Understanding the Elasto-Plasticity of Crystals

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Overview

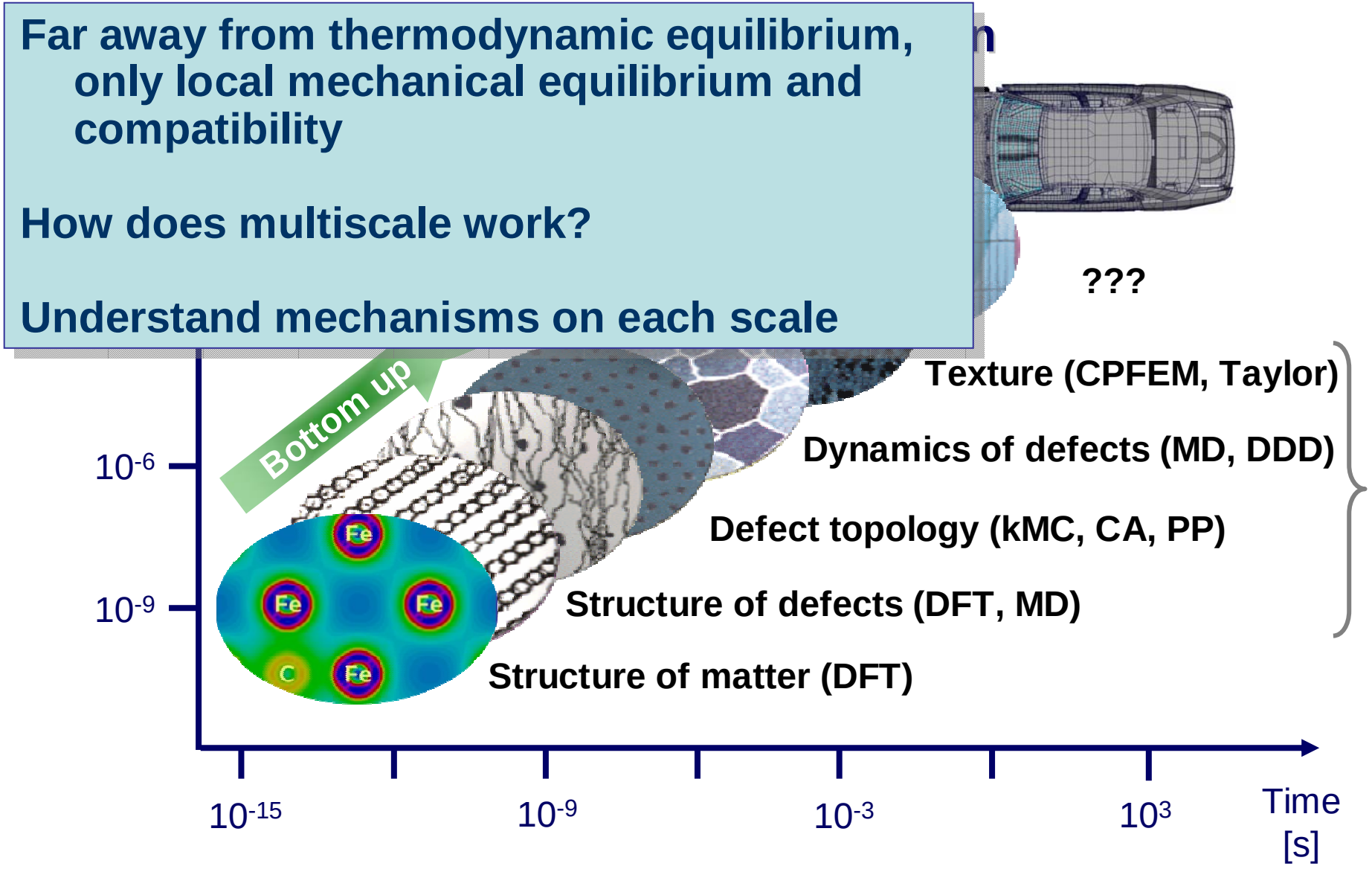
- **Scales in elasto-plasticity, MMM input** ←
- **Polycrystal elasto-plasticity homogenization (single phase, focus on kinematics, and b.c.)**
- **Limits in plasticity continuum models (small scale crystal plasticity)**

Multiscale Models: Scales, Methods

Far away from thermodynamic equilibrium, only local mechanical equilibrium and compatibility

How does multiscale work?

Understand mechanisms on each scale



Multiscale approaches in crystal plasticity

Parameter transfer / Scale hoping:
Elastic constants (Homogenization, feedback, inverse modeling: M. Friak, A. Counts, M. Petrov, J. Neugebauer, L. Limperakis)

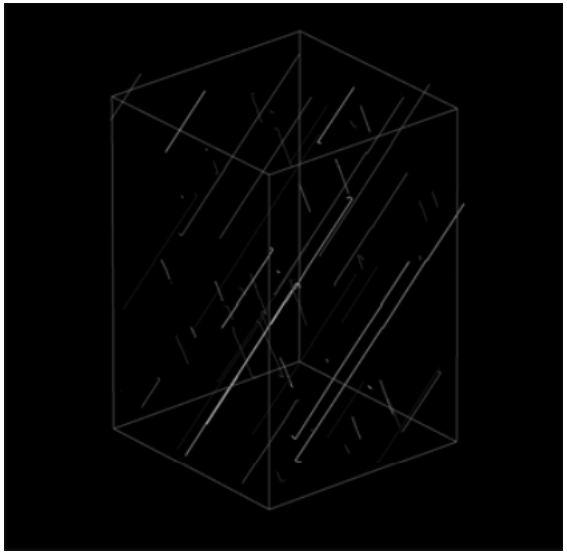
Coarse Graining / Statistics:
Statistical dislocation theory (pattern, defect structure formation: F. Roters, P. Dondel, S. Müller)

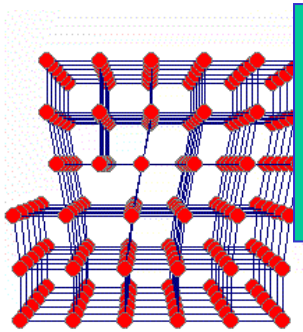
Polycrystal homogenization theory
Averages mechanical quantities for polycrystals (complex interaction, unknown local b.c., multiple phases, transformations: P. Eisenlohr, M. Friak, J. Neugebauer)

Multiscale, crystal plasticity: coarse graining

- Brief example (kinetics): dislocation evolution + dislocation-stress relation (talk of F. Roters)

Motivation: Fundamentals of crystal mechanics





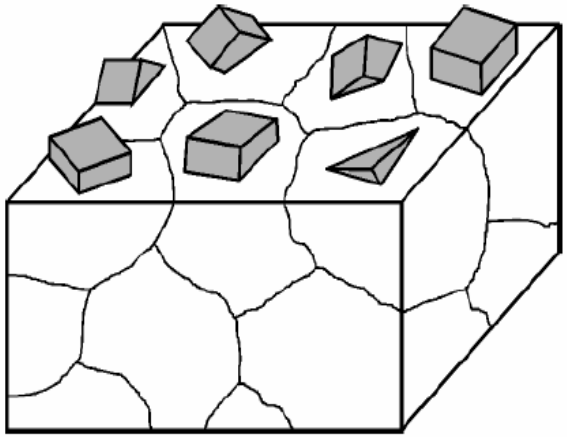
Lattice defects kinematics (dyadics of the shear DOF) plus boundary conditions

Lattice defect kinetics (Franz Roters)

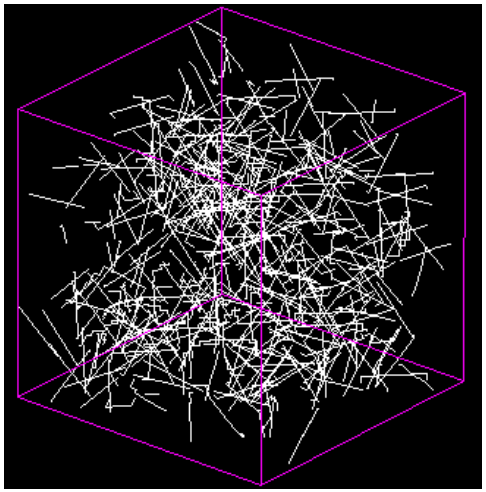
one dislocation

mesoscopic boundary conditions (grain / orientation neighborhood)

parallel loops (Kubin)



reactions (Kubin)



spin (orientation change)

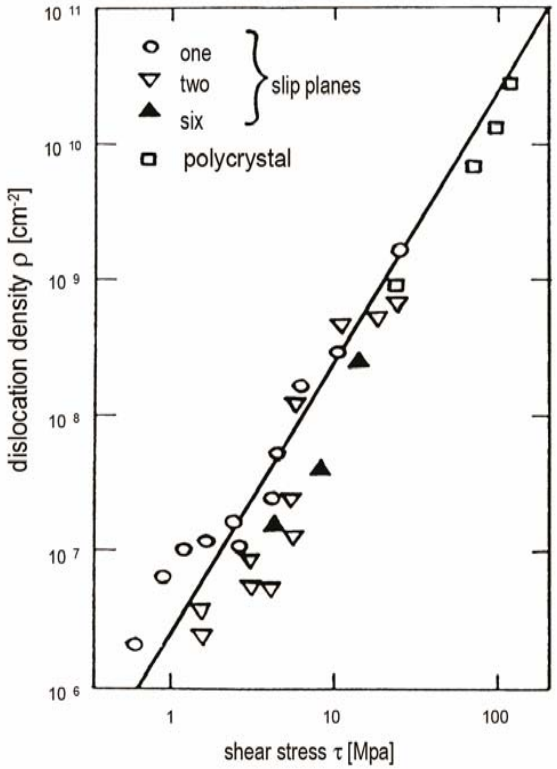
Motivation: Fundamentals of crystal mechanics

kinetics: collective dislocation behaviour

- **kinetic equation of state**

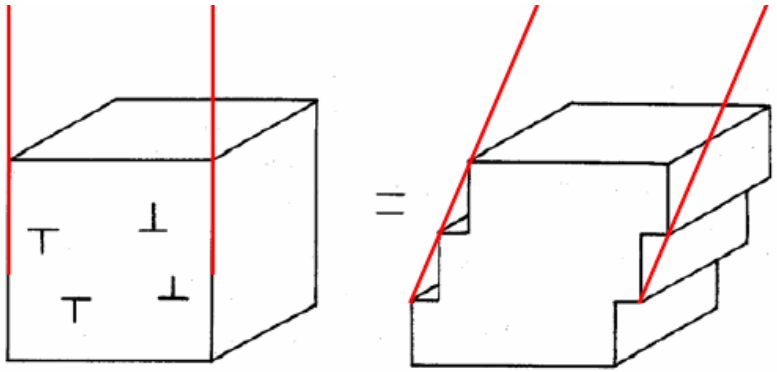
- **structure evolution**

$$\frac{d\rho}{d\gamma} = A\rho^{+} + B\rho^{-}$$



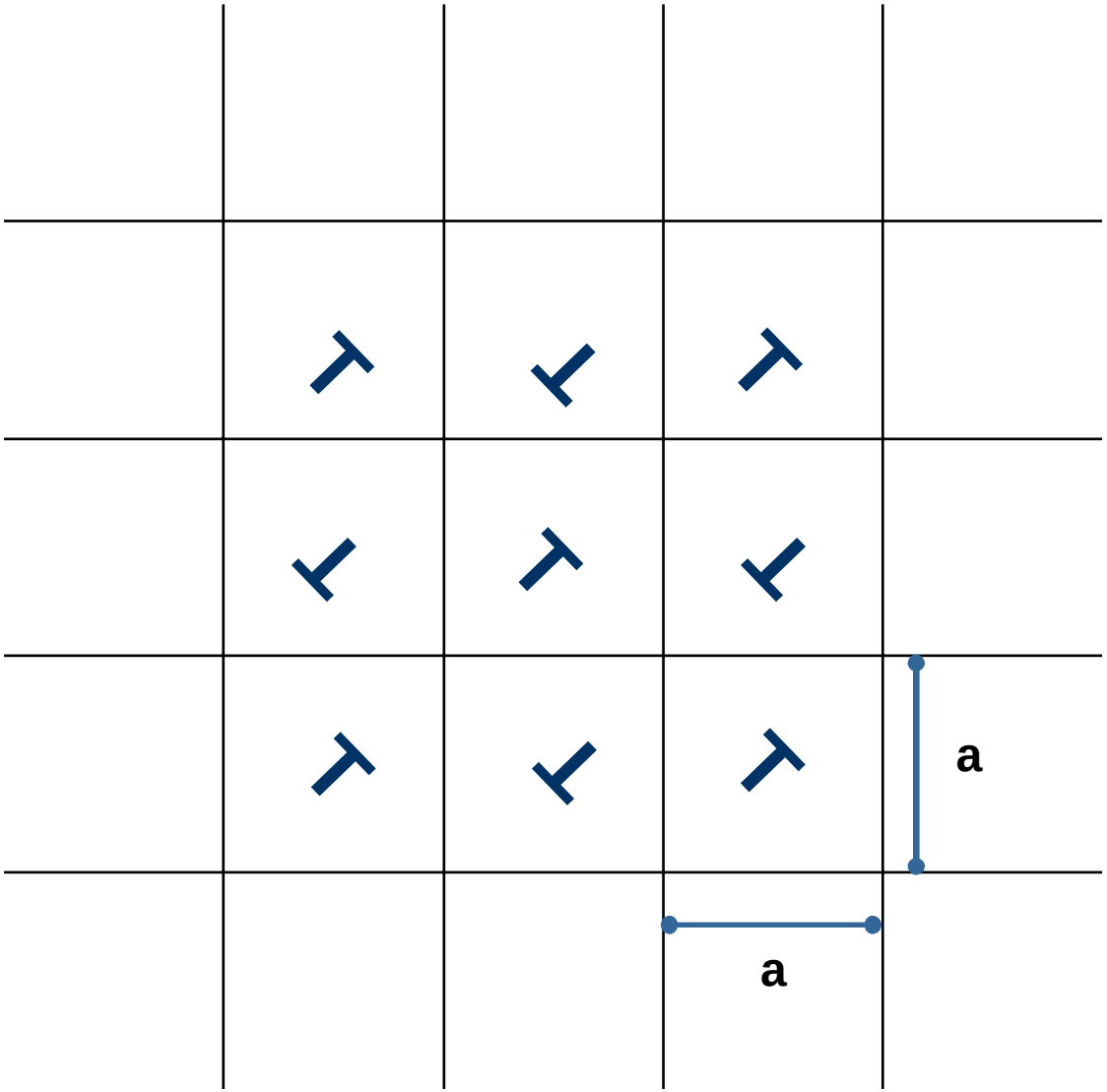
$$\tau = \alpha G b \sqrt{\rho}$$

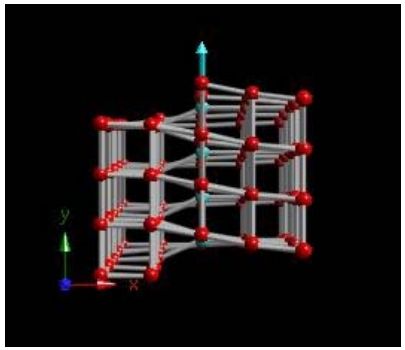
- **coupling to imposed shape change**



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

Coarse Graining: flow stress only



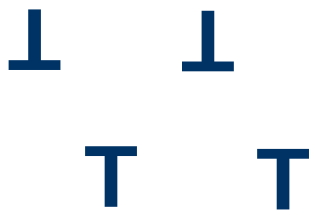


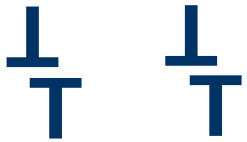
$$\tau = G\gamma = \frac{Gb}{2\pi r}$$

$$\rho = \frac{1}{a^2}$$

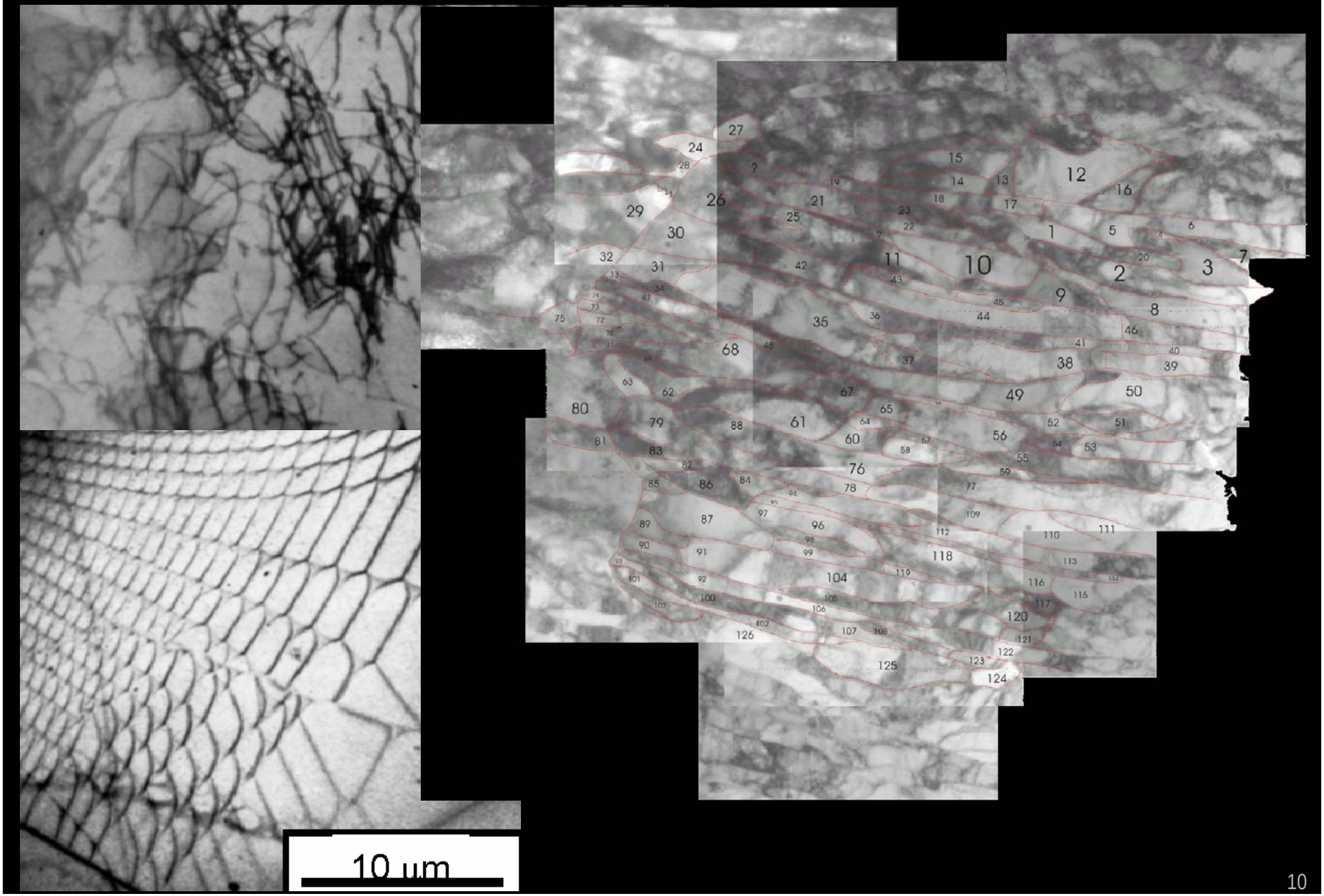
$$\tau = \frac{Gb}{2\pi a} = \frac{Gb}{2\pi}\sqrt{\rho}$$

