



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)**

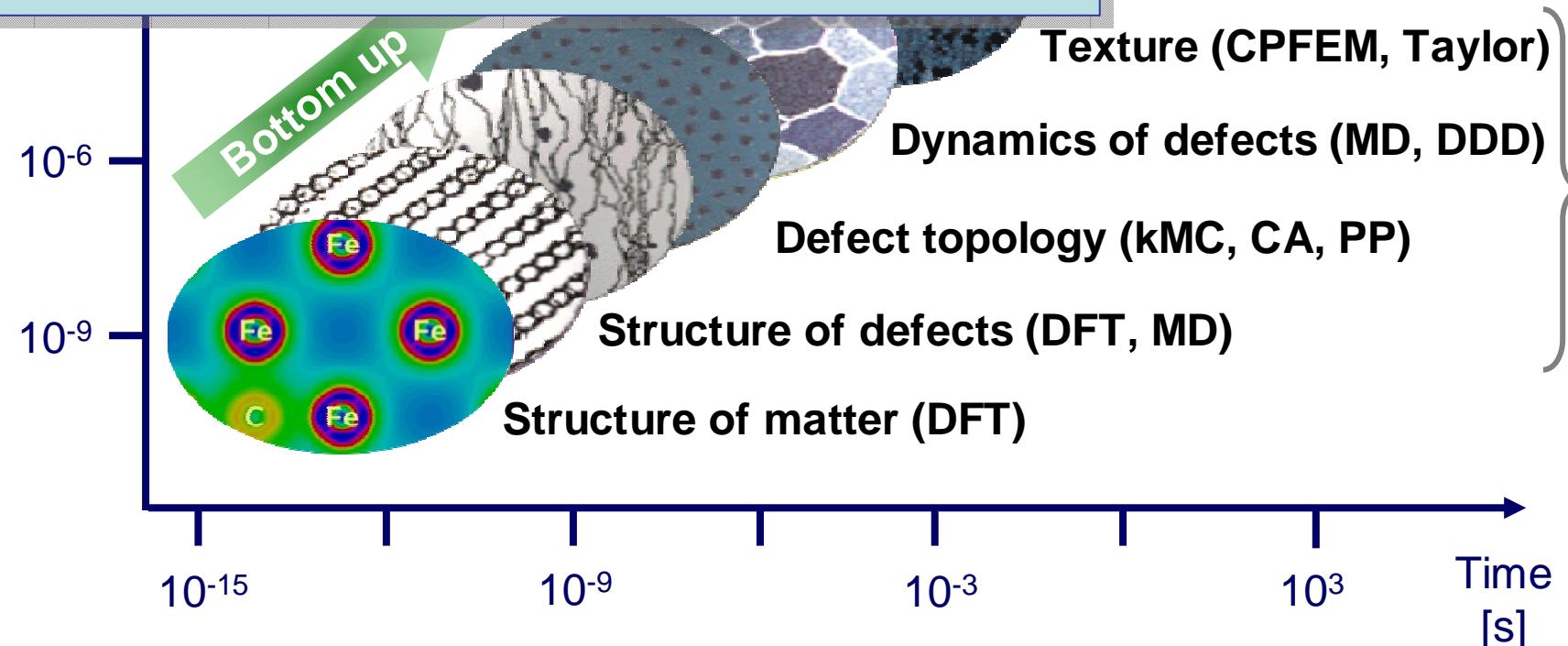


Multiscale Models: Scales, Methods

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 hopping:

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)



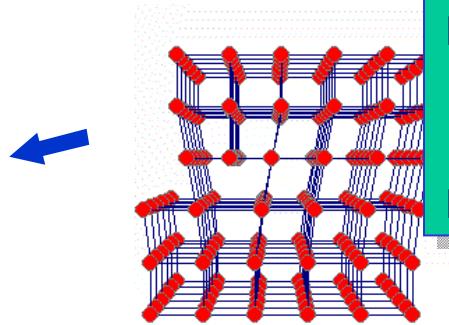
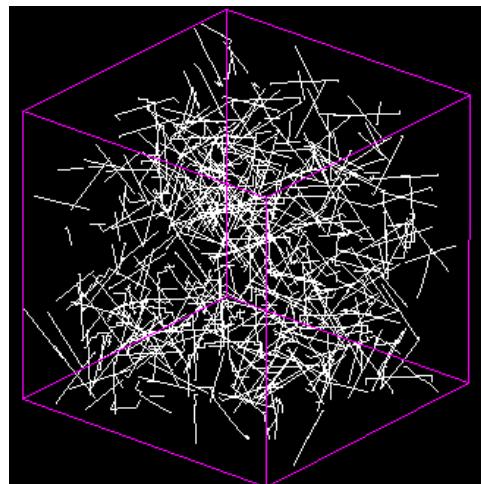
Multiscale, crystal plasticity: coarse graining

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

Motivation: Fundamentals of crystal mechanics



parallel loops (Kubin)
reactions (Kubin)

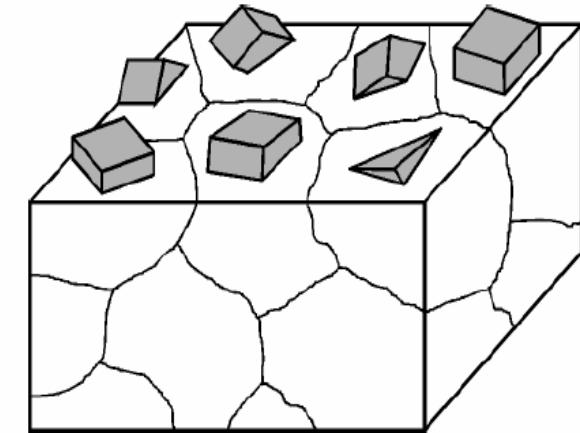


one dislocation

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

Lattice defect kinetics (Franz Roters)

mesoscopic boundary conditions (grain / orientation neighborhood)



spin (orientation change)



