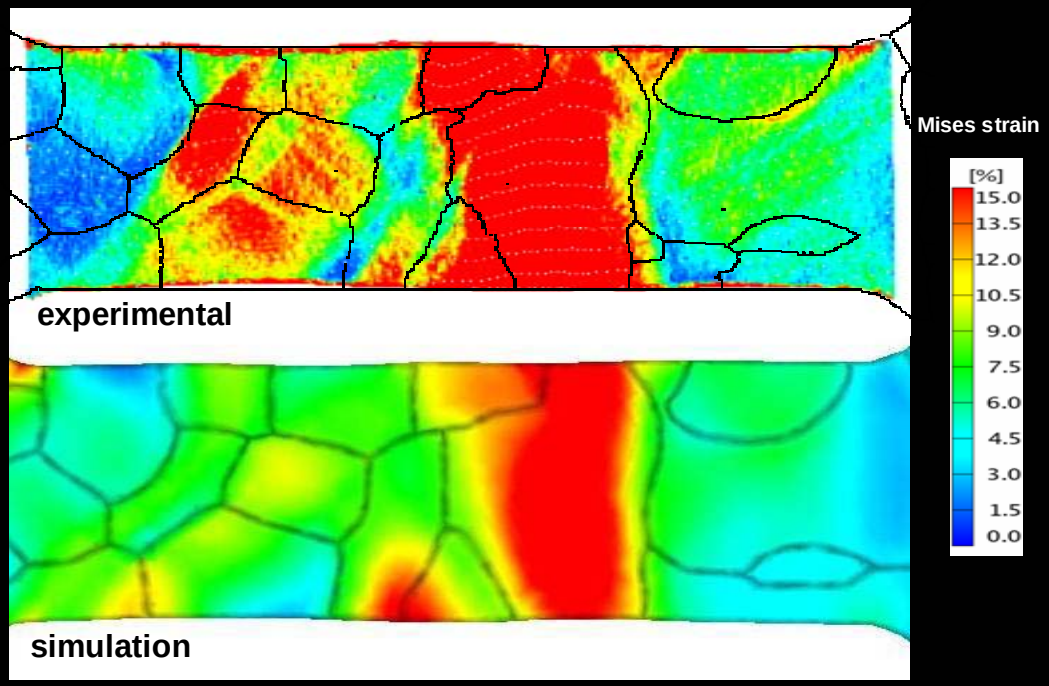
Experiment
(DIC, EBSD)
v Mises strain

Simulation
(CP-FEM)