Coarse graining, problems





Coarse graining, problems



Typical issues

Continuum scale coarse graining:

- **How much physics is included in a model ?**
- **How transparent are the assumptions ?**
- **What was left out and why ?**
- **Simplify complex systems**
- **Is there any experimental / theoretical proof ?**
- **Are the experiments trustworthy (better make your own, create new experiments)?**

Overview

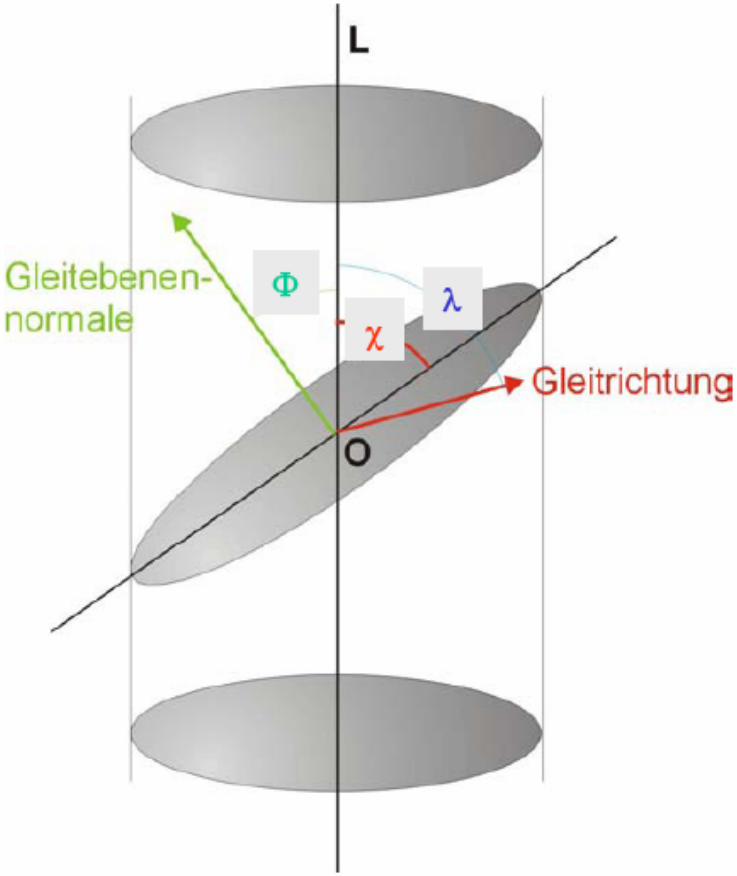
- **Scales in elasto-plasticity, MMM input**
- **Polycrystal elasto-plasticity homogenization (single phase, focus on kinematics, and b.c.)** ←
- **Limits in plasticity continuum models (small scale crystal plasticity)**

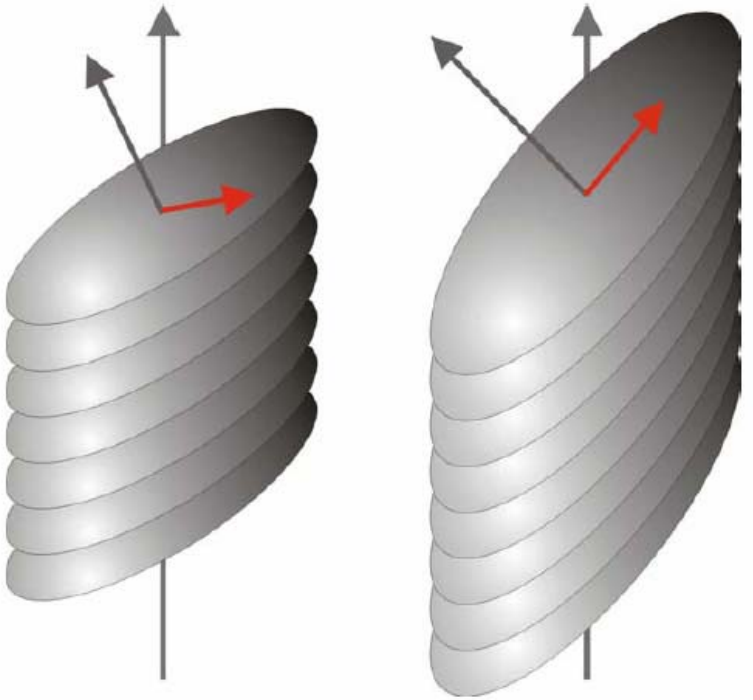
Crystal mechanics and anisotropy

single crystal level

single crystal level: stress homogenization

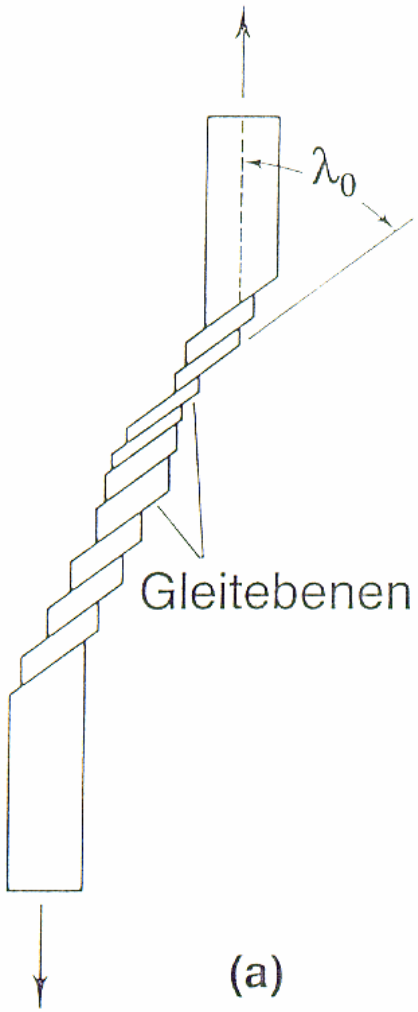
Origin of plastic anisotropy





single crystal level: stress homogenization

kinematics:
shape change (symmetric part of displacement gradient)



kinematics:
rotation / texture (antisymmetric part of displacement gradient)

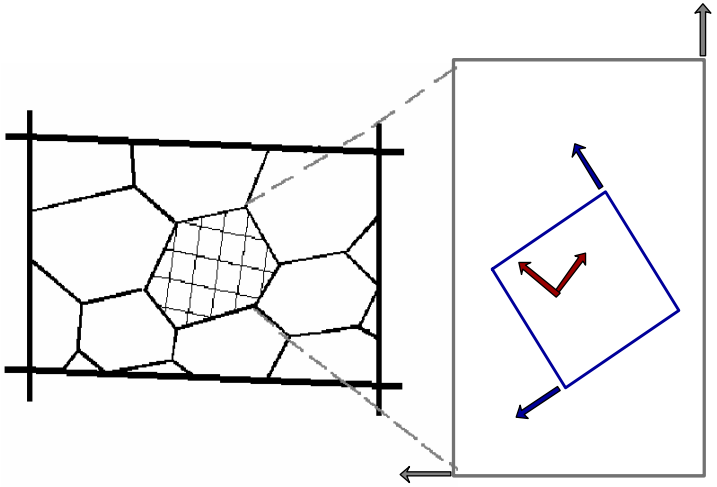
Plastically stretched zinc single crystal.

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.*

single crystal level: stress homogenization

1 crystal, 1 slip system:



slip systems

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

crystal (k,l)

$m_{kl} = n_k b_l$

sample (i,j)

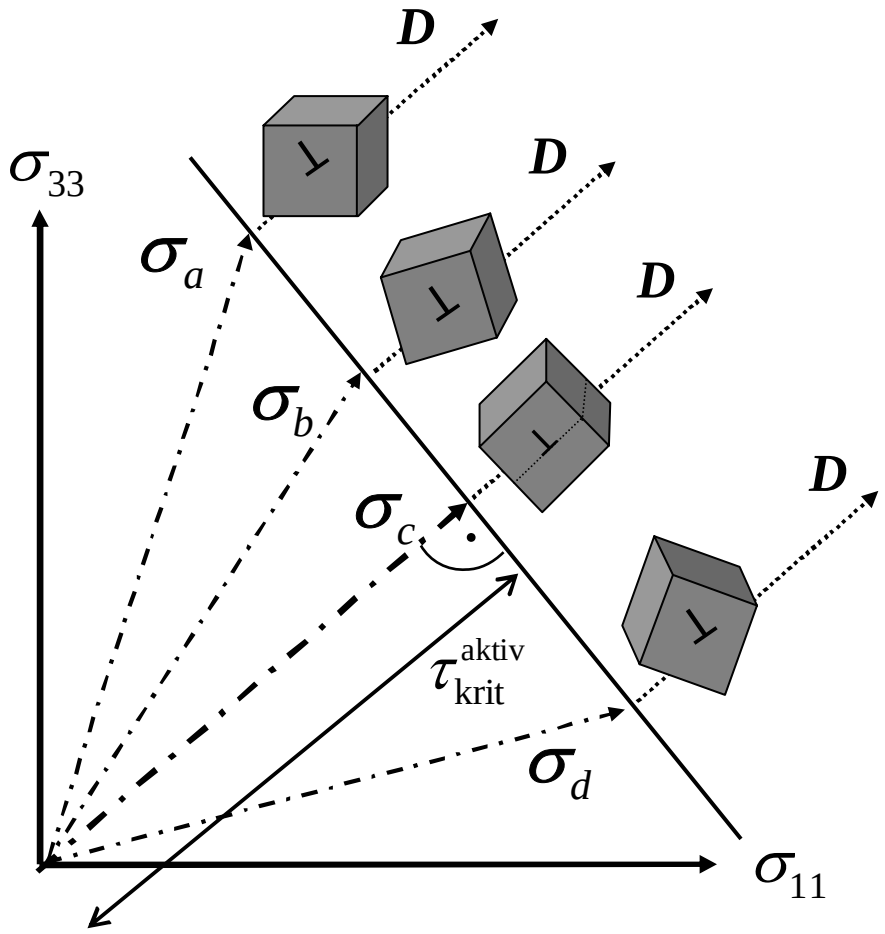
$m_{ij} = a_{ik} n_k \; a_{jl} b_l$

kinematics **kinetics**

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

single crystal level: stress homogenization

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



1 crystal, 1 slip system:

single crystal level: stress homogenization

slip system s

n_i^s , b_i^s

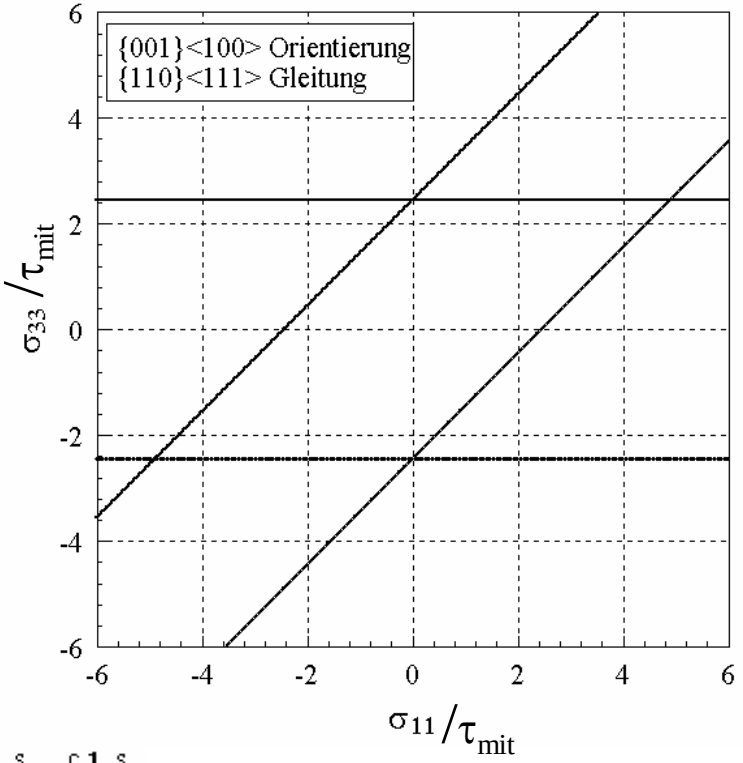
kinematics **kinetics**

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

orientation factor for s

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

1 crystal, 2 slip systems



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)

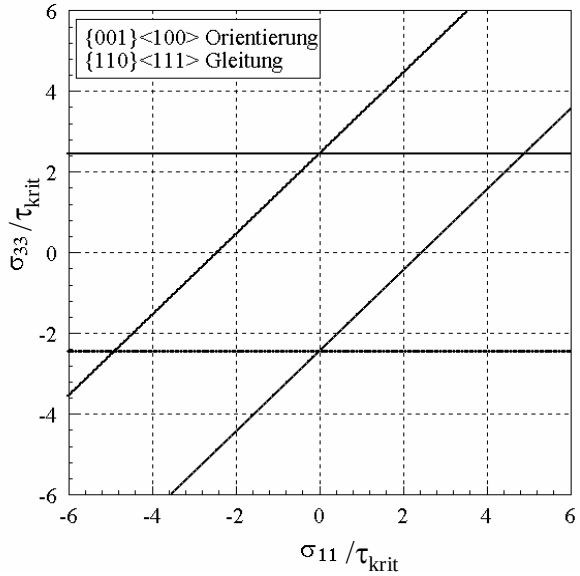
$$m_{kl}^{sym,s=aktiv}\sigma_{kl} = \sigma_{aufg}^s = \tau_{krit,(+)}^{s=aktiv}$$

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

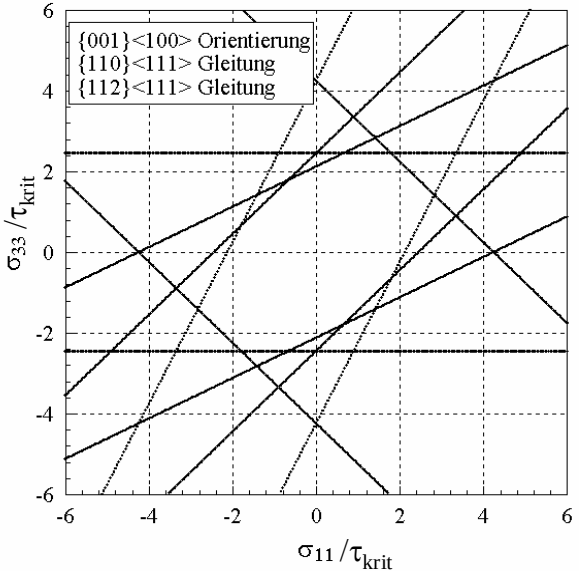
(non-active systems)