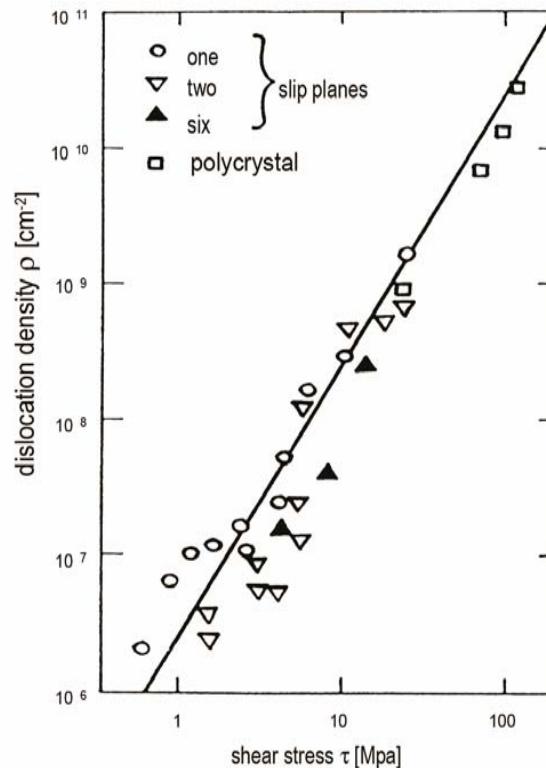
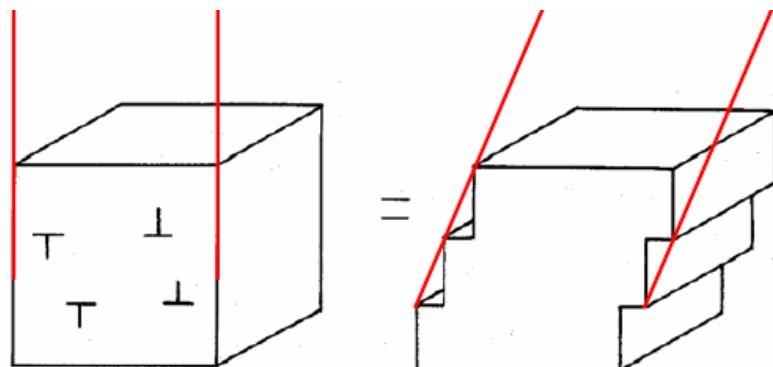
Motivation: Fundamentals of crystal mechanics

kinetics: collective dislocation behaviour

- kinetic equation of state
- structure evolution

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

- coupling to imposed shape change

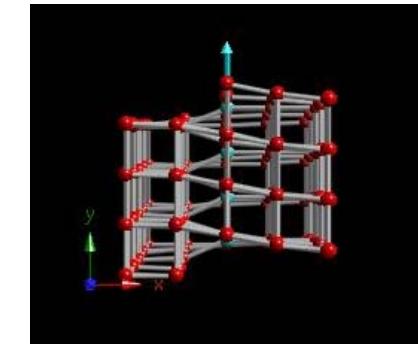
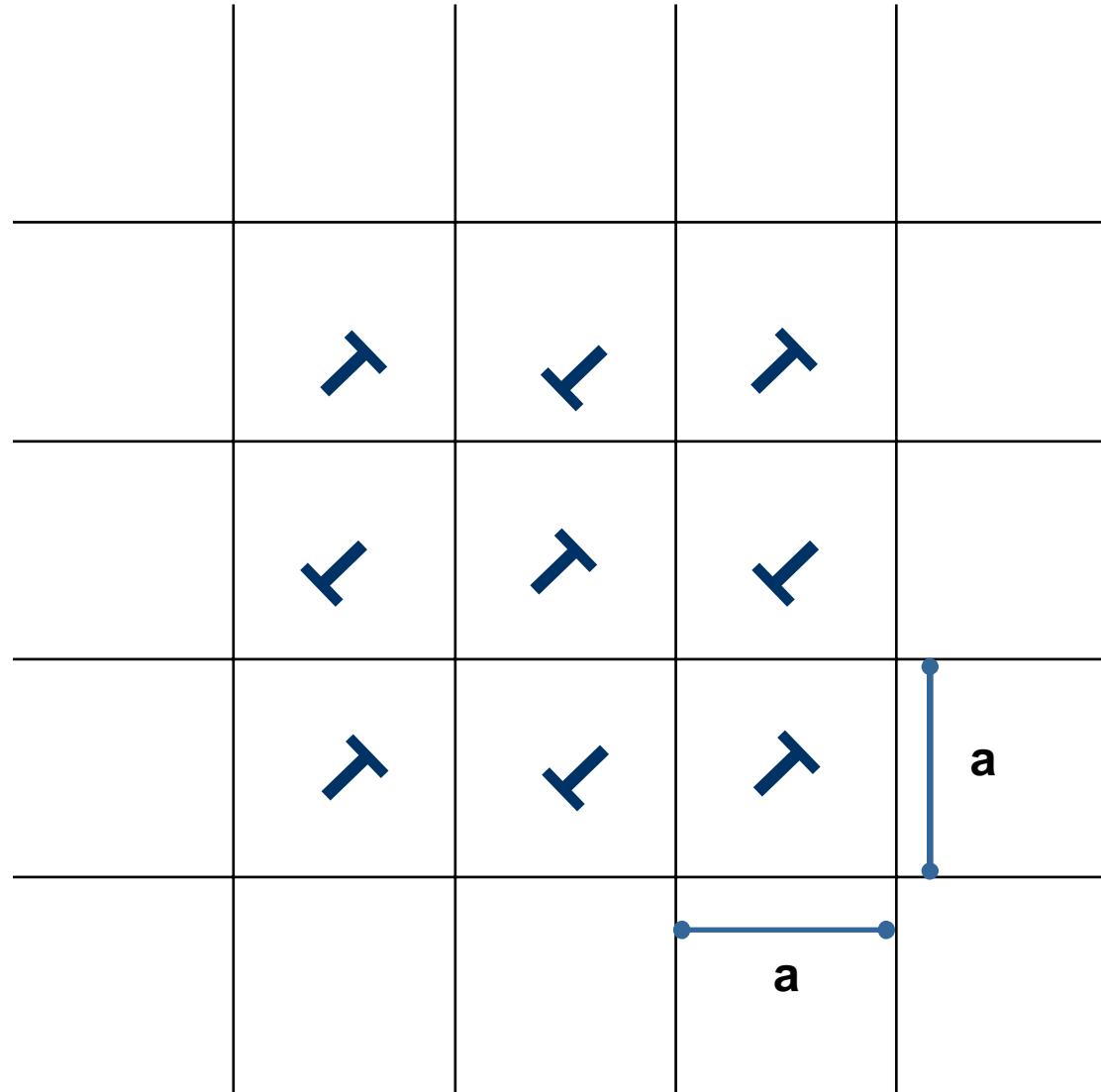


$$\tau = \alpha G b \sqrt{\rho}$$

$$\dot{\gamma} = \frac{d\gamma}{dt} = n \frac{dx}{X Z} \frac{b}{dt} \frac{1}{\rho_m b v} = \rho_m b v$$