v Mises strain

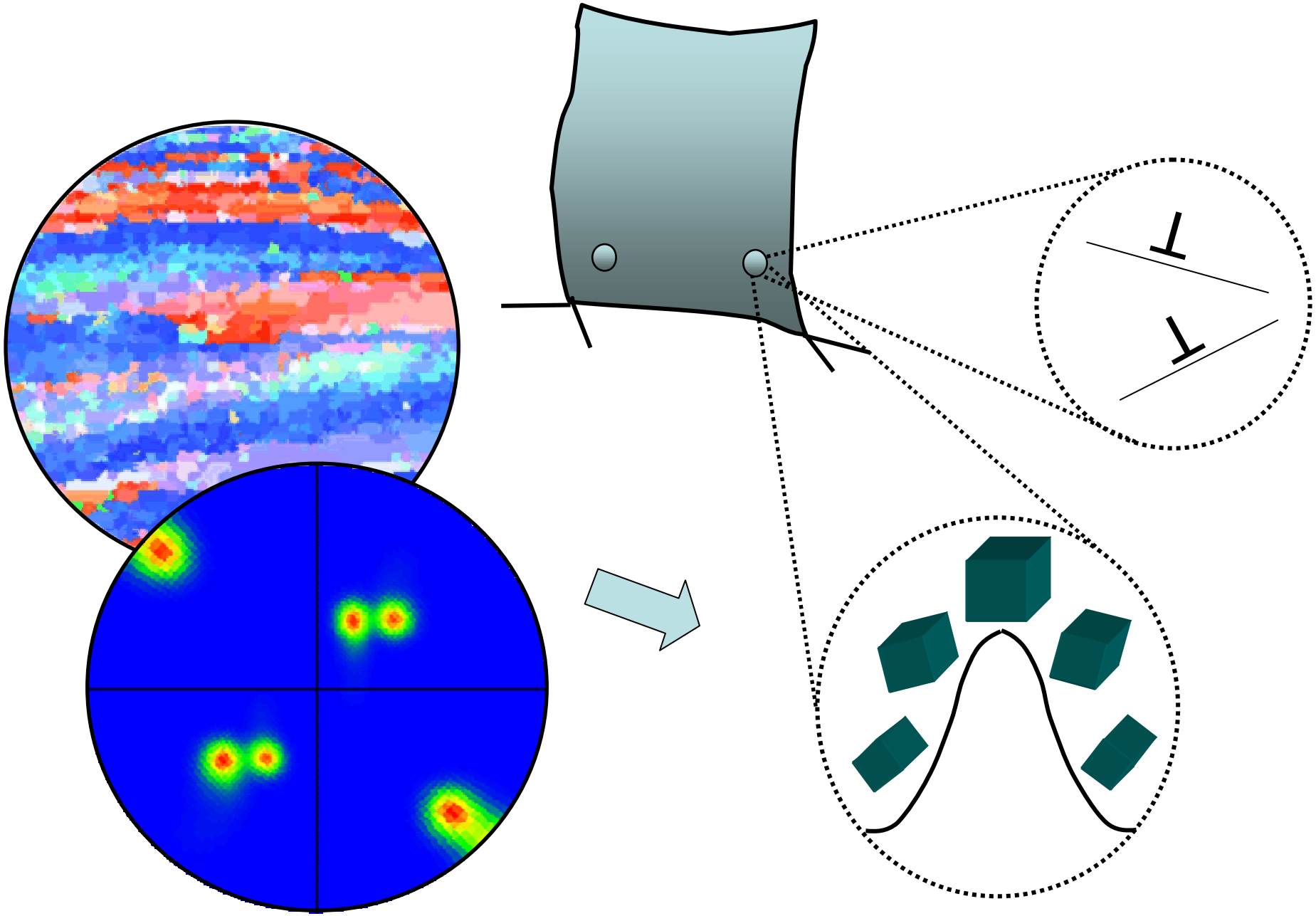
Crystal Mechanics FEM, grain scale mechanics (3D)