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

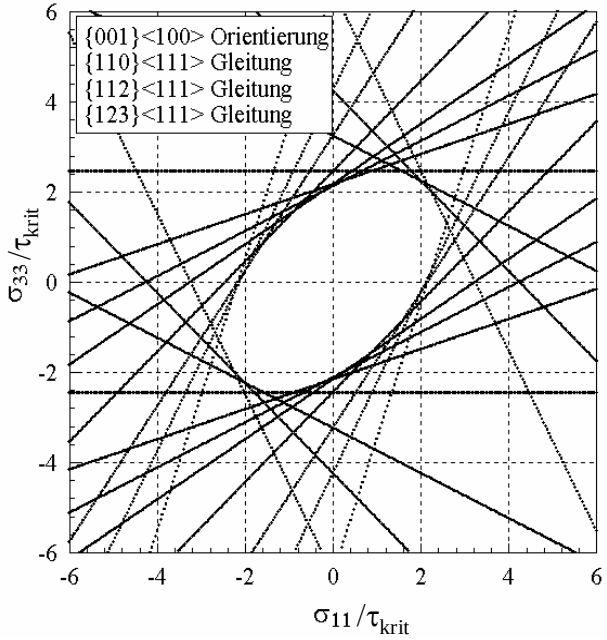
single crystal level: stress homogenization



krz, kfz, Schnitt



krz, 24 Systeme, Schnitt



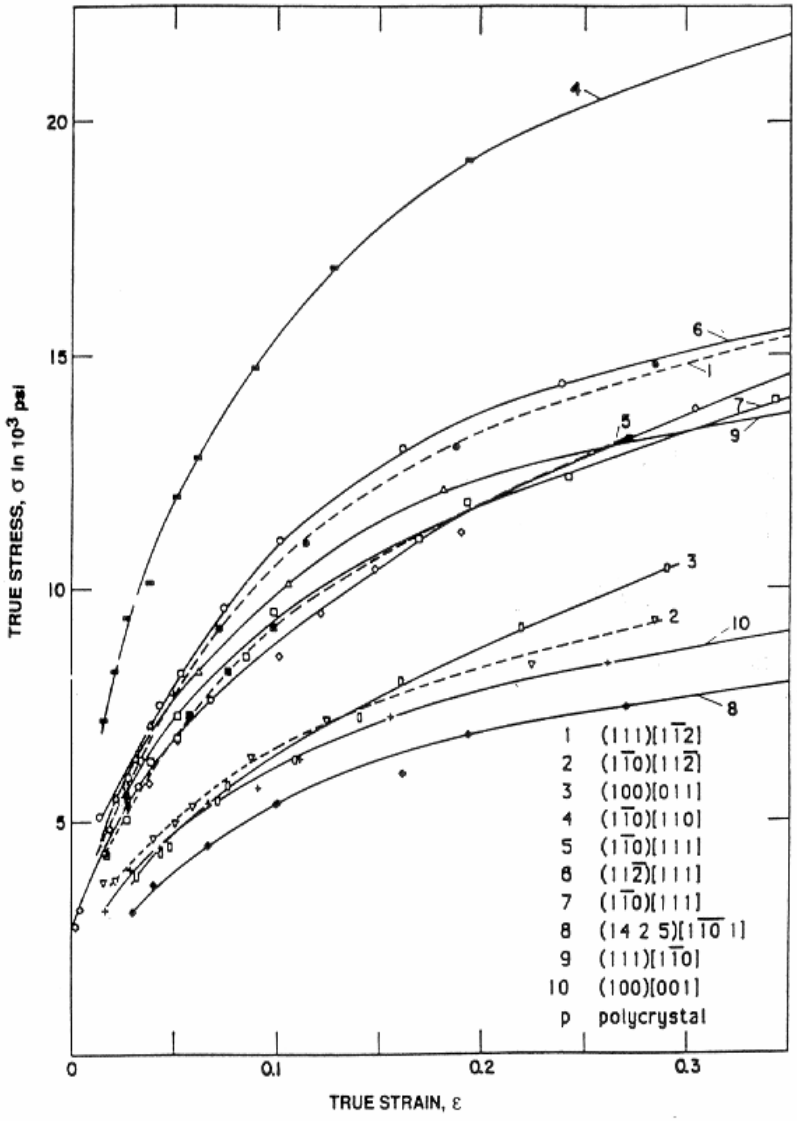
krz, 48 Systeme, Schnitt

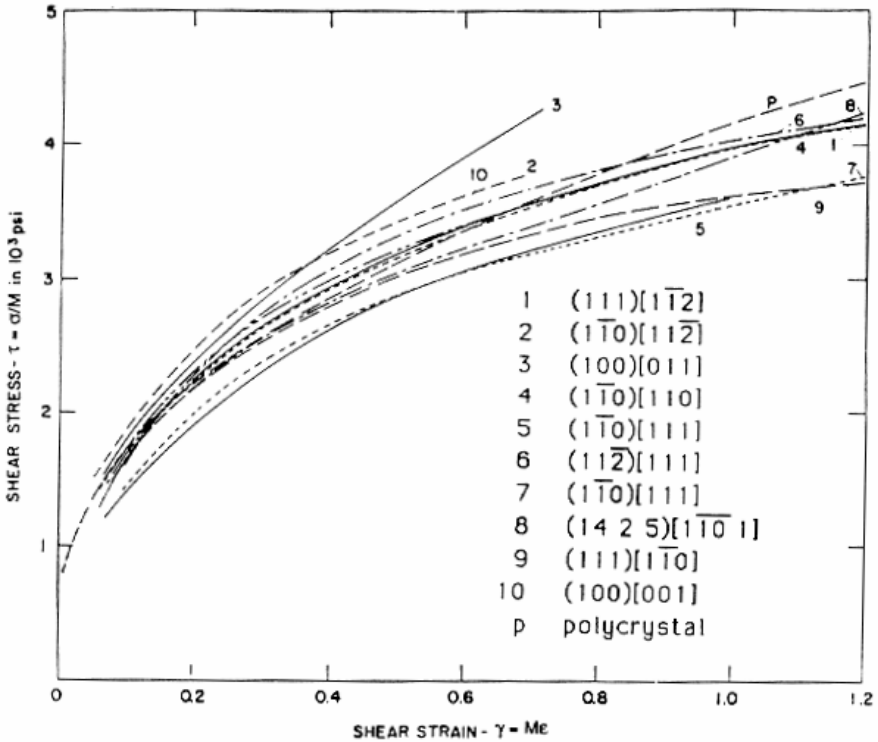
1 crystal, many slip systems

yield surface, bcc

single crystal, bcc, (001)[100]

single crystal level: stress homogenization



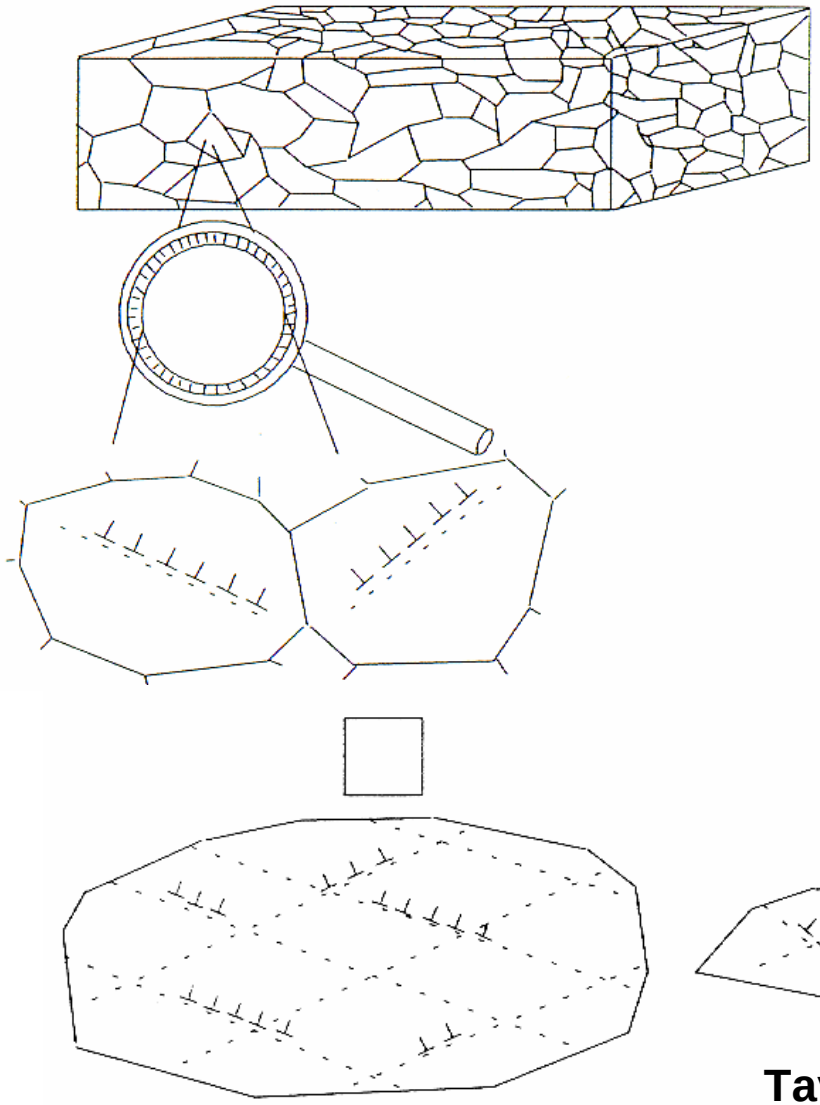


Hosford

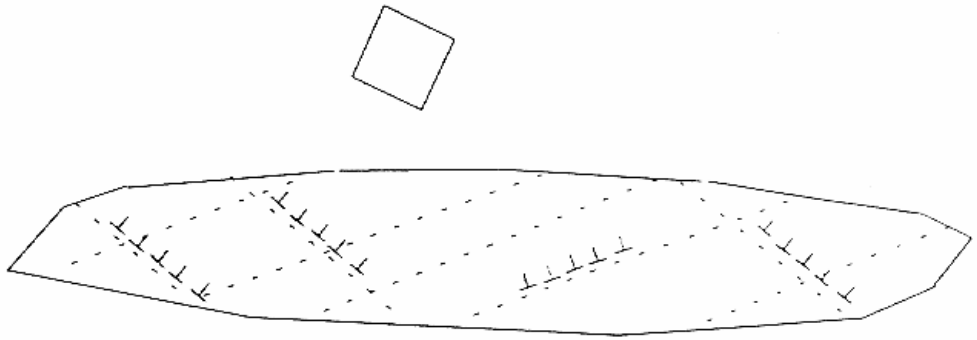
Crystal mechanics and anisotropy

polycrystal level

polycrystal: strain homogenization

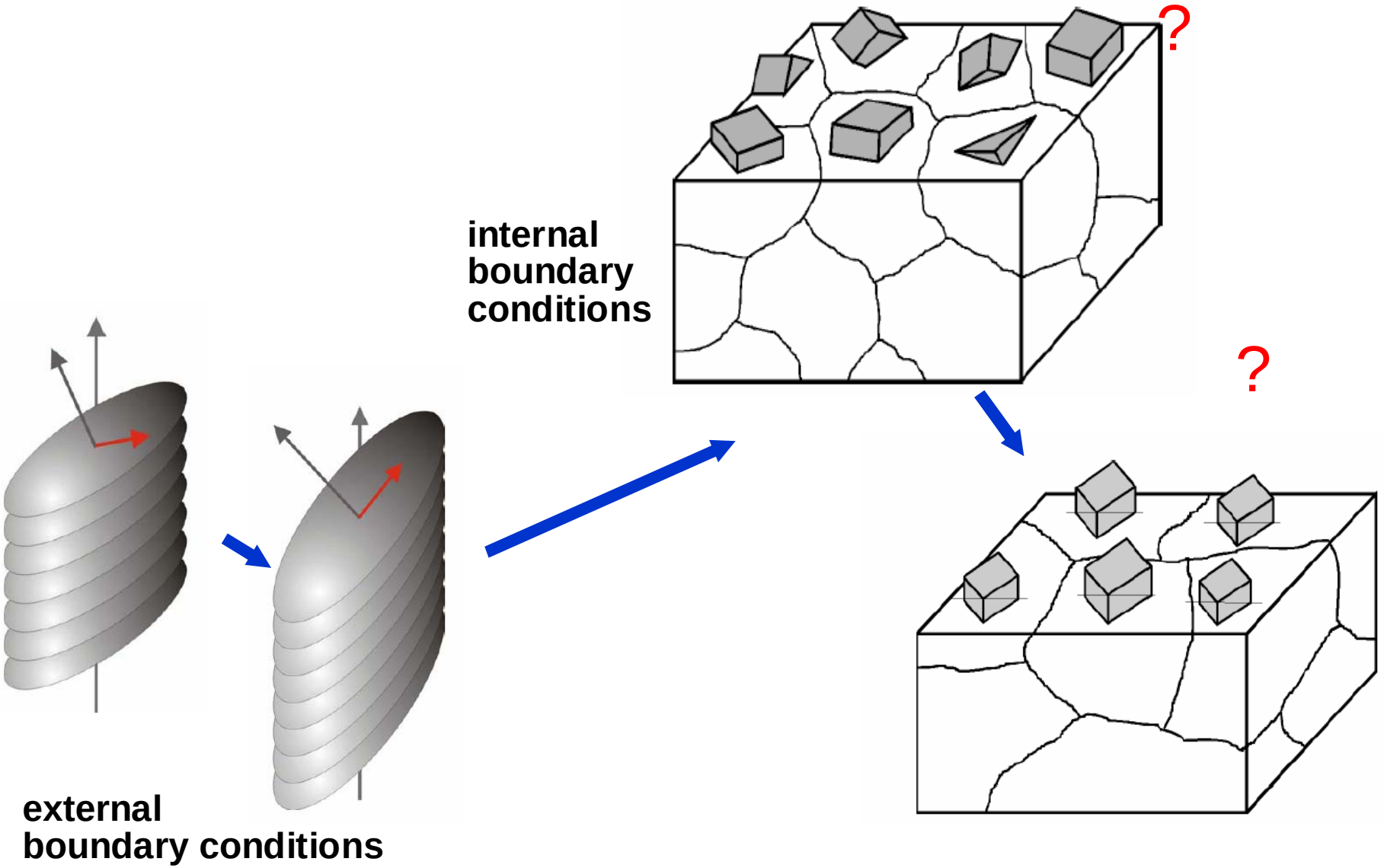


$$\varepsilon_{ij} = \frac{1}{2}\sum_{s=1}^{5}\left(n_i^s b_j^s + n_j^s b_i^s\right)\gamma^s$$

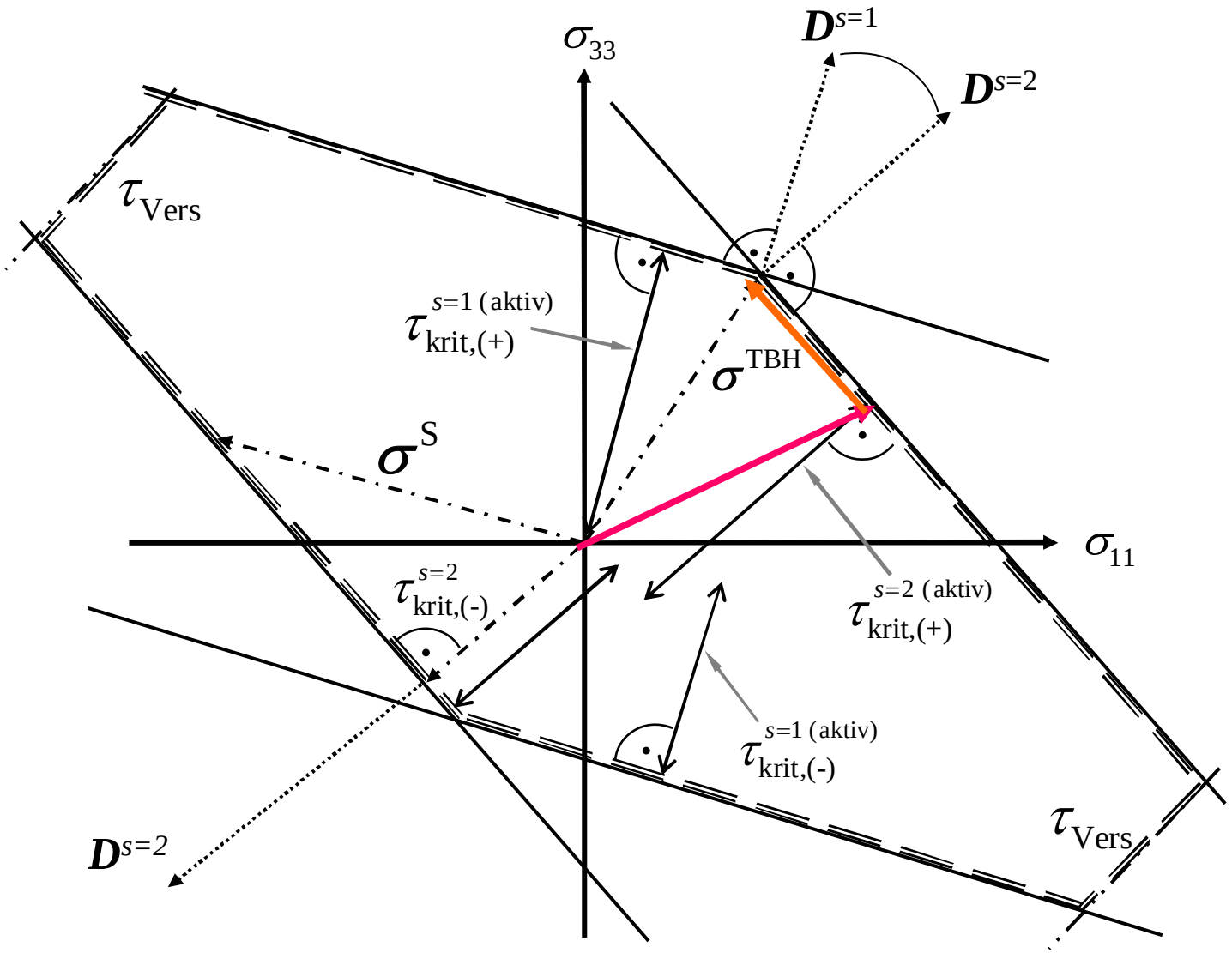


Taylor-Model

polycrystal: strain homogenization ?