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

↓ ↓
T T

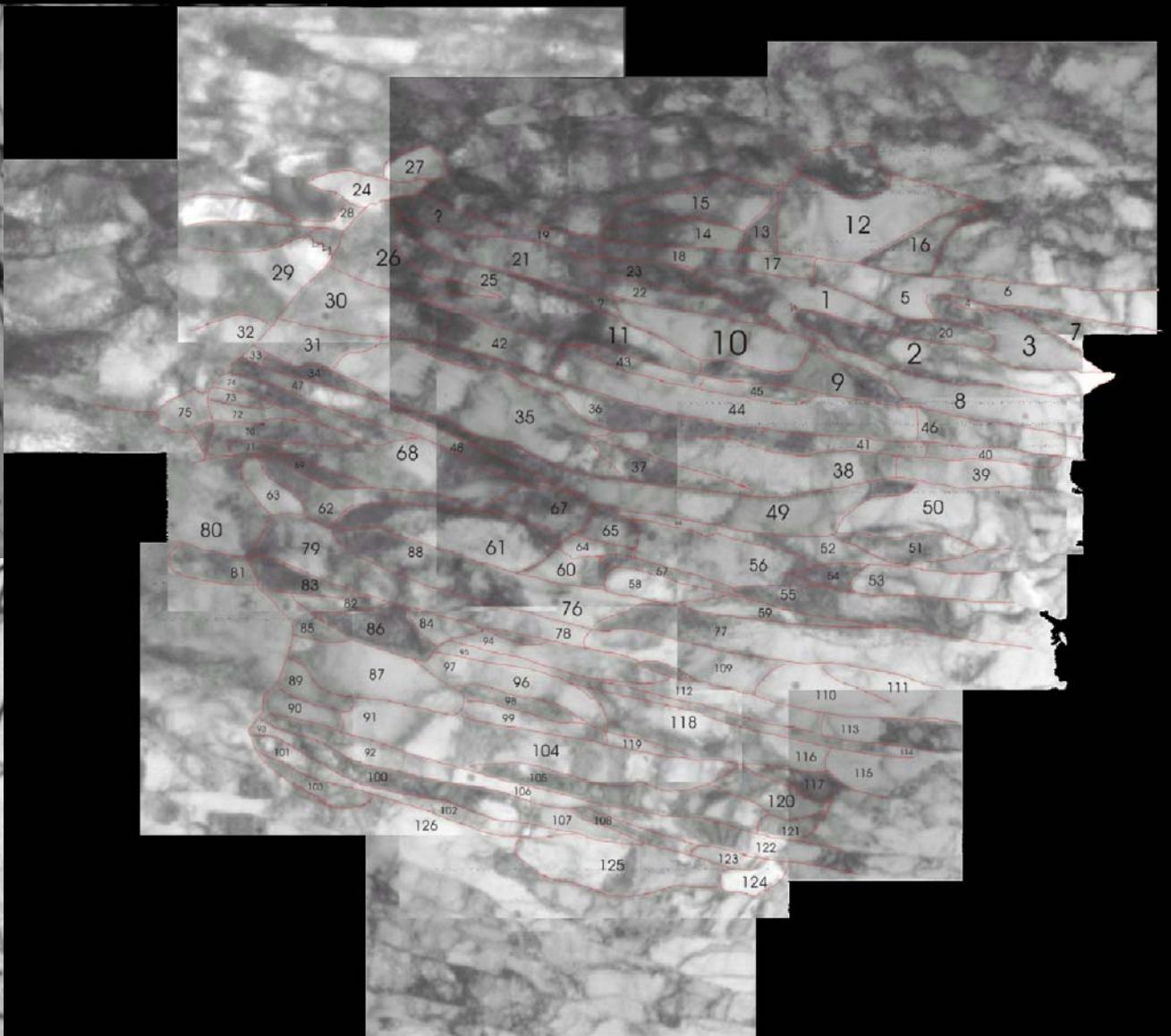
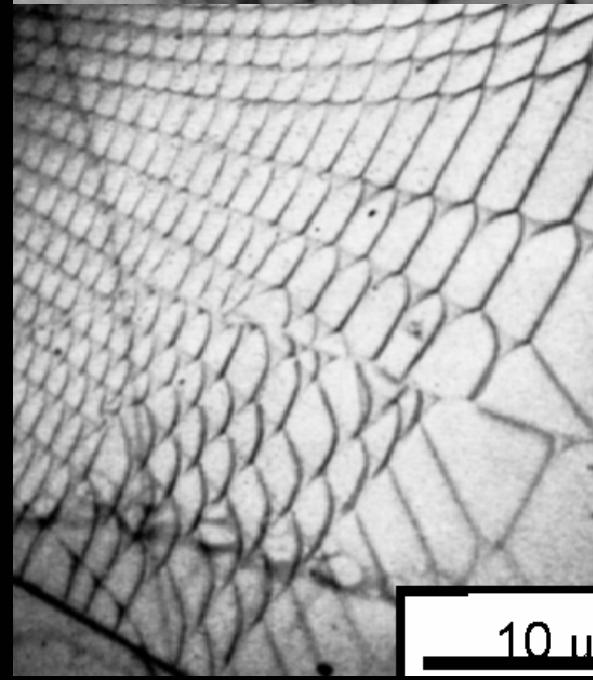
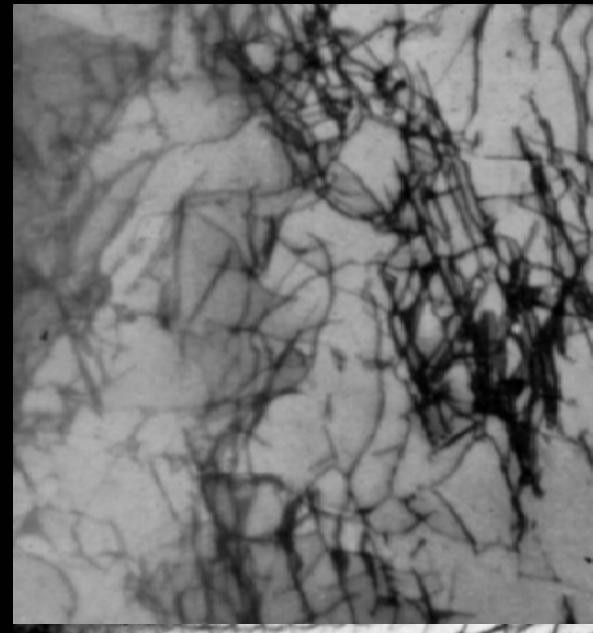
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T T