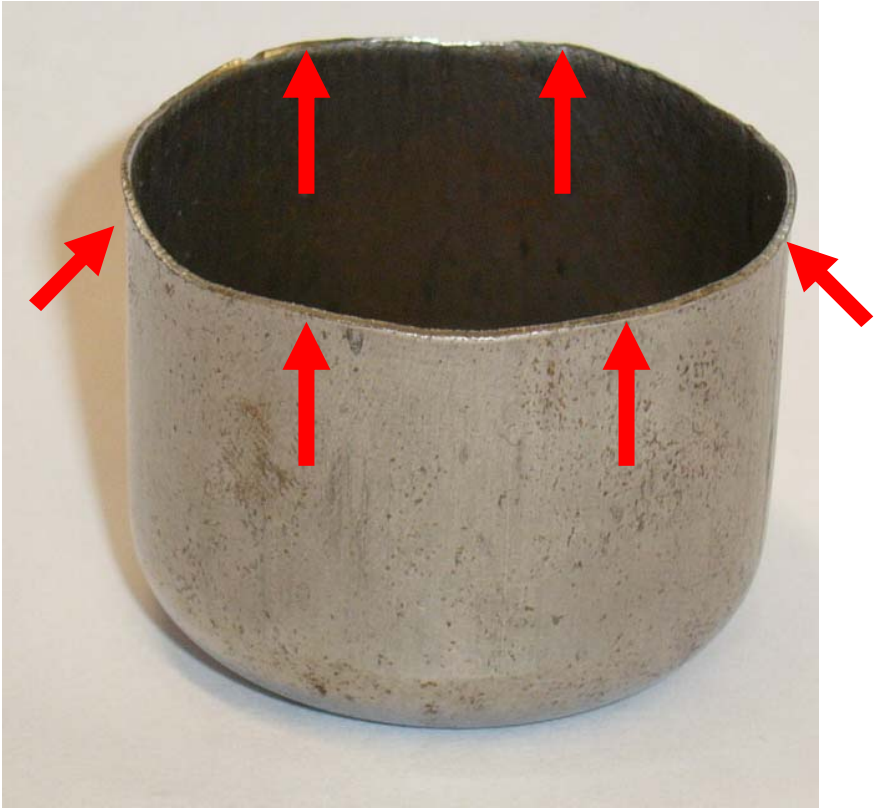


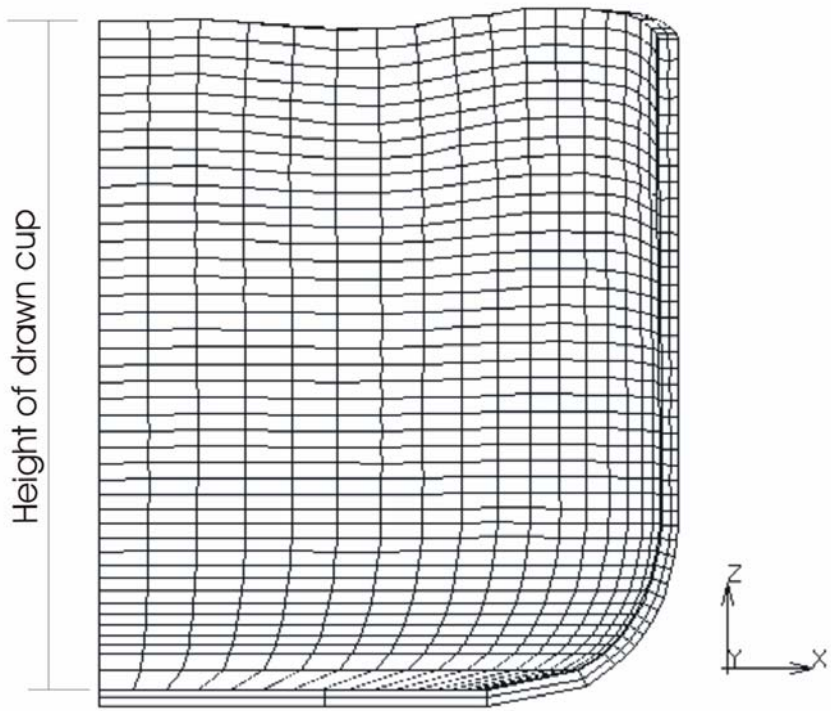


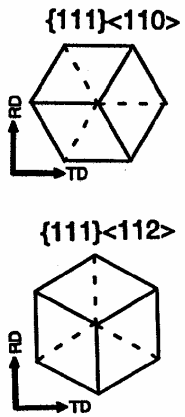


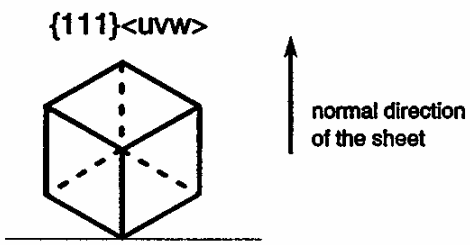
map texture functions into FEM

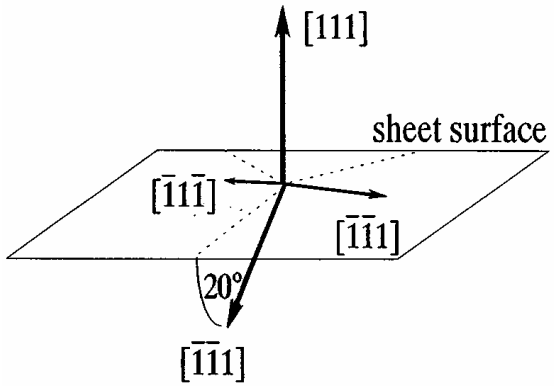






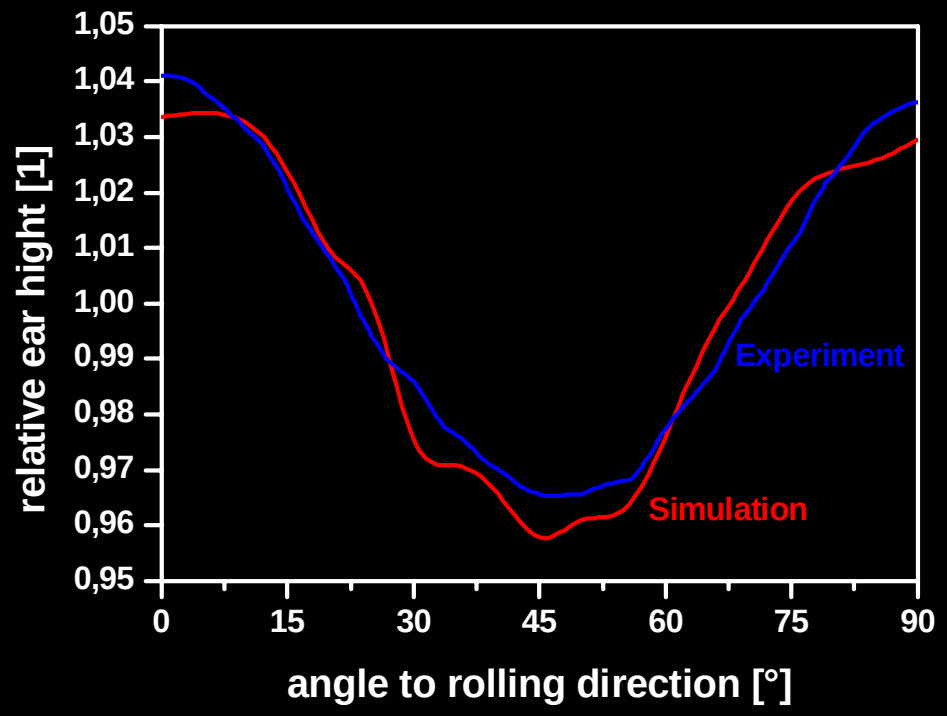


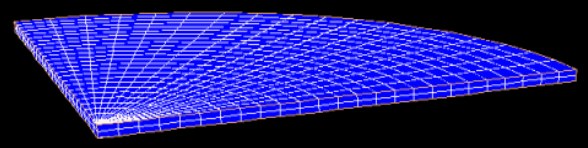




position of slip directions

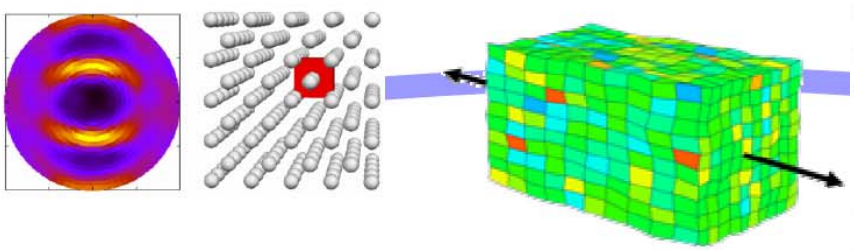
Crystal Plasticity FEM