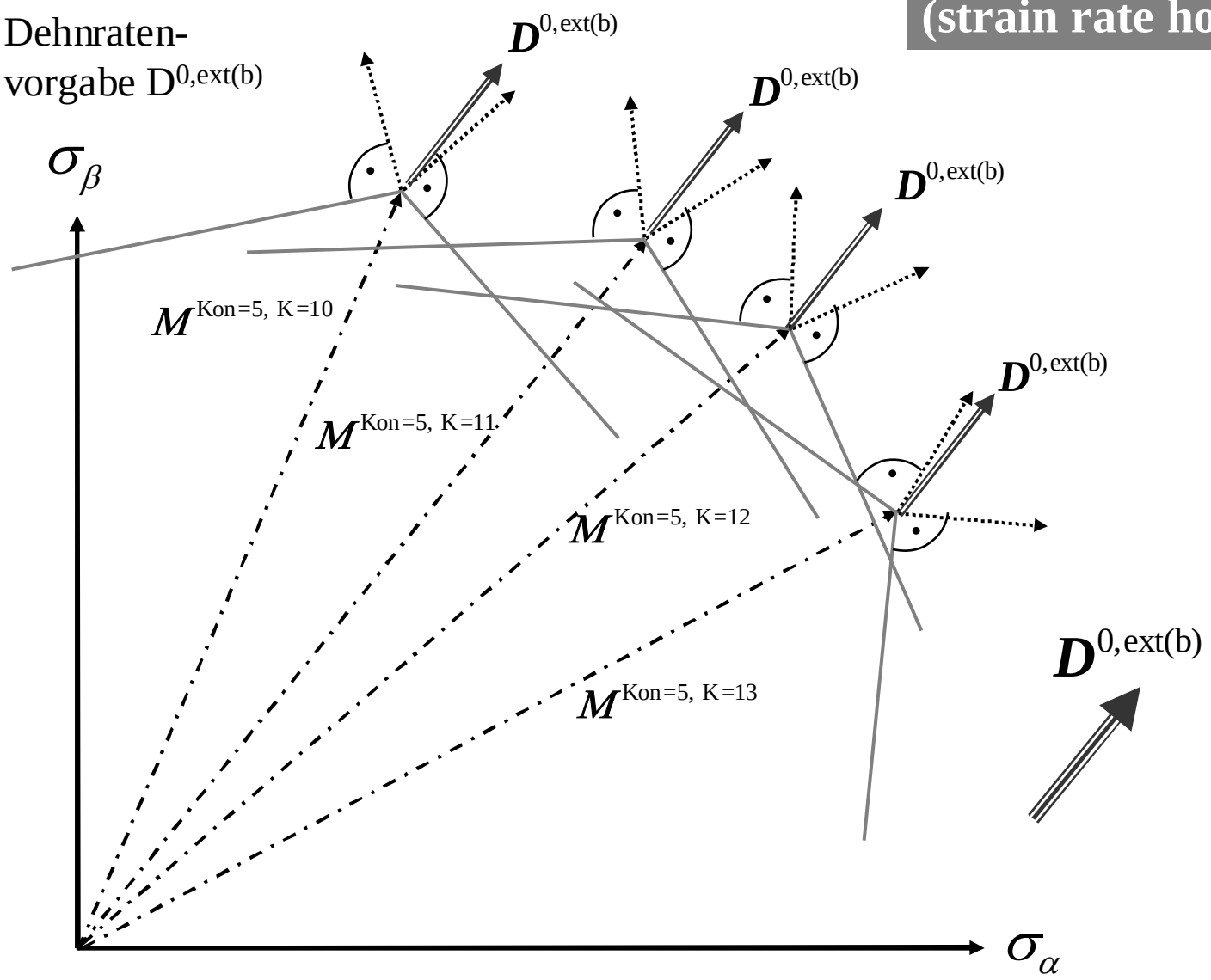
polycrystal : strain homogenization



1 grain, many systems (stress space)

polycrystal: strain homogenization

many grains, 2 systems (strain rate homogenization)

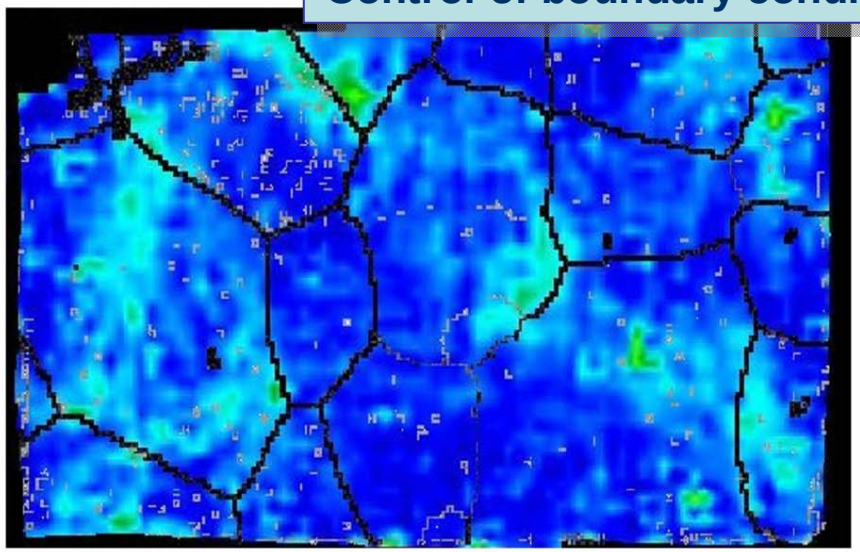


polycrystal reality

Crystal-scale homogeneity does not exist

Control of boundary conditions essential

3%



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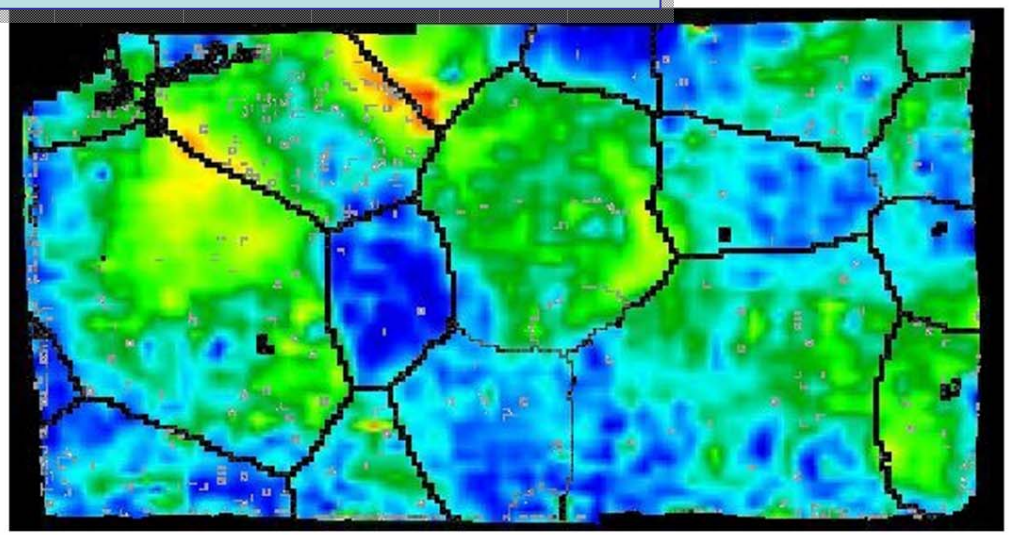

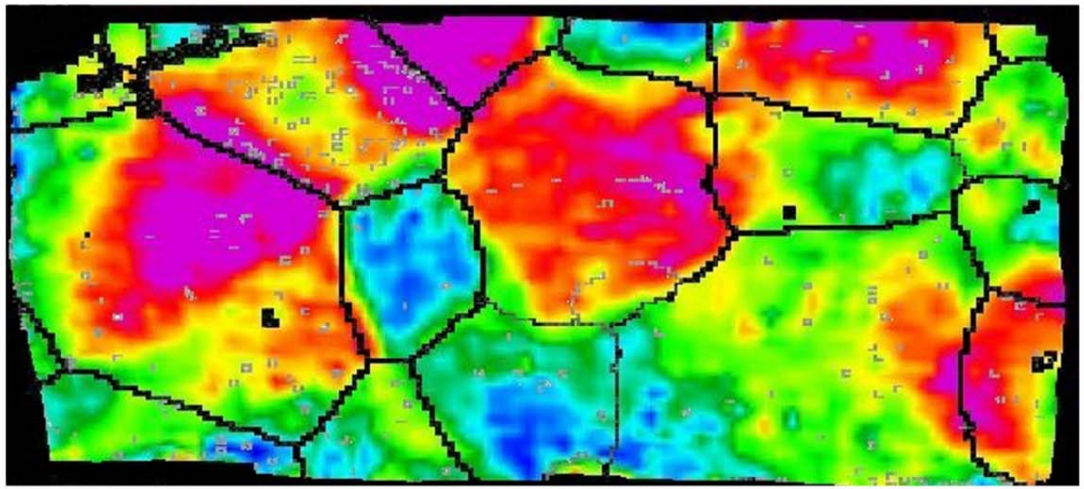

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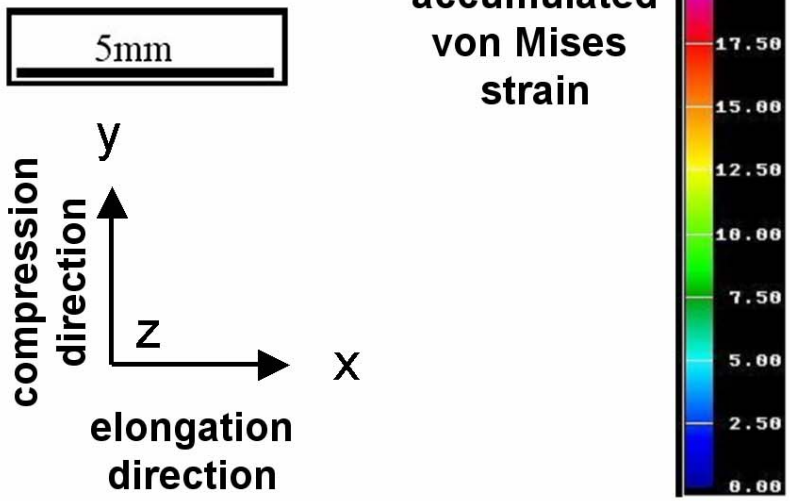


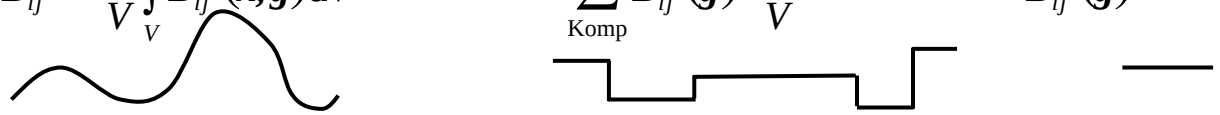
polycrystal: homogenization

averages $\left\langle \sigma_{ij} \right\rangle = \frac{1}{V}\int_V \sigma_{ij}(\boldsymbol{x},\boldsymbol{g})\mathrm{d}V$ $\left\langle D_{ij} \right\rangle = \frac{1}{V}\int_V D_{ij}(\boldsymbol{x},\boldsymbol{g})\mathrm{d}V$

typical boundary conditions

$D_{ij}^{\mathrm{ext}} = \left\langle D_{ij} \right\rangle = \frac{1}{V}\int_V D_{ij}^{\mathrm{K}}(\boldsymbol{x},\boldsymbol{g})\mathrm{d}V,$ problem: $D_{ij}^{\mathrm{K}}(\boldsymbol{x},\boldsymbol{g})$ $\sigma_{ij}^{\mathrm{K}}(\boldsymbol{x},\boldsymbol{g})$

$D_{ij}^{\mathrm{ext}} = \frac{1}{V}\int_V D_{ij}^{\mathrm{K}}(\boldsymbol{x},\boldsymbol{g})\mathrm{d}V \approx \sum_{\mathrm{Komp}} D_{ij}^{\mathrm{K}}(\boldsymbol{g})\frac{V^{\mathrm{Komp}}}{V} \approx D_{ij}^{\mathrm{K}}(\boldsymbol{g})$



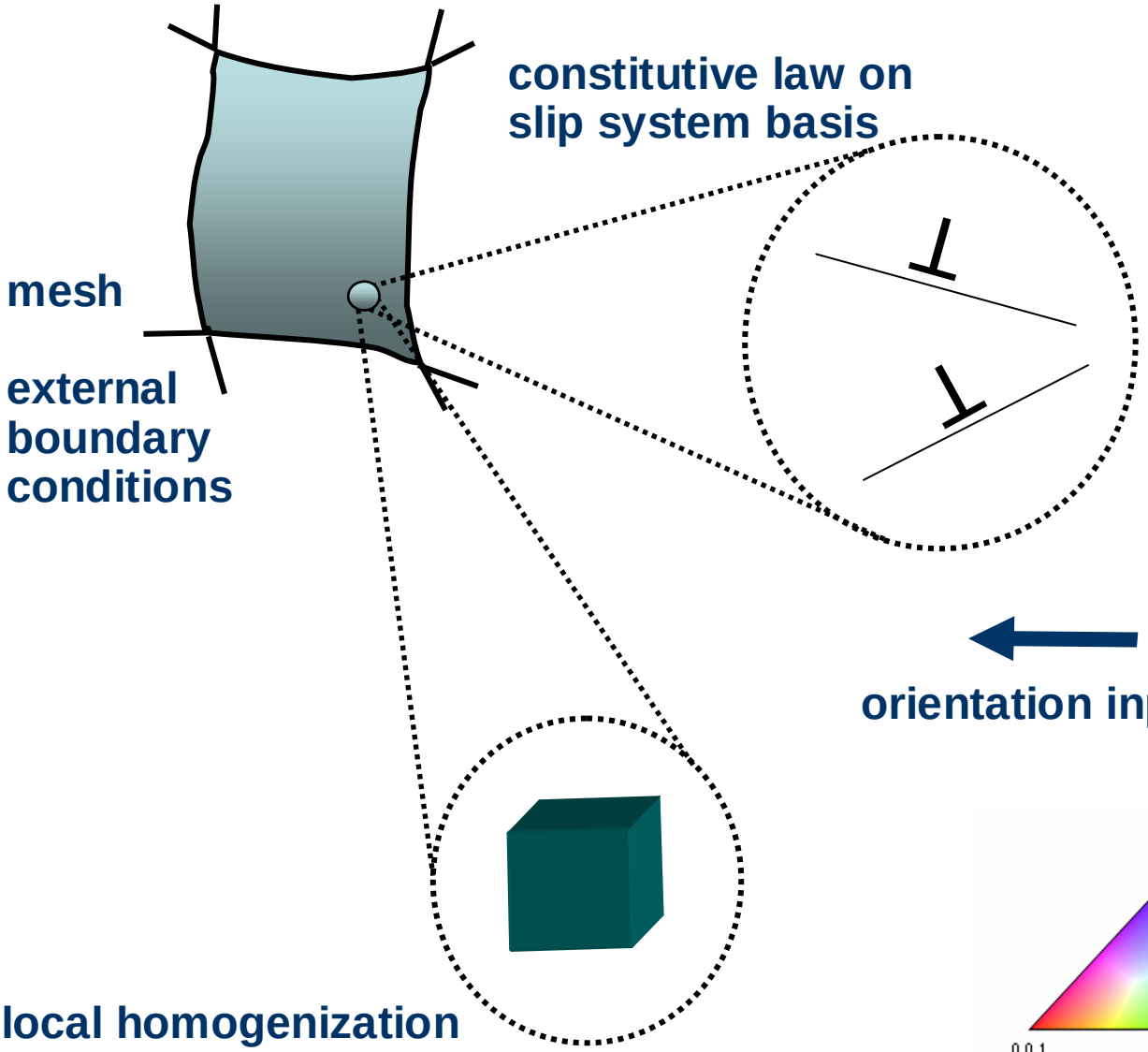
less typical boundary conditions

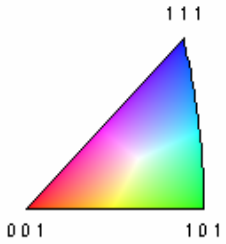
$\sigma_{ij}^{\mathrm{ext}} = \left\langle \sigma_{ij} \right\rangle = \frac{1}{V}\int_V \sigma_{ij}^{\mathrm{K}}(\boldsymbol{x},\boldsymbol{g})\mathrm{d}V,$ Problem: $\sigma_{ij}^{\mathrm{K}}(\boldsymbol{x},\boldsymbol{g})$

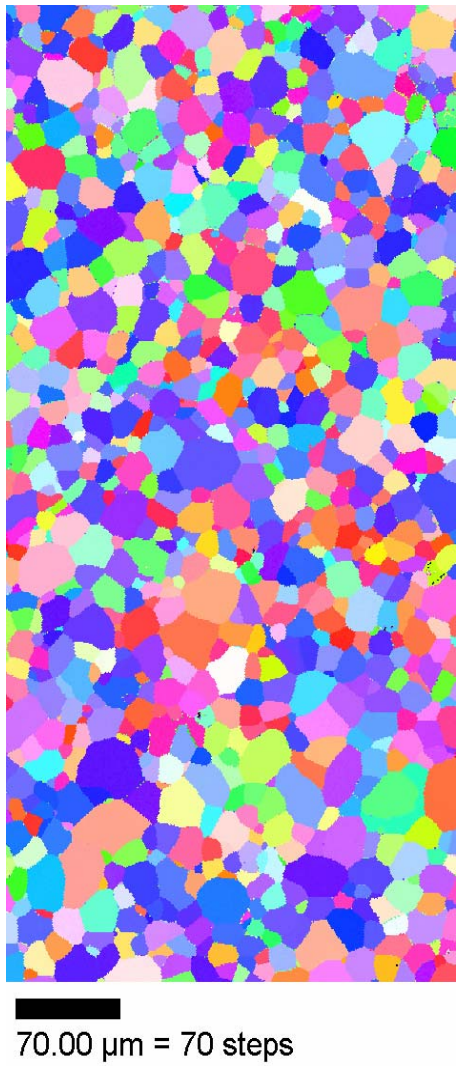
D. Raabe, P. Klose, B. Engl, K.-P. Imlau, F. Friedel, F. Roters: Advanced Engineering Materials 4 (2002) 169-180
„Concepts for integrating plastic anisotropy into metal forming simulations”
D. Raabe, Z. Zhao, W. Mao: Acta Materialia 50 (2002) 4379–4394
„On the dependence of in-grain subdivision and deformation texture of aluminium on grain interaction”

Crystal Mechanics FEM (General)