Coarse graining, problems



10 µm



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)?**



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- **Limits in plasticity continuum models (small
scale crystal plasticity)**



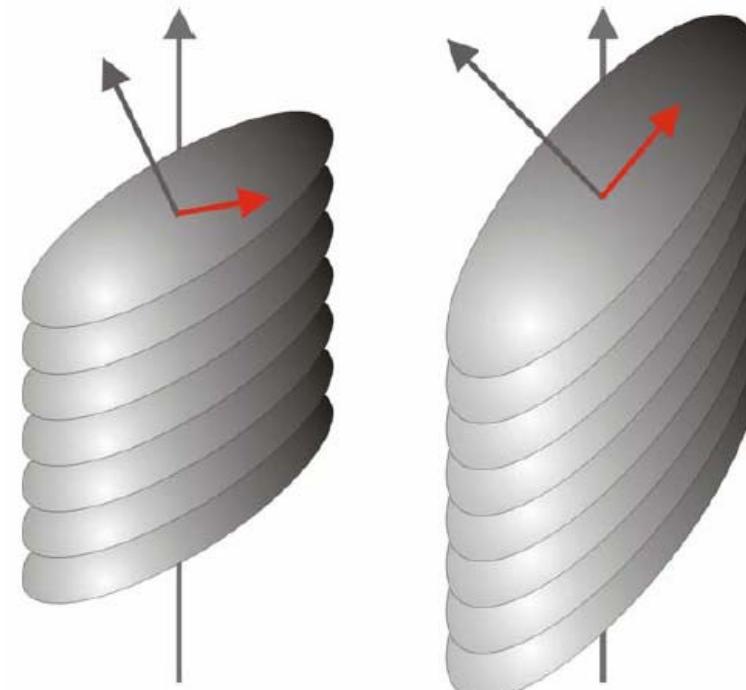
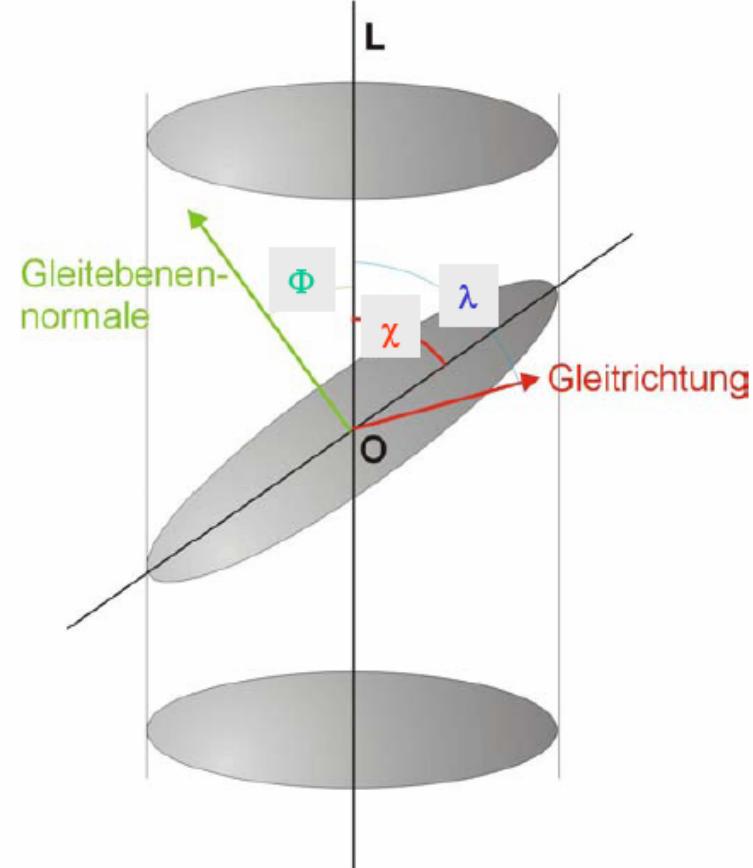
Crystal mechanics and anisotropy

single crystal level

single crystal level: stress homogenization



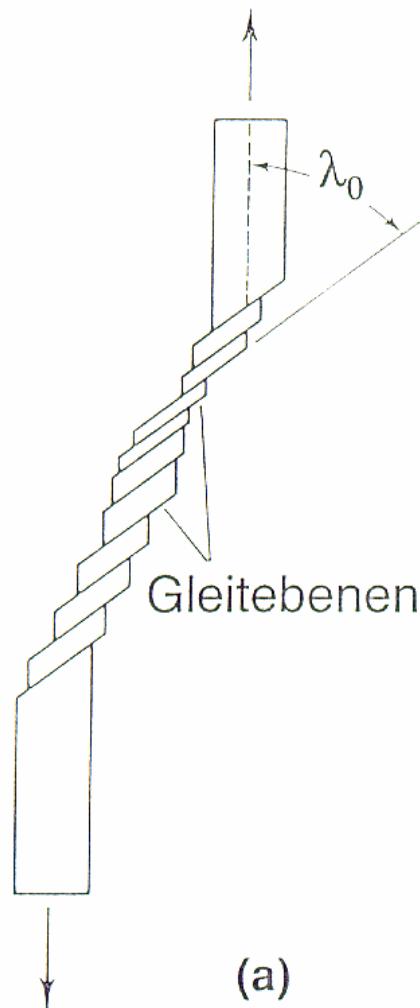
Origin of plastic anisotropy



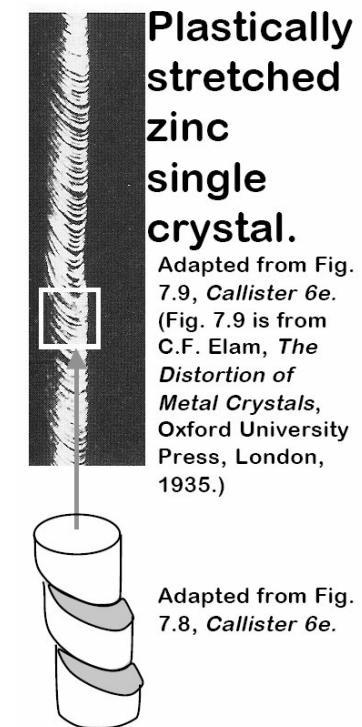


single crystal level: stress homogenization

kinematics:
shape change (symmetric part
of displacement gradient)