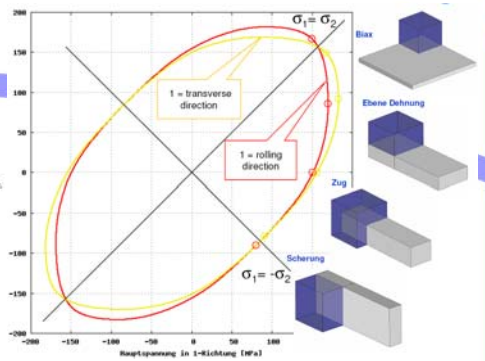


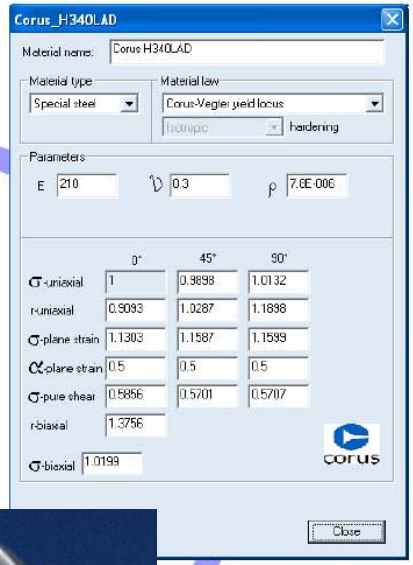


Example: automotive modeling

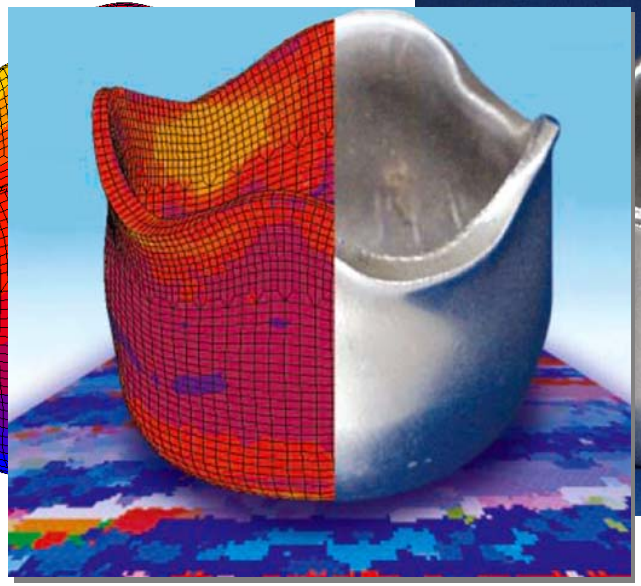
From Crystal Plasticity to Deep Drawing







- **Virtual Material Testing**
  - Representative Volume Element
  - Virtual test program – extrapolation of calibration tests
  - Parameter fit of the macro material model