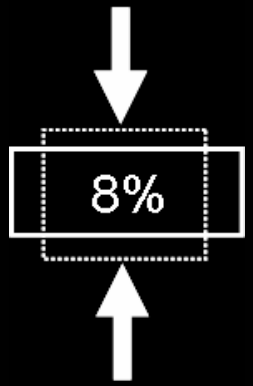
complex b.c.: Crystal Plasticity FEM (CPFEM) - Family

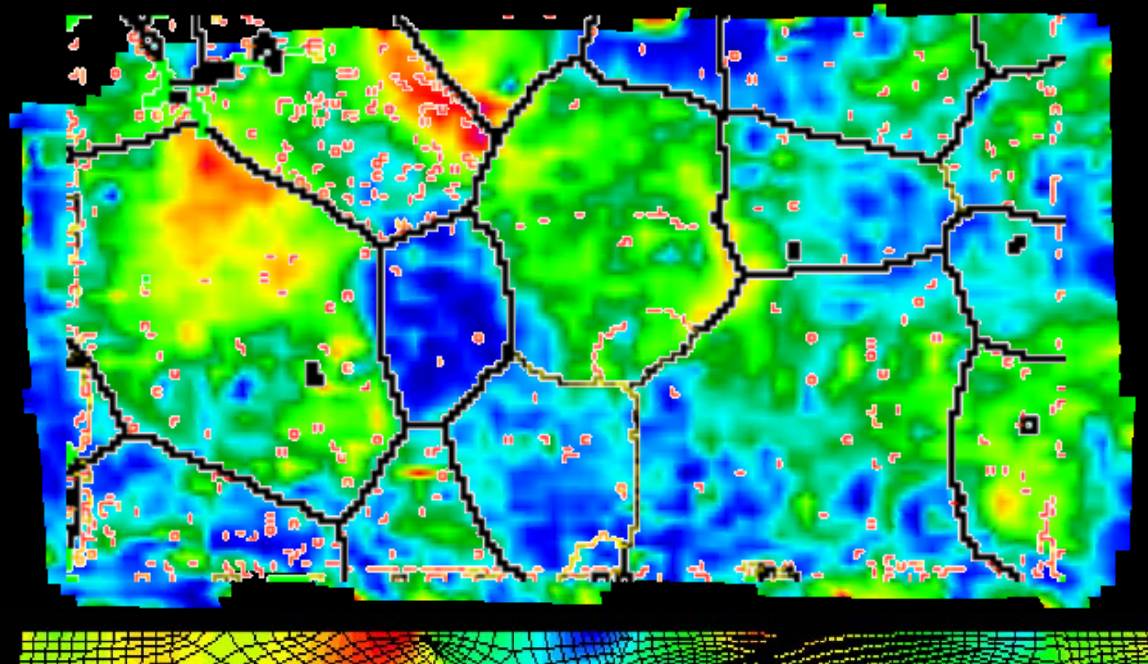




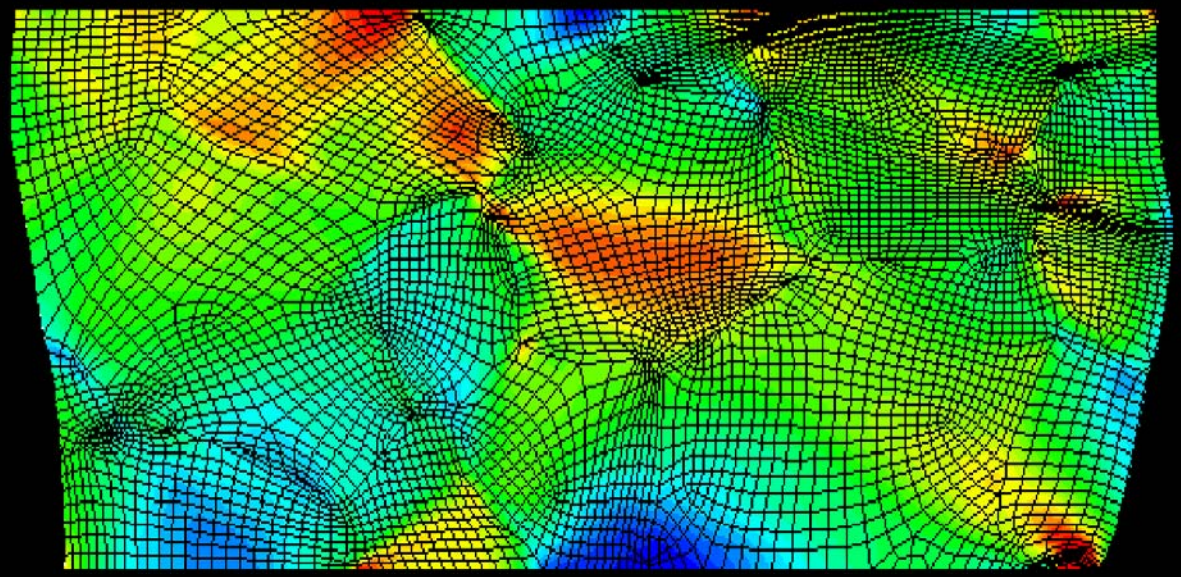


Crystal Mechanics FEM, grain scale mechanics (2D)

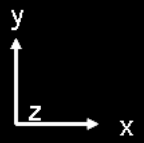




Experiment
(DIC, EBSD)
v Mises strain

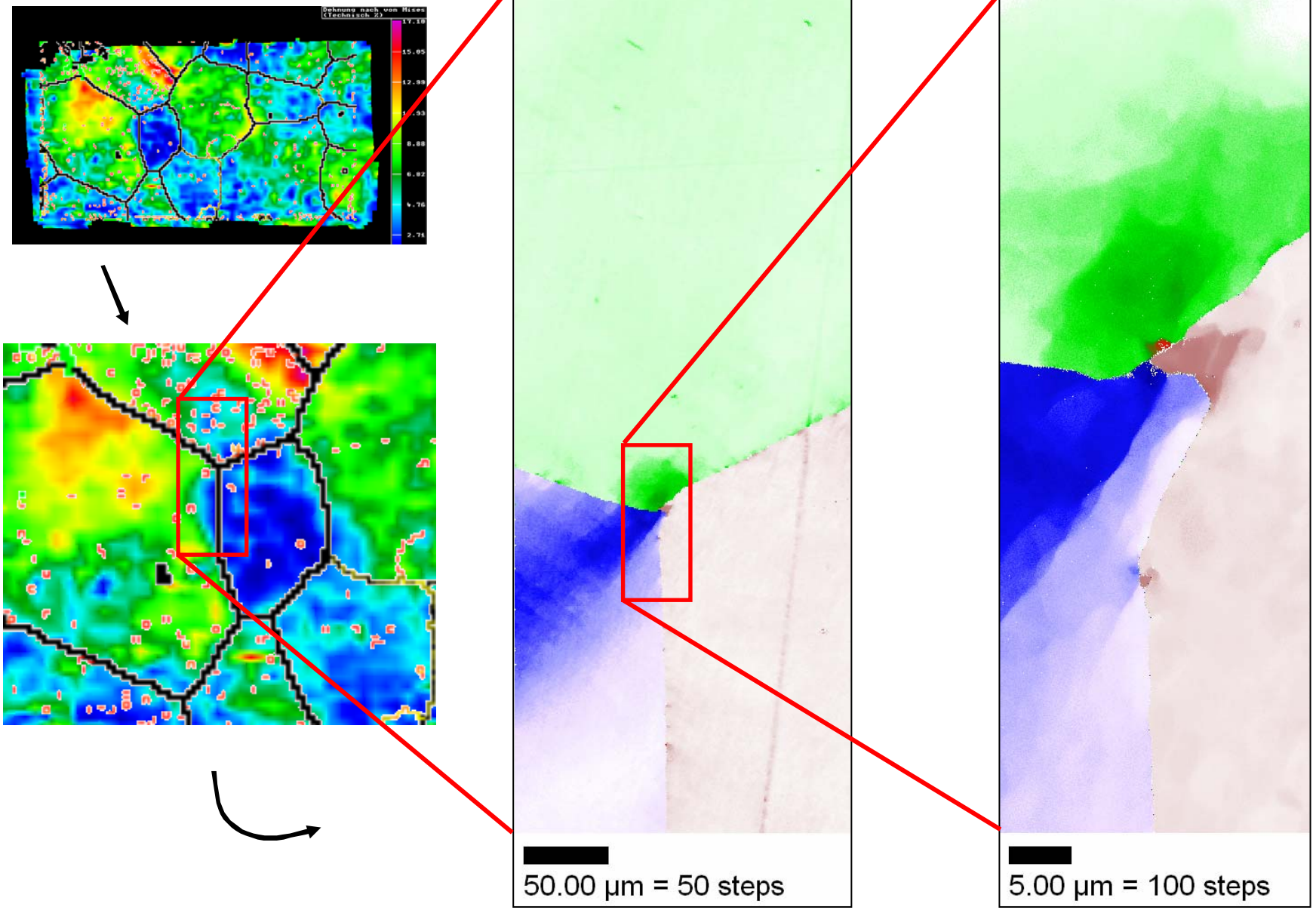


Simulation
(CP-FEM)
v Mises strain



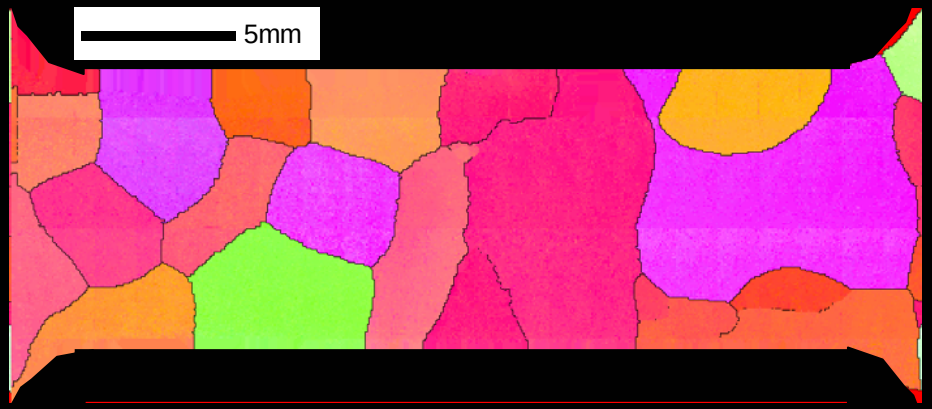
D. Raabe, M. Sachtleber, Z. Zhao, F. Roters, S. Zaefferer: Acta Materialia 49 (2001) 3433–3441
„Micromechanical and macromechanical effects in grain scale polycrystal plasticity experimentation and simulation"

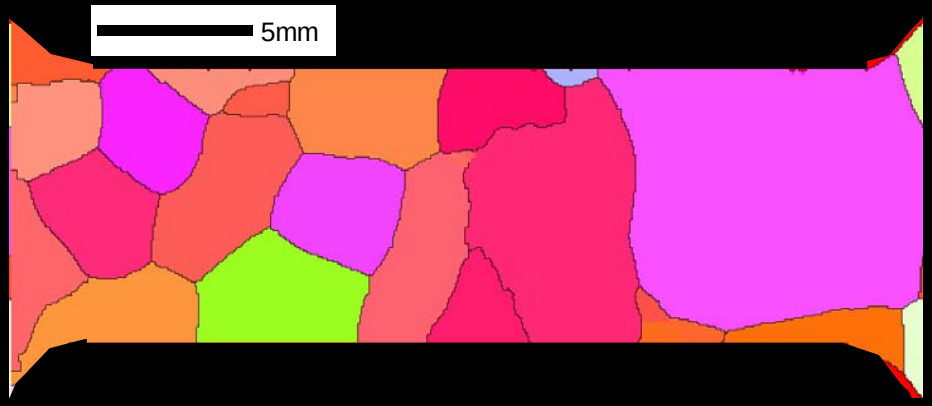
Inhomogeneity

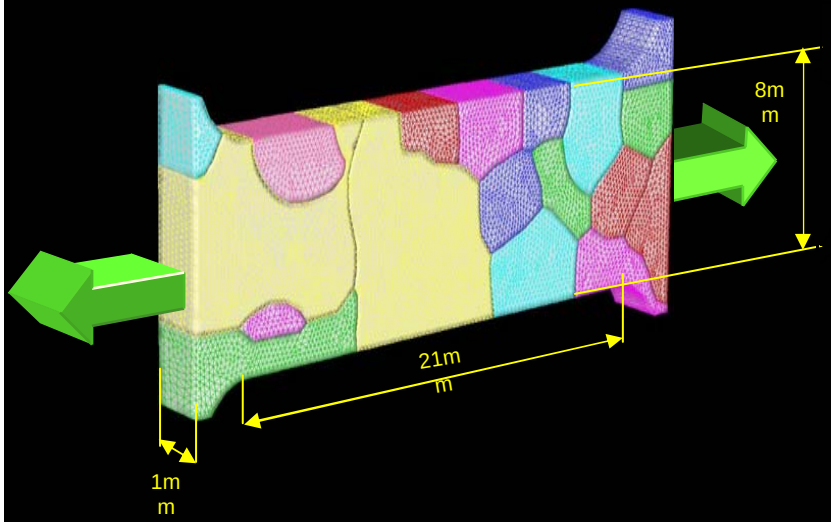


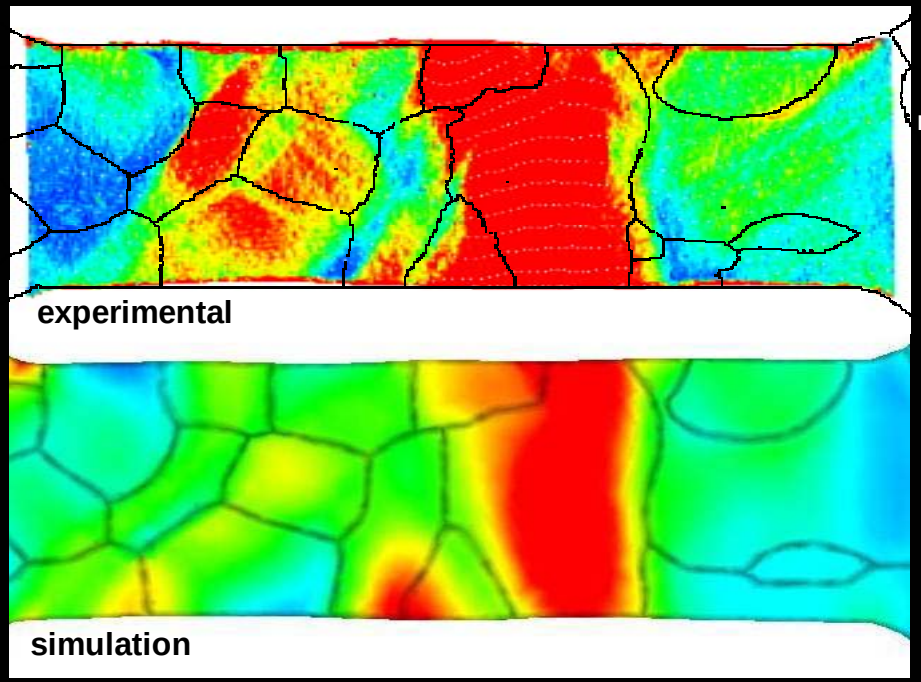
1000 nm **50 nm**

Crystal Mechanics FEM, grain scale mechanics (3D)