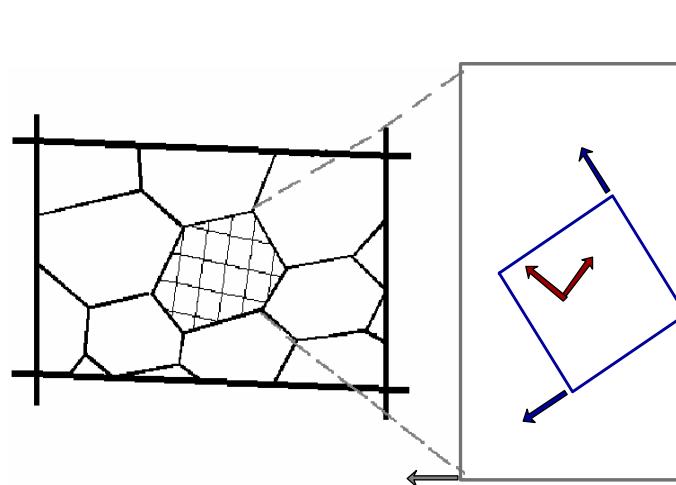
kinematics:
rotation / texture (antisymmetric part
of displacement gradient)





single crystal level: stress homogenization

1 crystal, 1 slip system:



slip systems
 $\bar{n} \bar{b}$

crystal (k,l)

$$m_{kl} = n_k b_l$$

sample (i,j)

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



kinematics

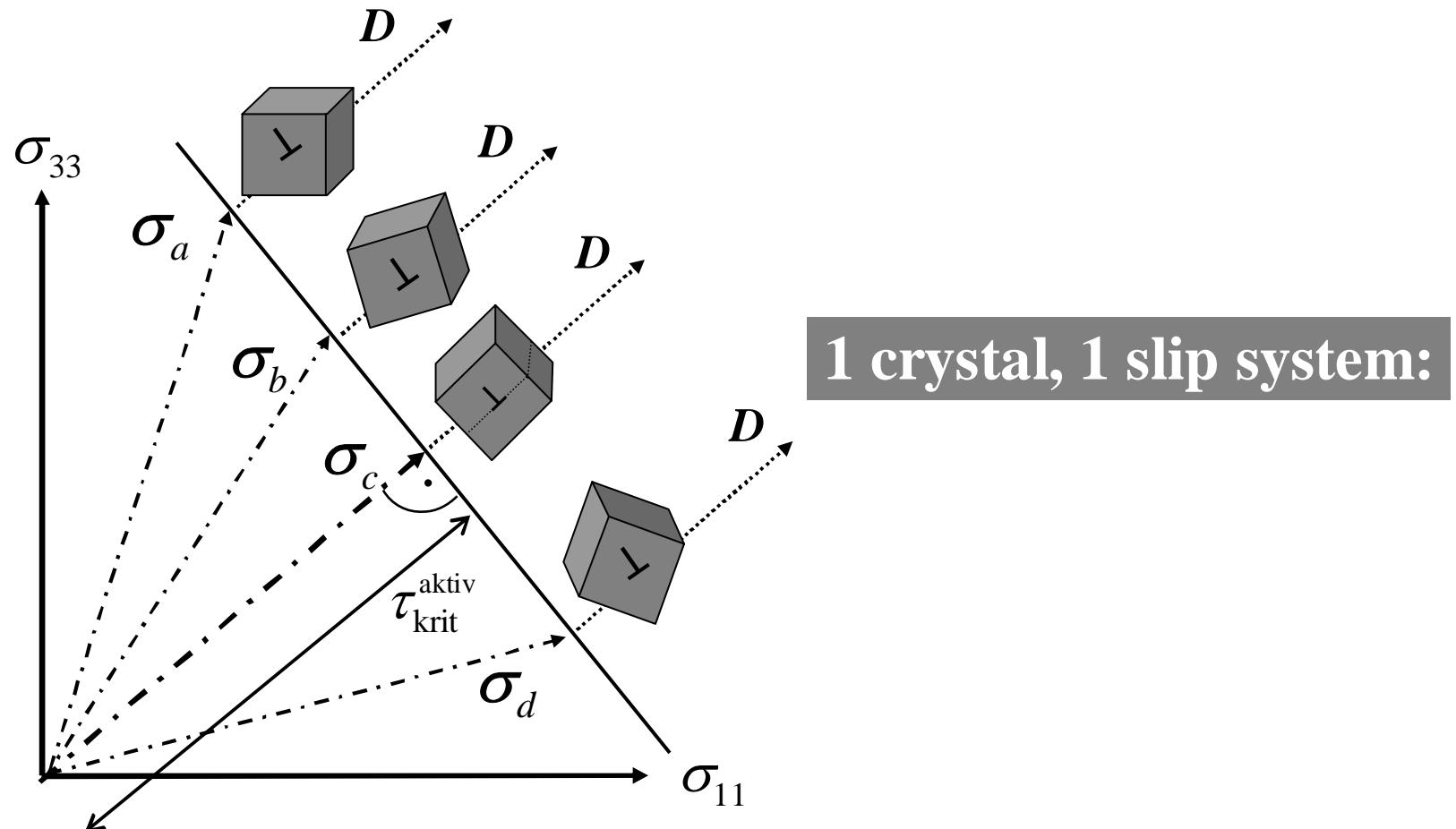
$$a_{ik} n_k a_{jl} b_l \sigma_{ij} = \tau^{crit}$$

kinetics



single crystal level: stress homogenization

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





single crystal level: stress homogenization

slip system s

$$\mathbf{n}_i^s, \mathbf{b}_i^s$$

kinematics

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

kinetics

orientation factor for s

$$m_{ij}^s = \mathbf{n}_i^s \cdot \mathbf{b}_j^s$$

1 crystal, 2 slip systems

symmetric part

$$m_{ij}^{sym,s} = \frac{1}{2} (\mathbf{n}_i^s \cdot \mathbf{b}_j^s + \mathbf{n}_j^s \cdot \mathbf{b}_i^s)$$

rotate crystal into sample

$$m_{kl}^s = a_{ki}^c \mathbf{n}_i^s \cdot a_{lj}^c \mathbf{b}_j^s$$

symmetric part

$$m_{kl}^{sym,s} = \frac{1}{2} (a_{ki}^c \mathbf{n}_i^s \cdot a_{lj}^c \mathbf{b}_j^s + a_{lj}^c \mathbf{n}_j^s \cdot a_{ki}^c \mathbf{b}_i^s)$$