  - No performance loss compared to classical deep drawing simulatio
  - Material behaviou ll in PamStamp 2G commercial FE co



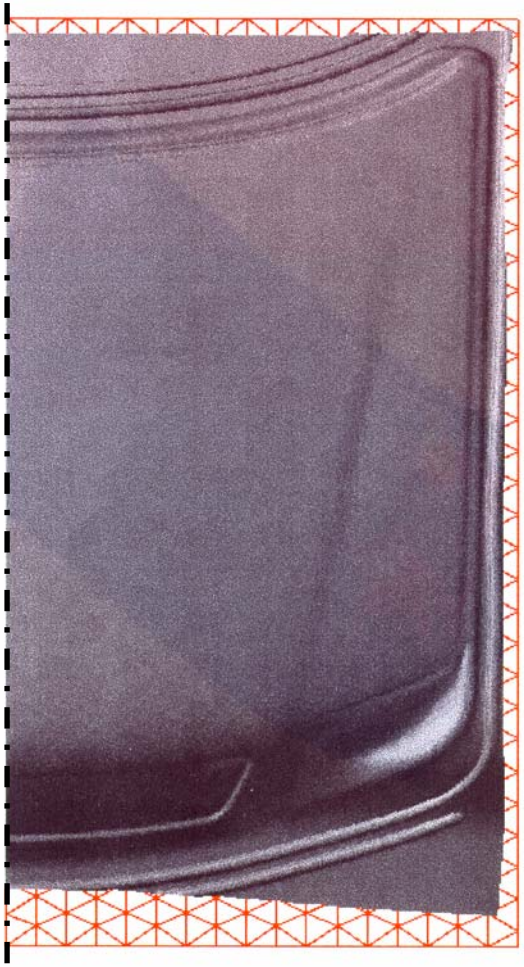
Beispiel einer Ziehsimulation

Frontklappe A6 (C5):

Halbsicht des gezogenen Teiles

Frontklappe A6 (grau) und ursprüngliche Form der Blechplatine (rotes Gitternetz):

Durch die Simulation kann u.a. der optimale Beschnitt der Platine festgelegt werden.



anisotropie of plasticity