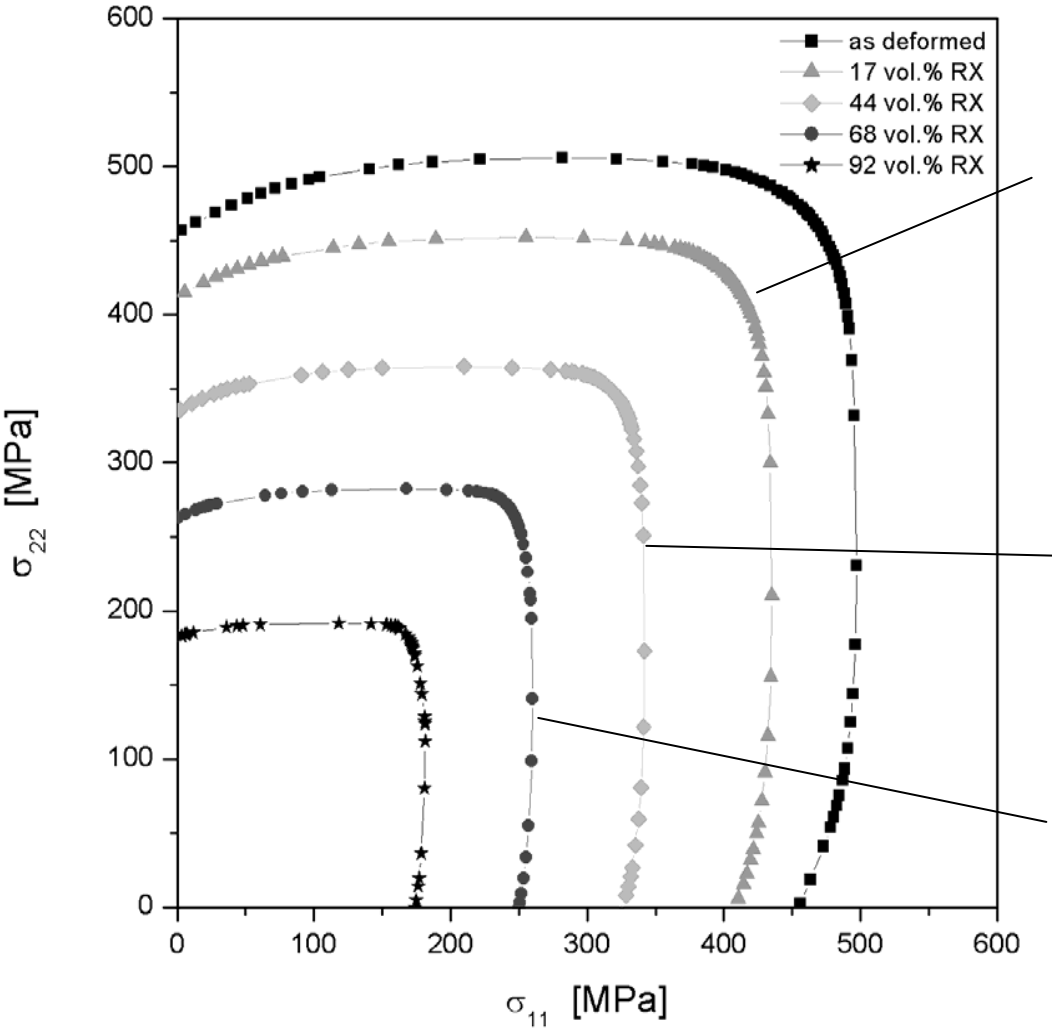


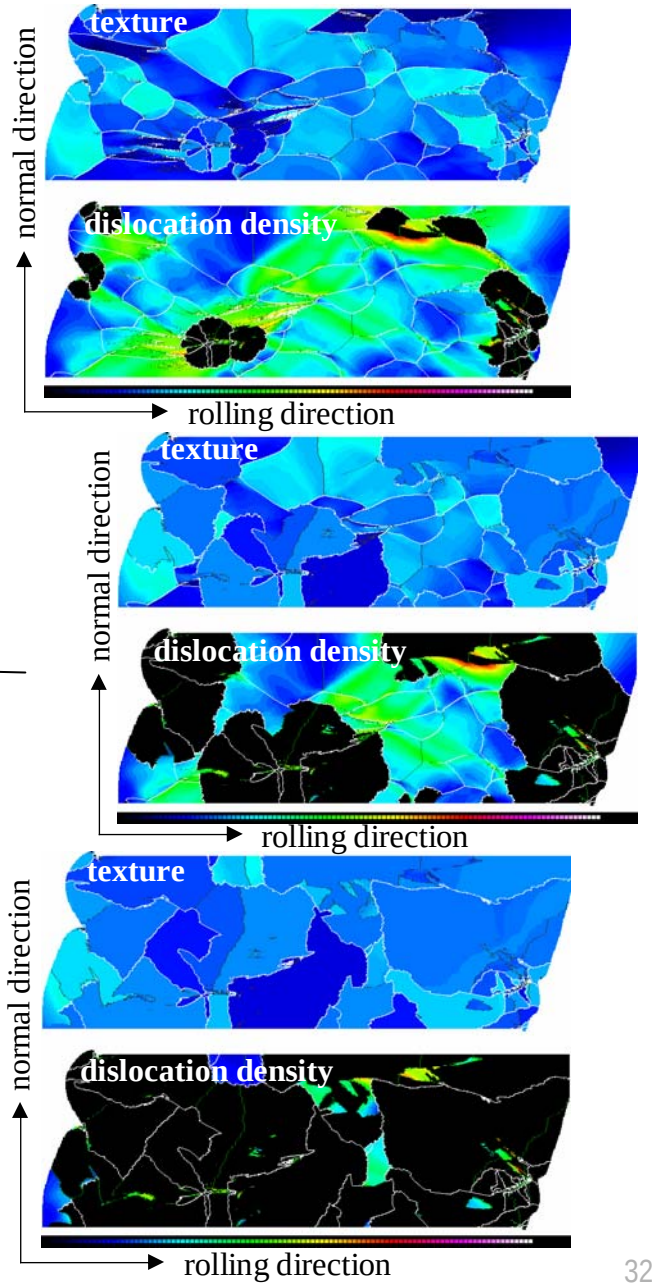




Crystal Mechanics FEM + transformation (recrystallization)

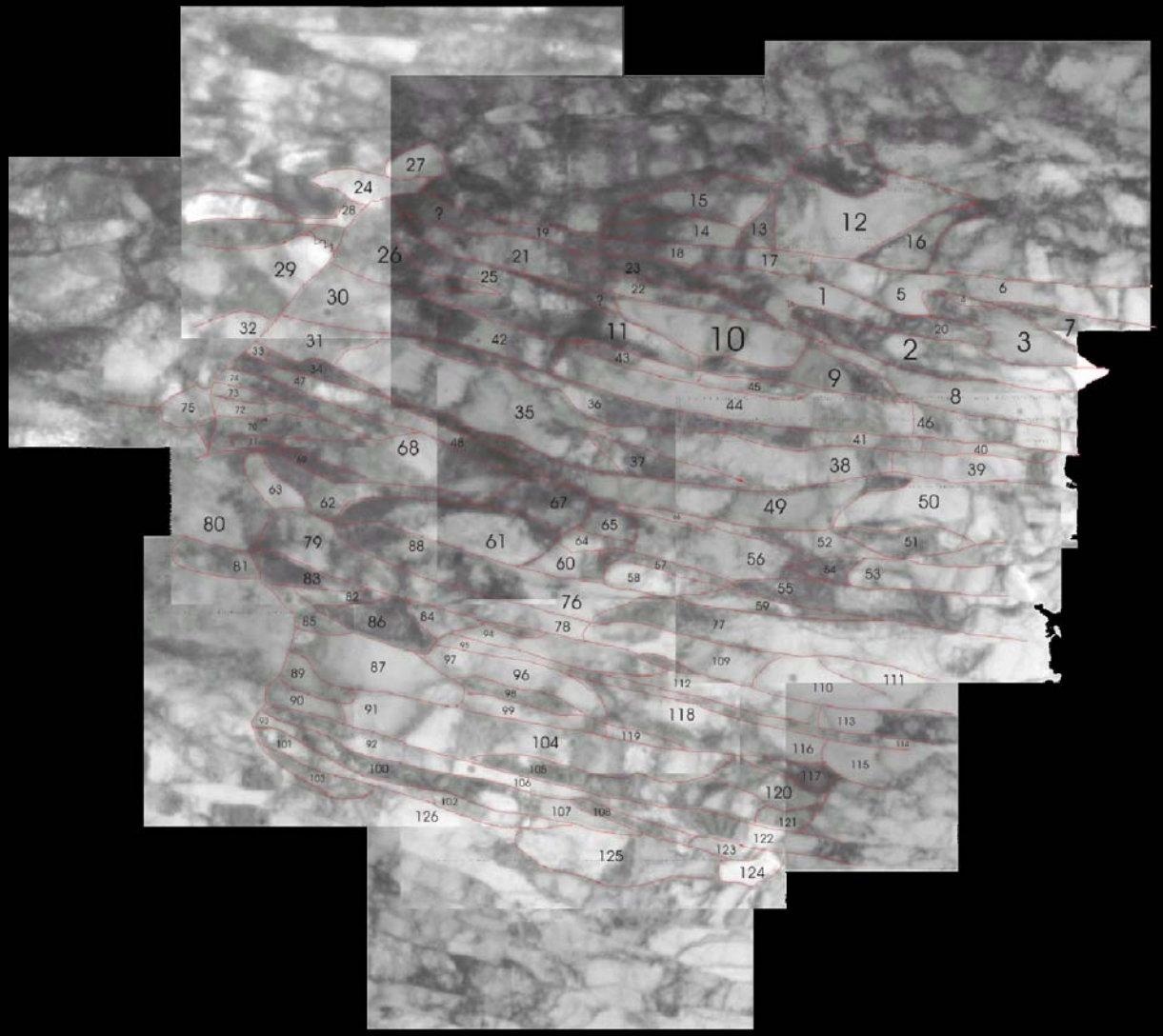
D. Raabe, R. Becker: Modelling and Simulation in Materials Science and Engineering 8 (2000) 445-462
„Coupling of a crystal plasticity finite element model with a probabilistic cellular automaton for simulating primary static recrystallization in aluminum“

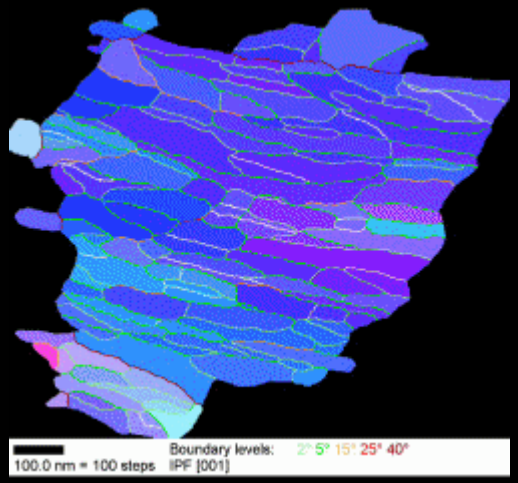


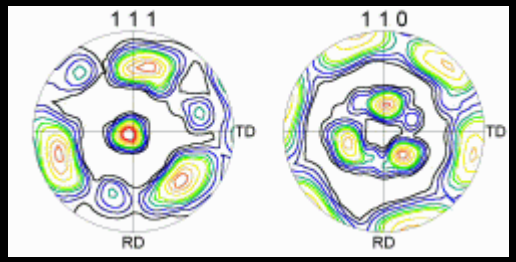


D. Raabe: Annual Review of Mater. Res. 32 (2002)

Nucleation in transformation (recrystallization)



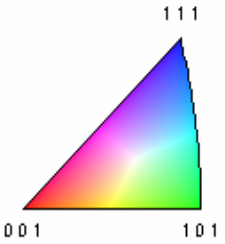


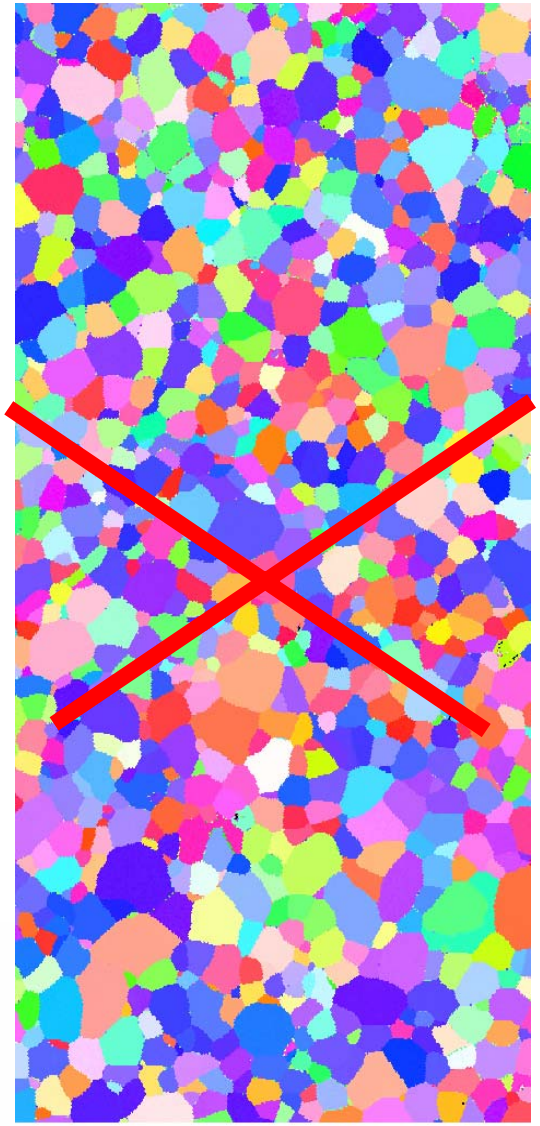


source: Stefan Zaefferer

10 billion grains

too many grains

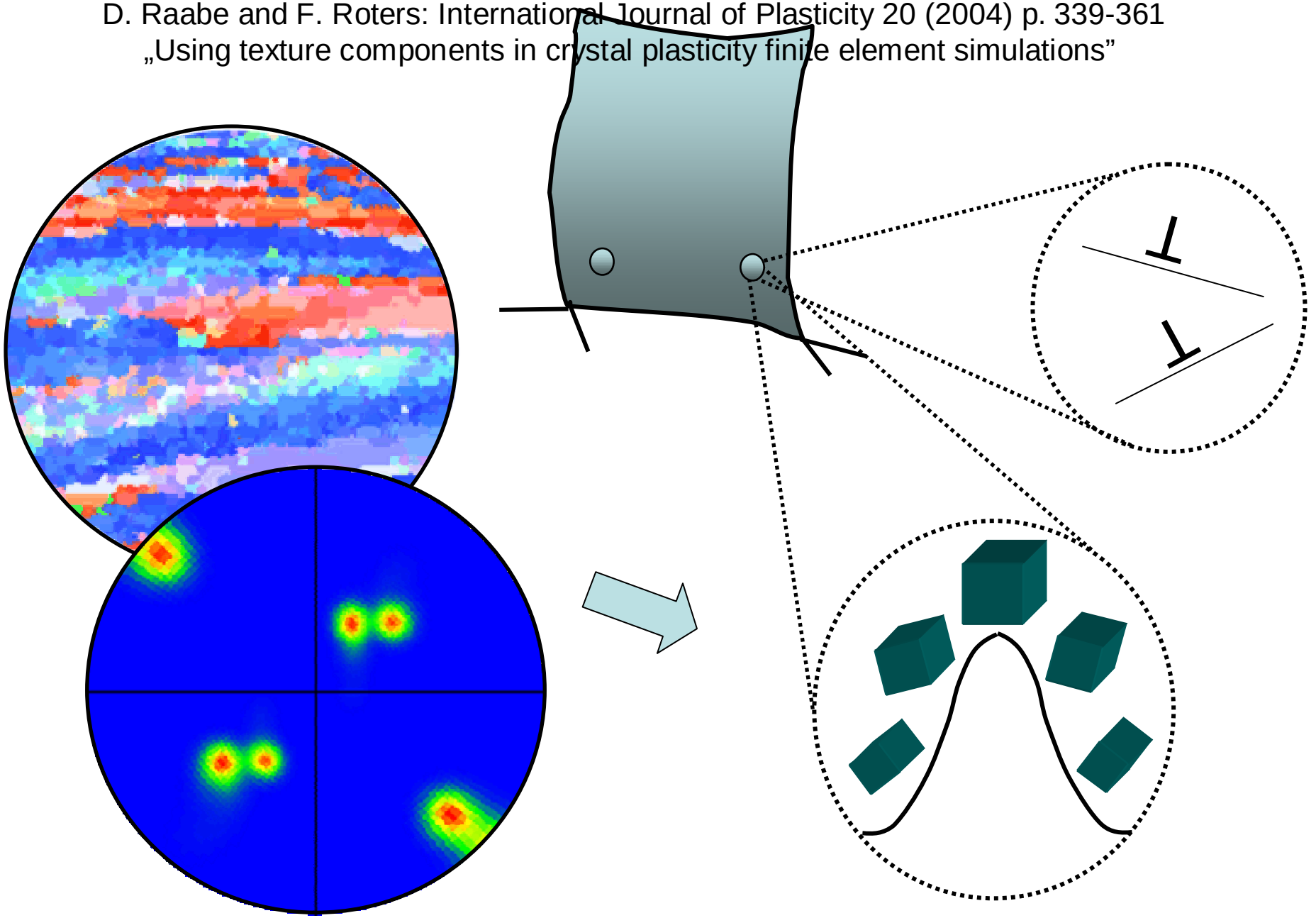




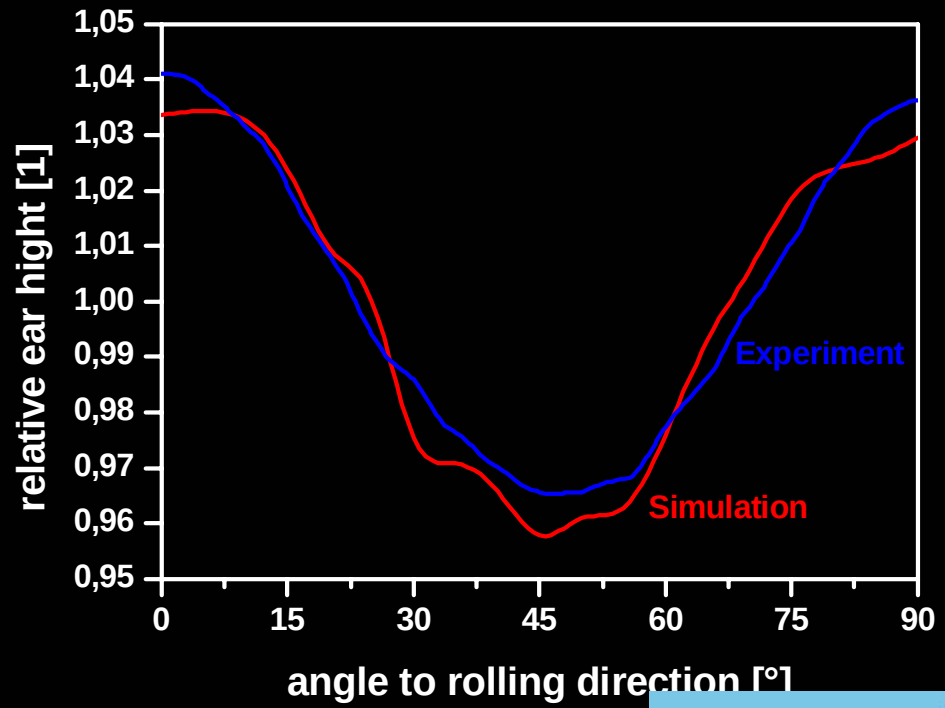
70.00 µm = 70 steps

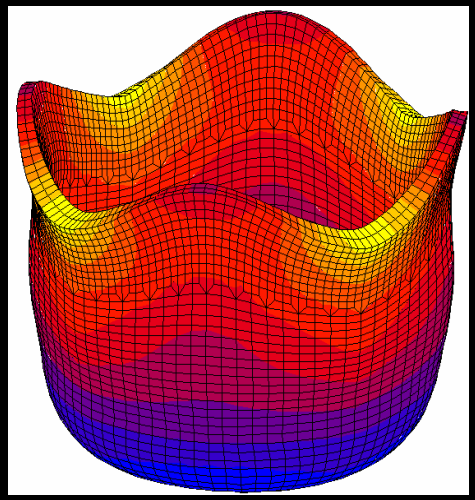
map texture functions into FEM

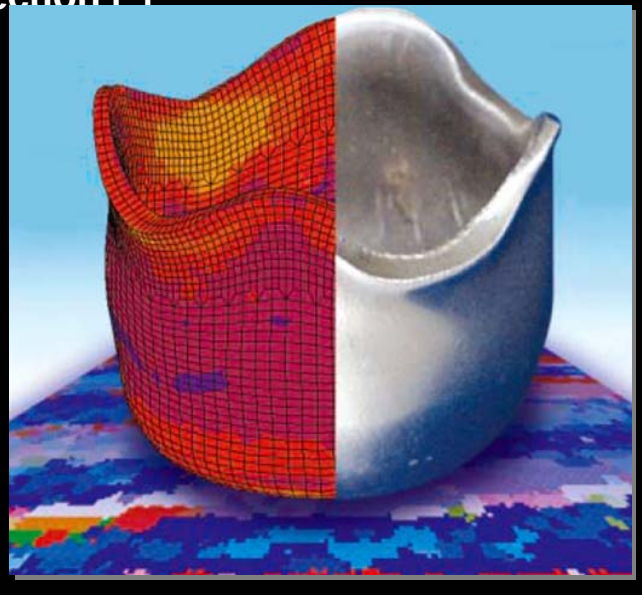
D. Raabe and F. Roters: International Journal of Plasticity 20 (2004) p. 339-361
„Using texture components in crystal plasticity finite element simulations”