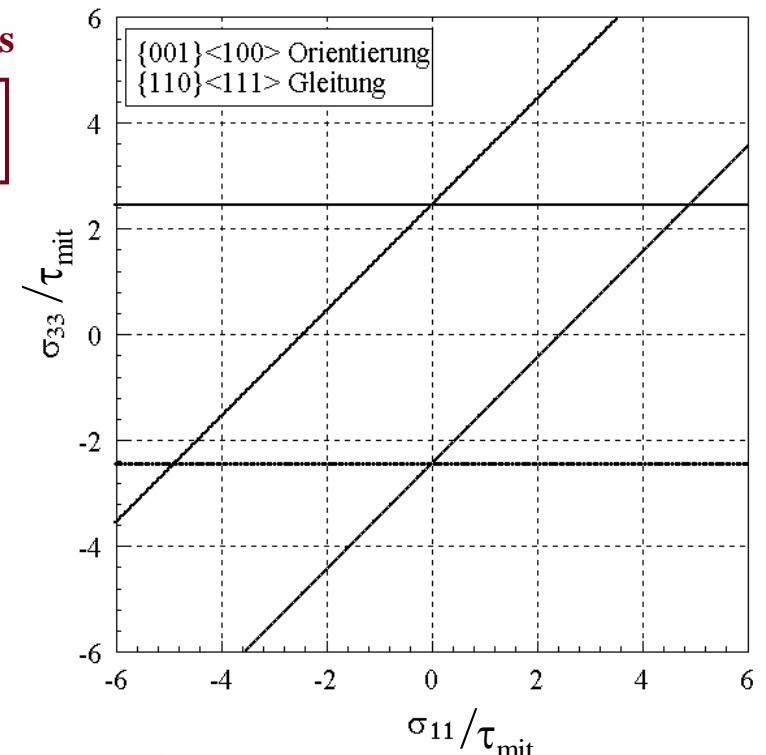
**yield surface
(active systems)**

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

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

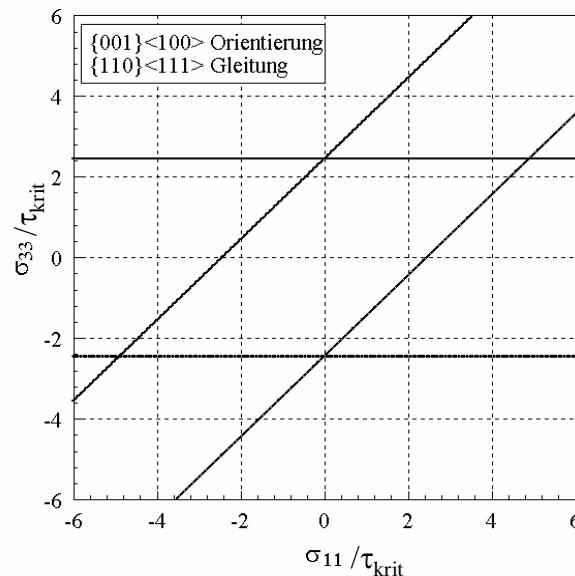
(non-active systems)

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

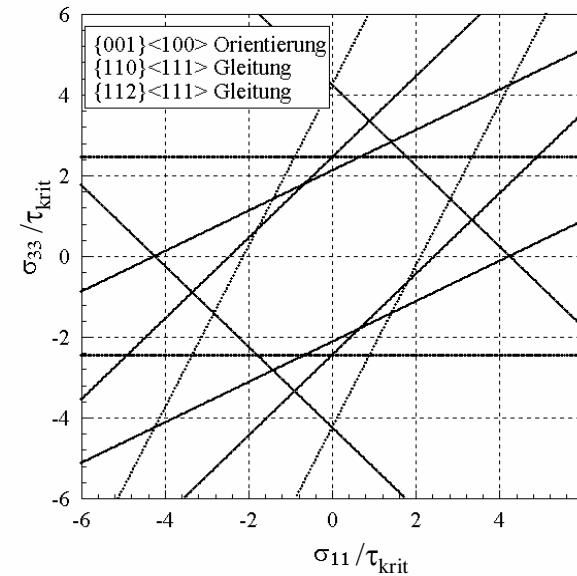




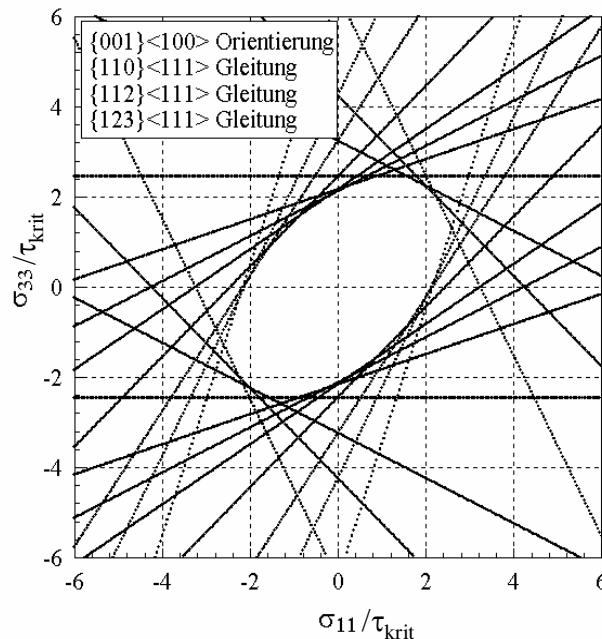
single crystal level: stress homogenization



krz, kfz,
Schnitt



krz, 24 Systeme,
Schnitt



krz, 48 Systeme,
Schnitt

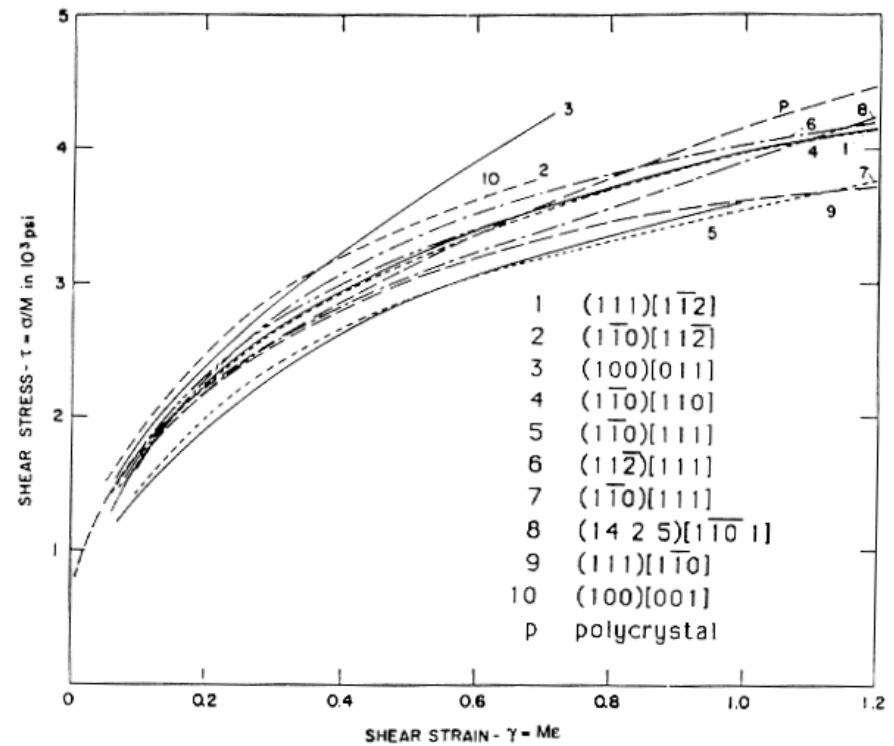
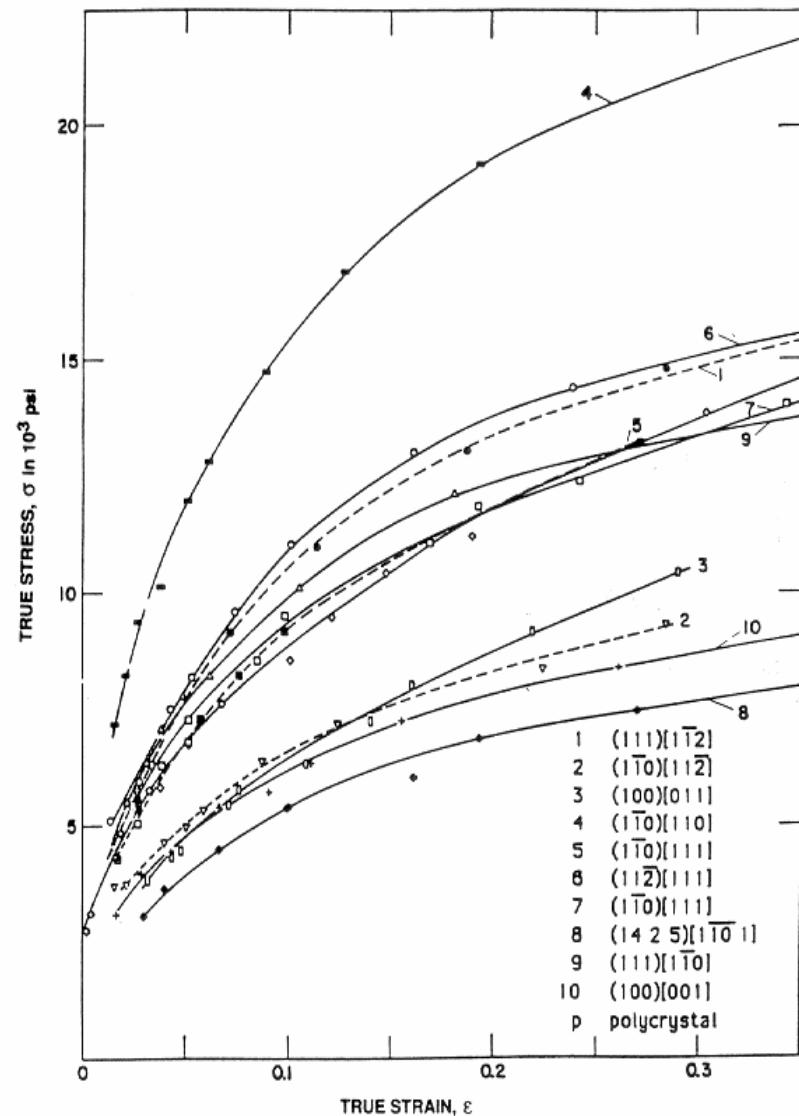
1 crystal, many slip systems

yield surface, bcc

single crystal, bcc, (001)[100]