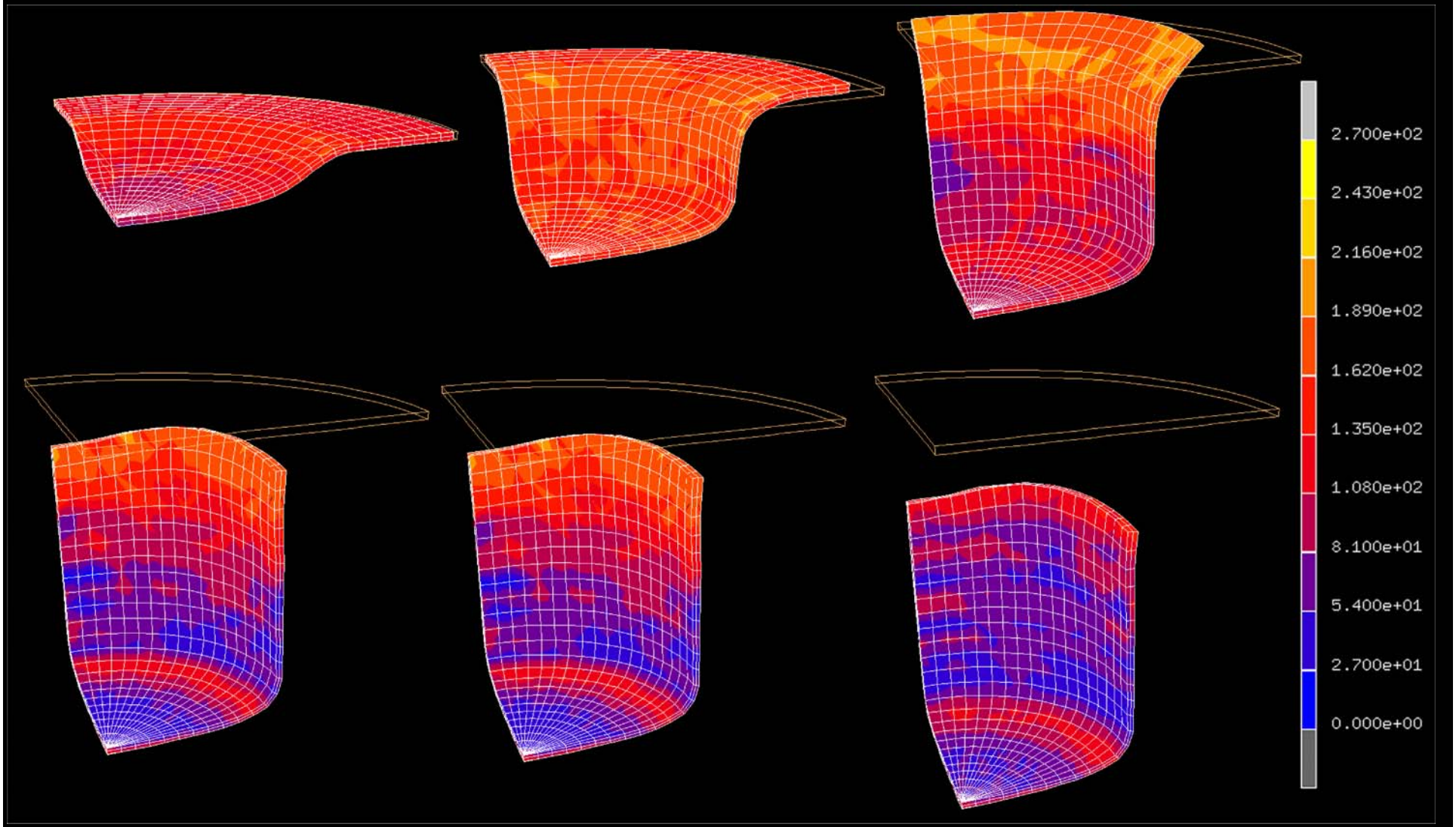
Crystal Plasticity FEM







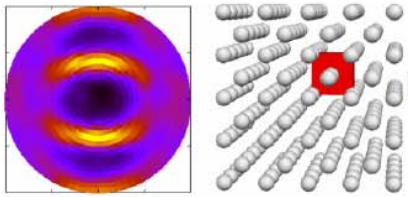
Crystal Plasticity FEM

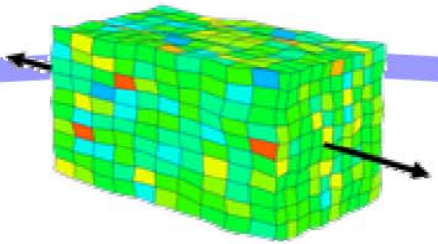


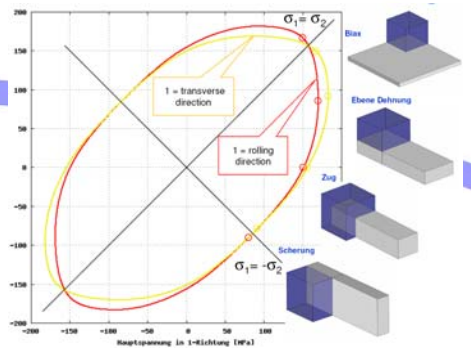
Example: Automobile (Coarse graining, Parametertransfer)

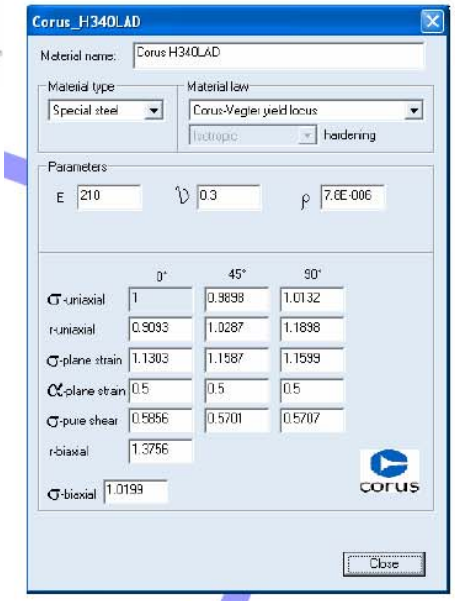
Numerical Laboratory

From Crystal Plasticity to Deep Drawing









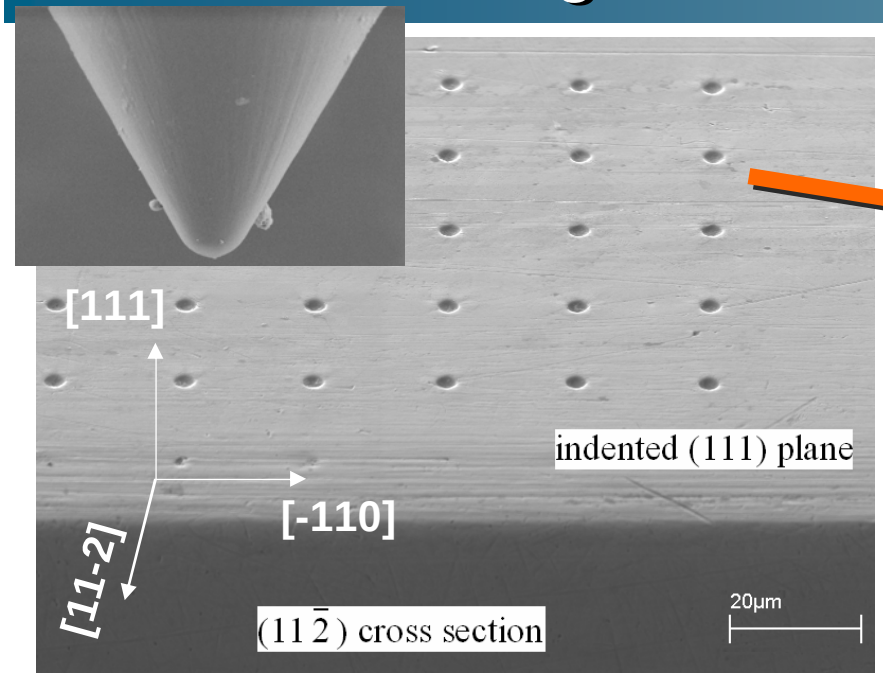
- **Virtual Material Testing**
  - Representative Volume Element
  - Virtual test program – extrapolation of calibration tests
  - Parameter fit of the macro material model
  - No performance loss compared to classical deep drawing simulation
  - Material behaviour limited to available models in commercial FE codes
  - Demonstrated by INPRO for (bcc) HSLA steel

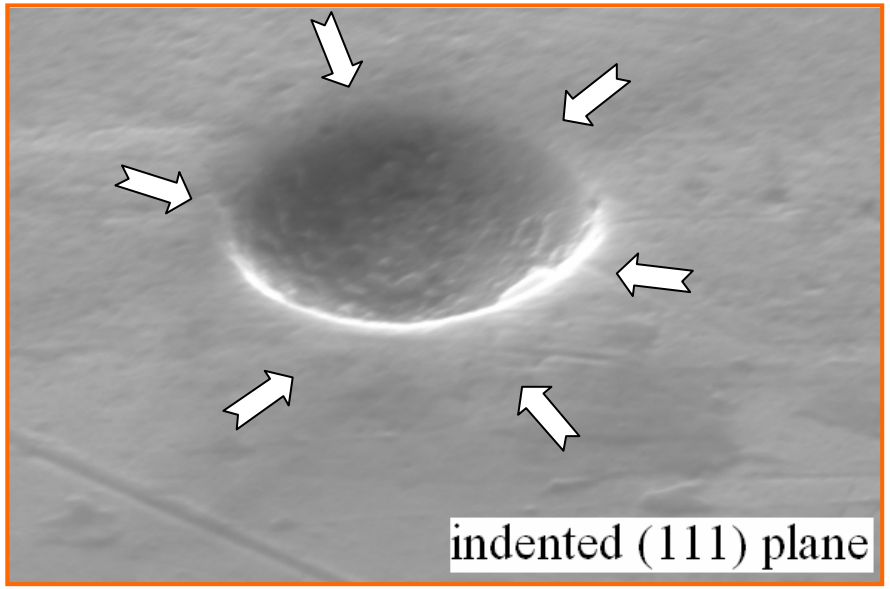
Vegter-Modell in PamStamp 2G

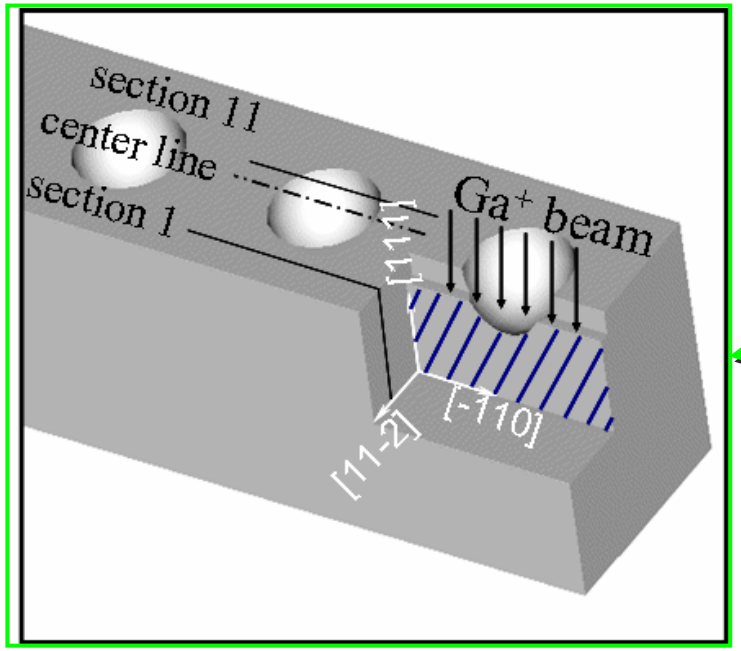
Overview

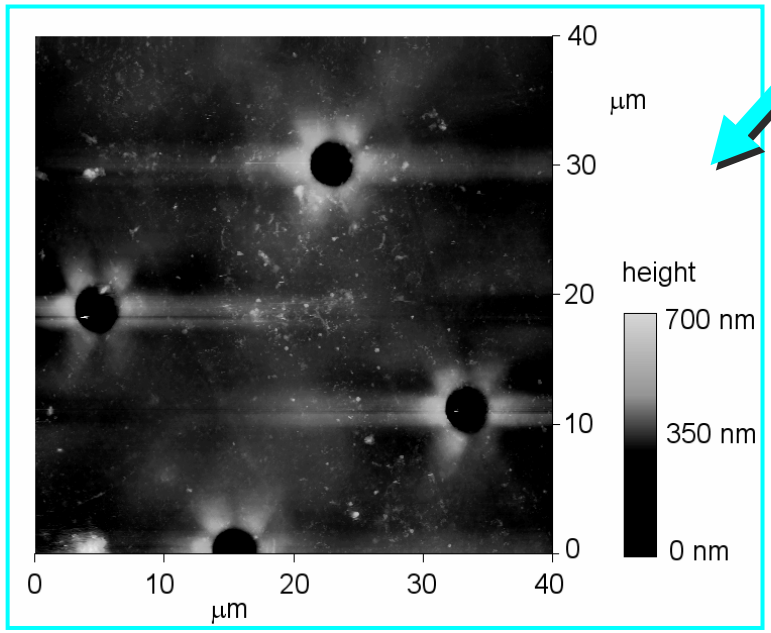
- **Scales in elasto-plasticity, MMM input**
- **Polycrystal elasto-plasticity homogenization (single phase, focus on kinematics, and b.c.)**
- **Limits in plasticity continuum models (small scale crystal plasticity)** ←

Nanoindentierung

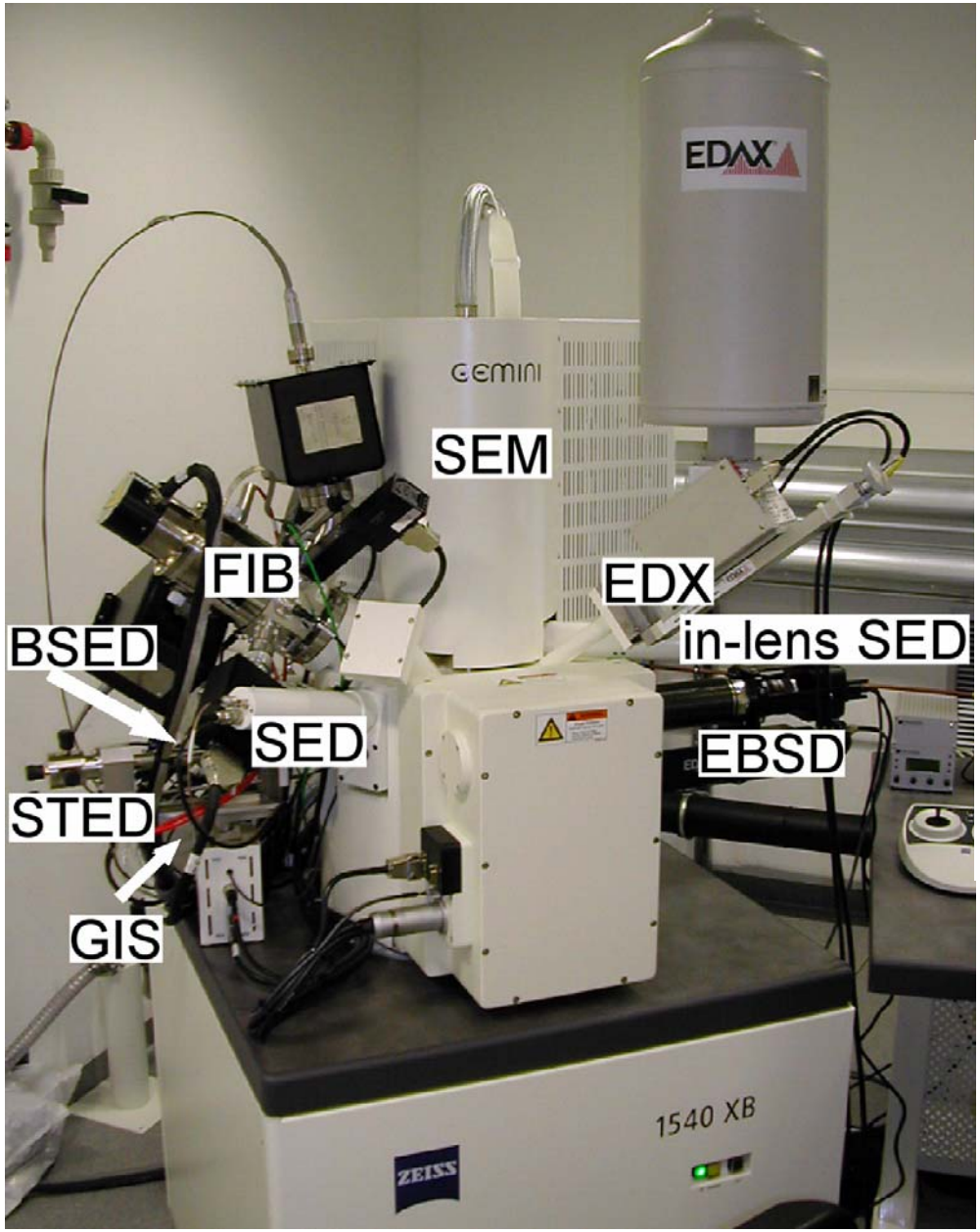


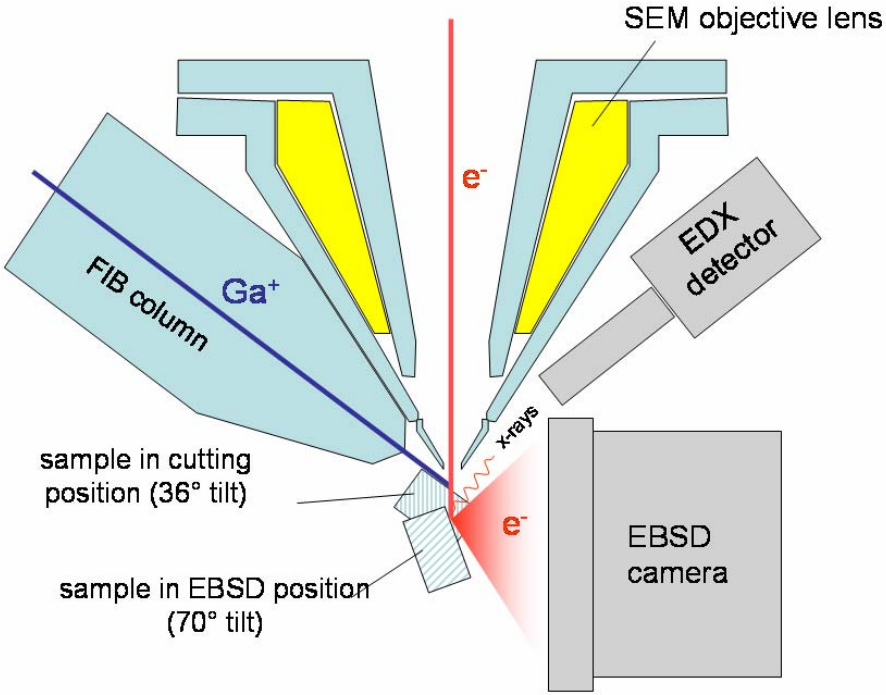






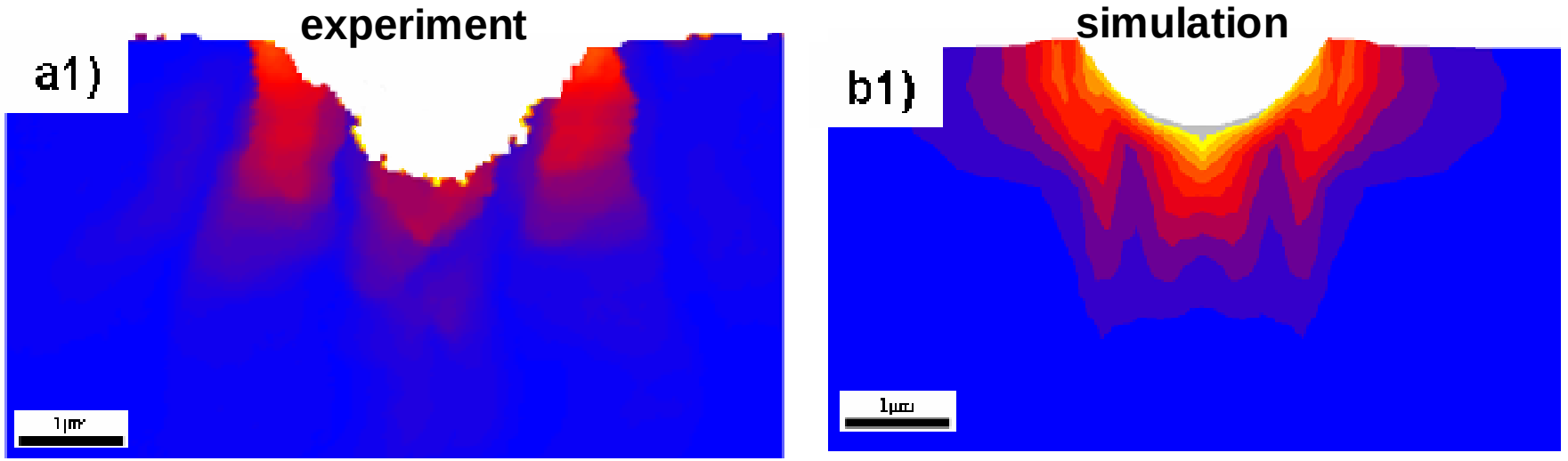
3D electron - microscopy

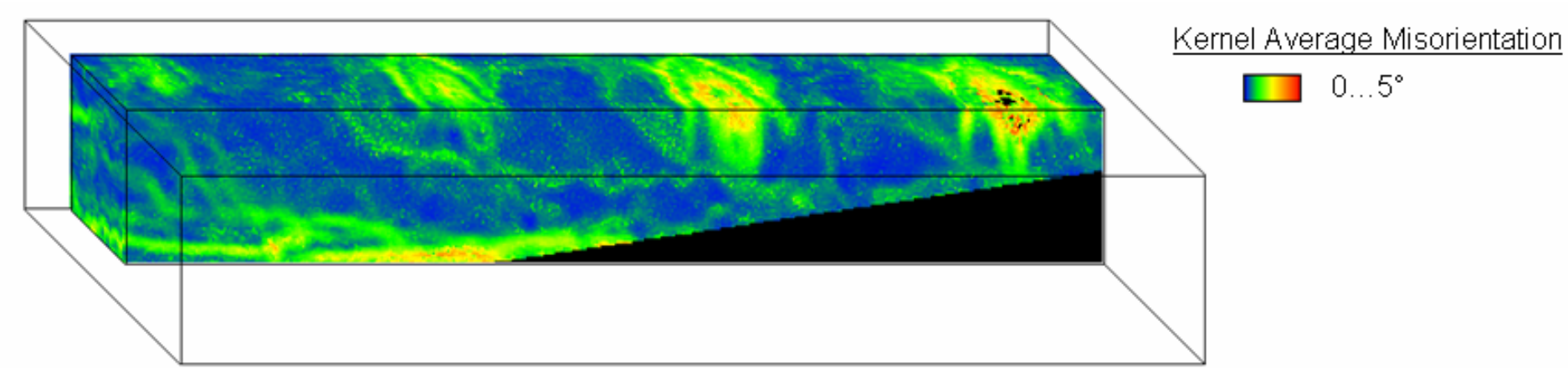




Misorientation map

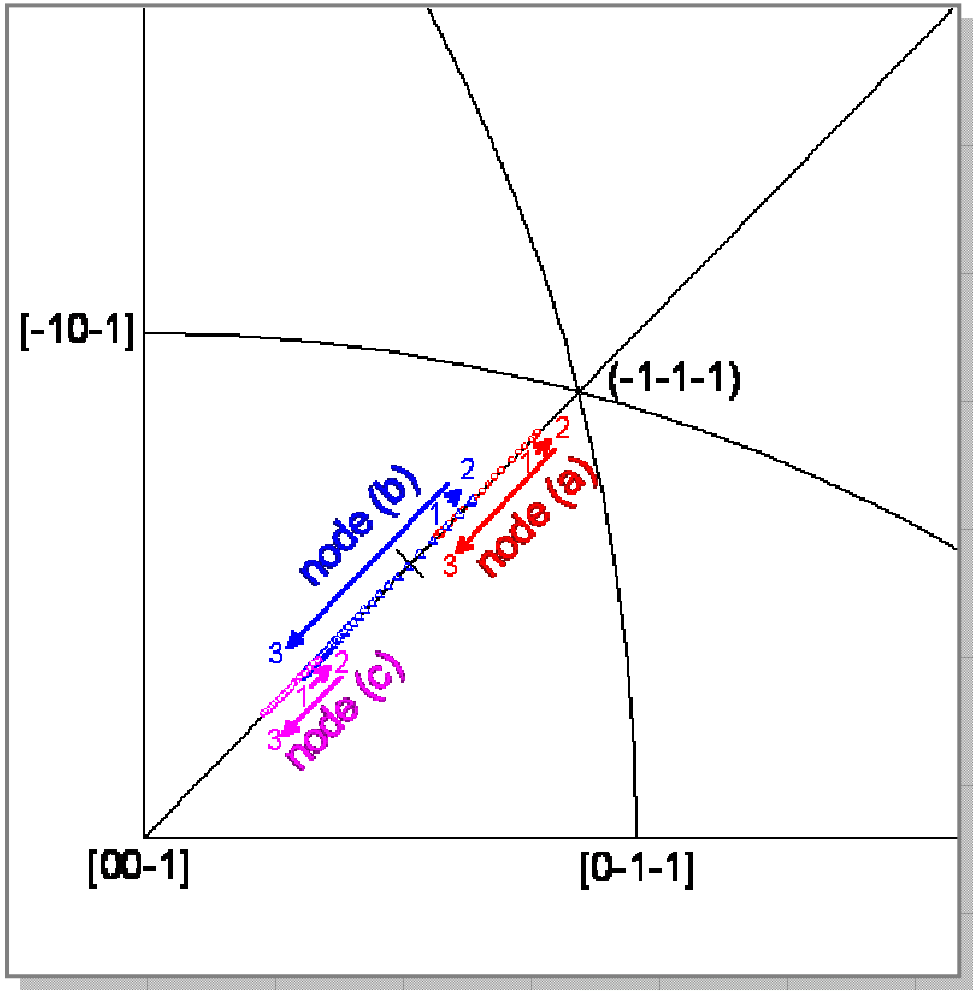
N. Zaafarani D. Raabe, R. N. Singh, F. Roters, S. Zaefferer,
Acta Materialia, Volume 54, Issue 7, Pages 1707-1994 (April 2006)
"Three dimensional investigation of the texture and microstructure below a nanoindent in a Cu single crystal using 3D EBSD and crystal plasticity finite element simulations"

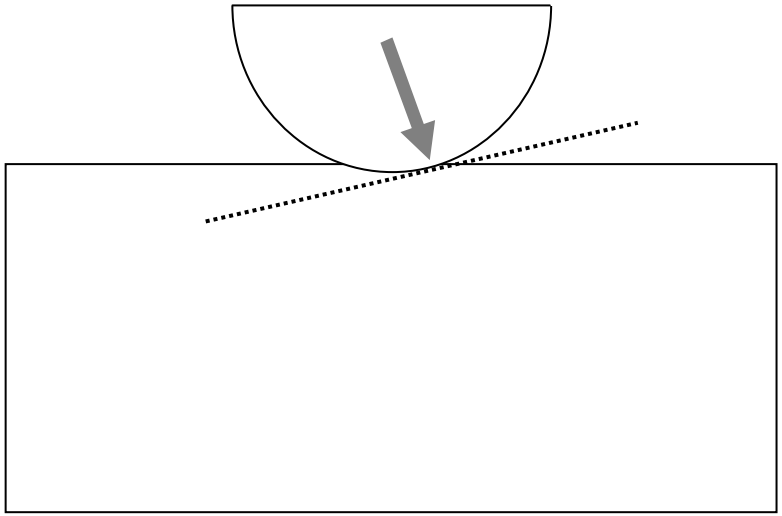


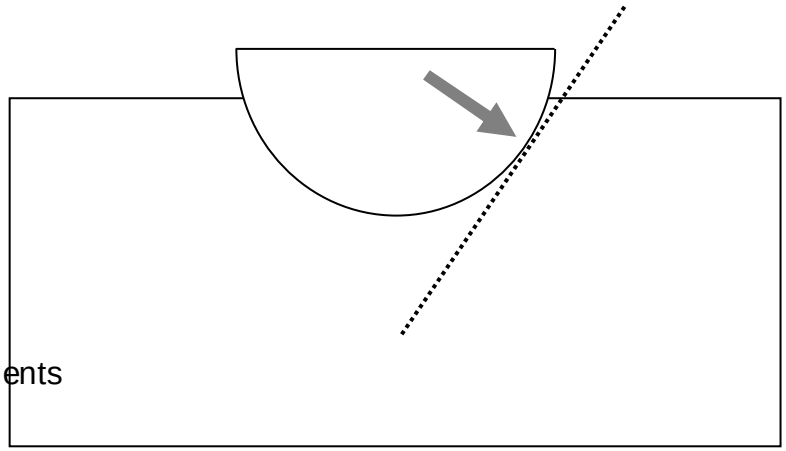


Forces: 4, 6, 8, and 10 mN

Simplify

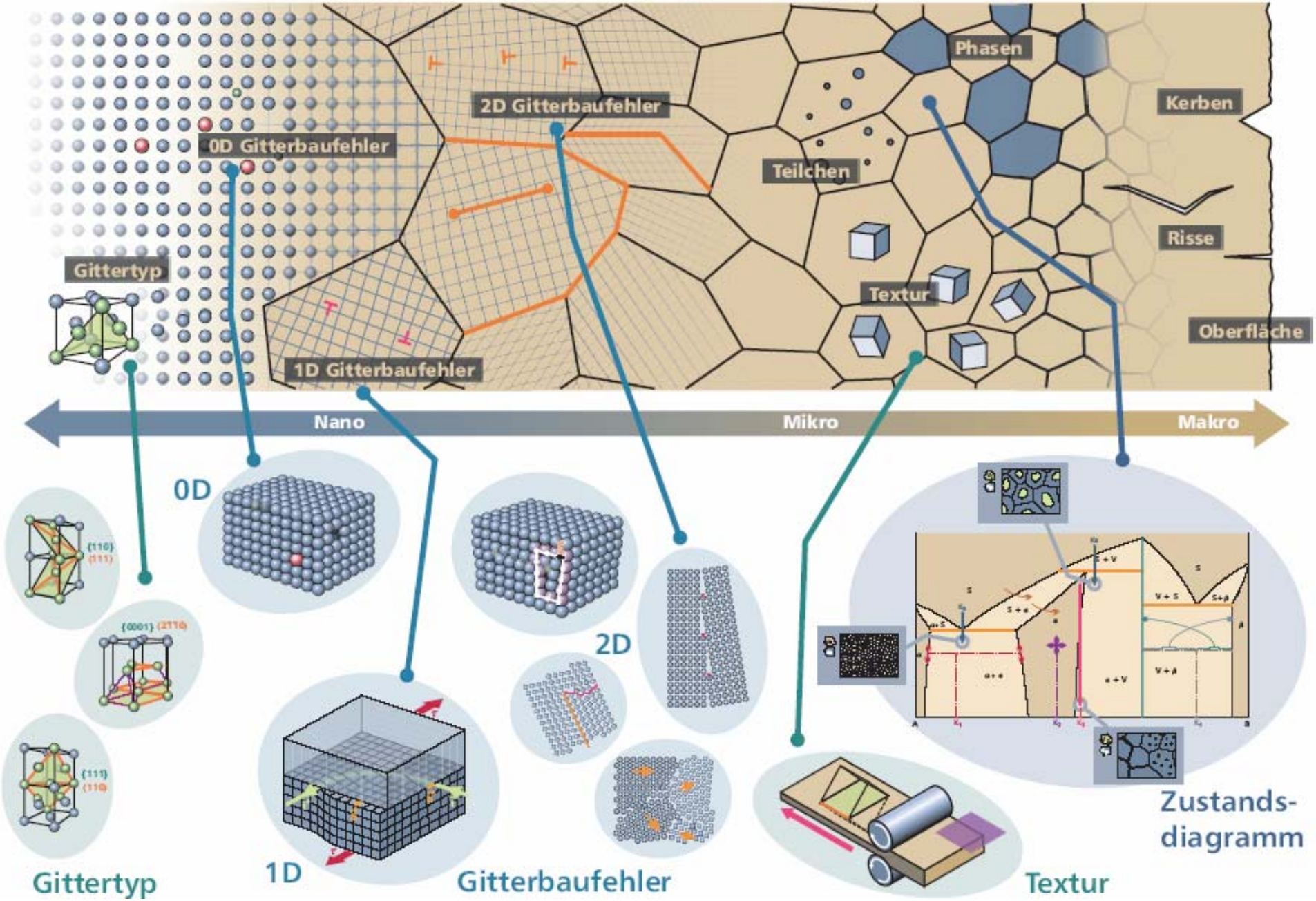






N. Zaafarani, D. Raabe, F. Roters and S. Zaefferer
Acta Materialia, Volume 56, Issue 1, January 2008, Pages 31-42
On the origin of deformation-induced rotation patterns below nanoindents

Multiscale approaches in crystal plasticity



Multiscale Models: Scales, Methods

MMM : input / handshake in Elasto-Plasticity

- **Structure of matter (DFT): TD of alloys, impurities, order, T>0K (talk of M. Friak)**
- **Structure of defects (DFT, MD); dislocation cores, dislocation motion, inertia, energy surface during motion, dislocation reactions, impurities, interface properties, T>0K (MD potentials, rates, loads !) (talk of L. Limperakis)**
- **Defect topology (DD, kMC, CA, PP): kinetics, Ostwald, clustering, interface dynamics: physics of interfaces and diffusion**
- **Dynamics of defects (MD, DD): mechanical reactions, interaction with interfaces, role of impurities (talk of L. Limperakis)**
- **Texture (CPFEM, Taylor): any intrinsic anisotropy**