single crystal level: stress homogenization



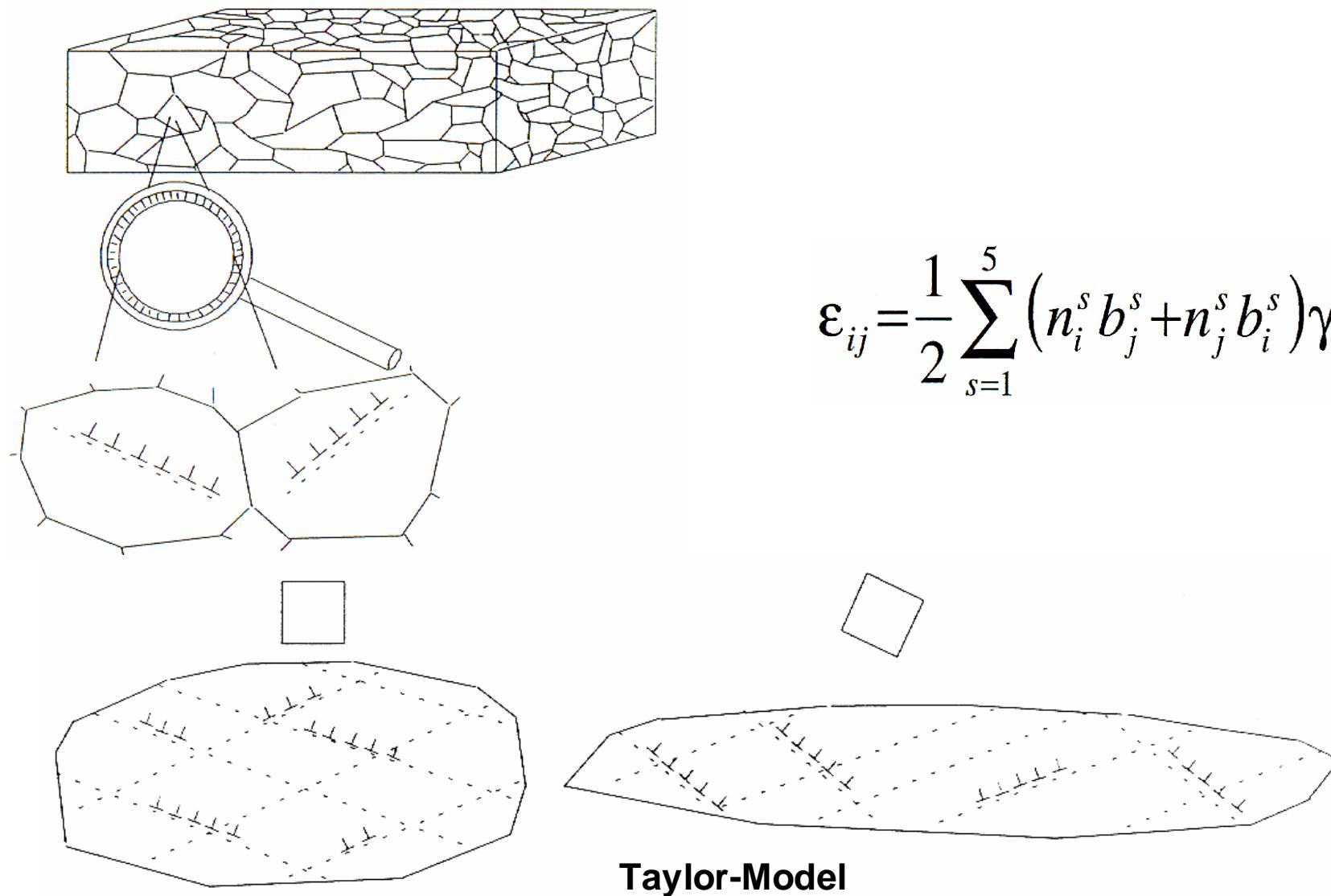


Crystal mechanics and anisotropy

polycrystal level

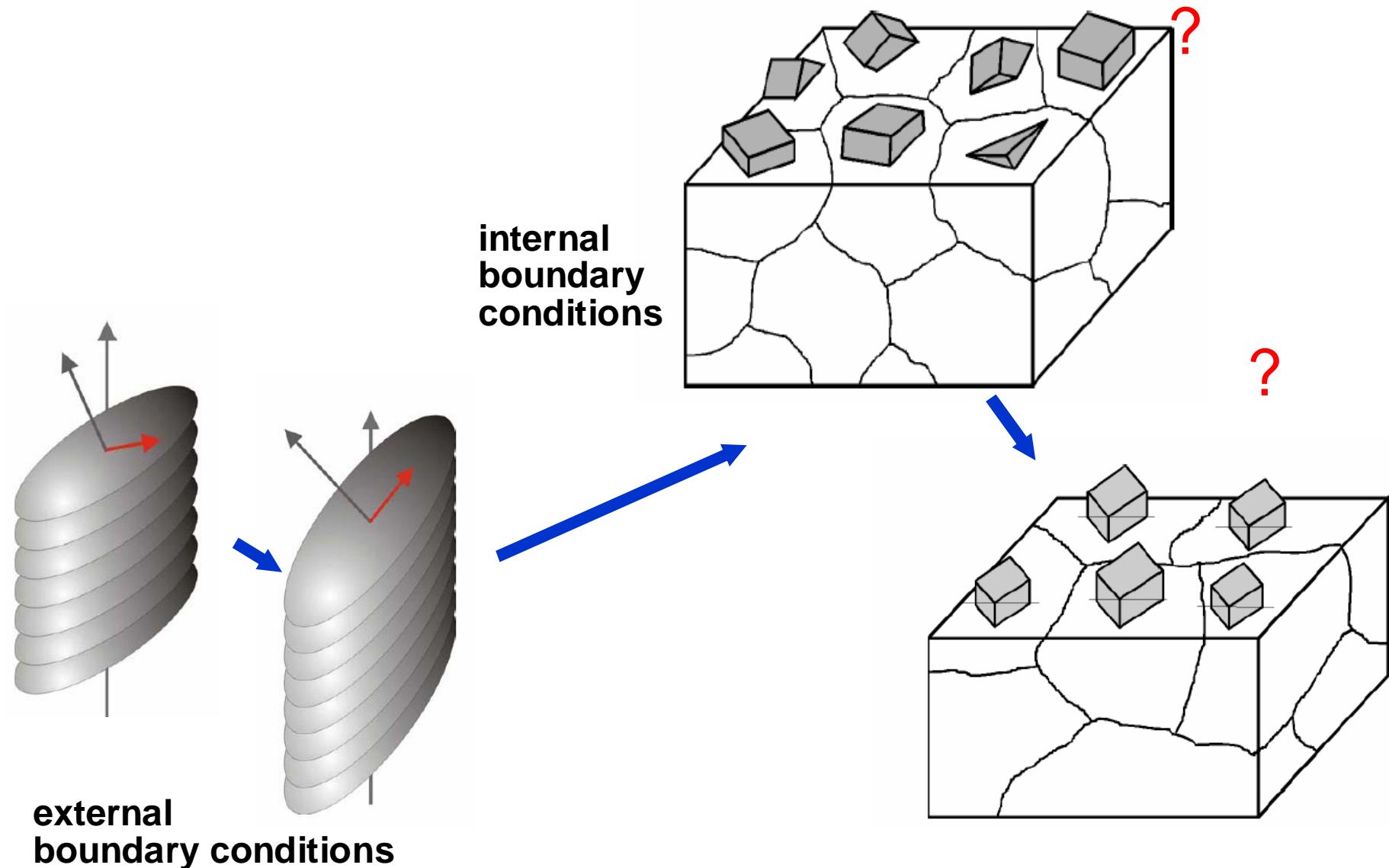


polycrystal: strain homogenization



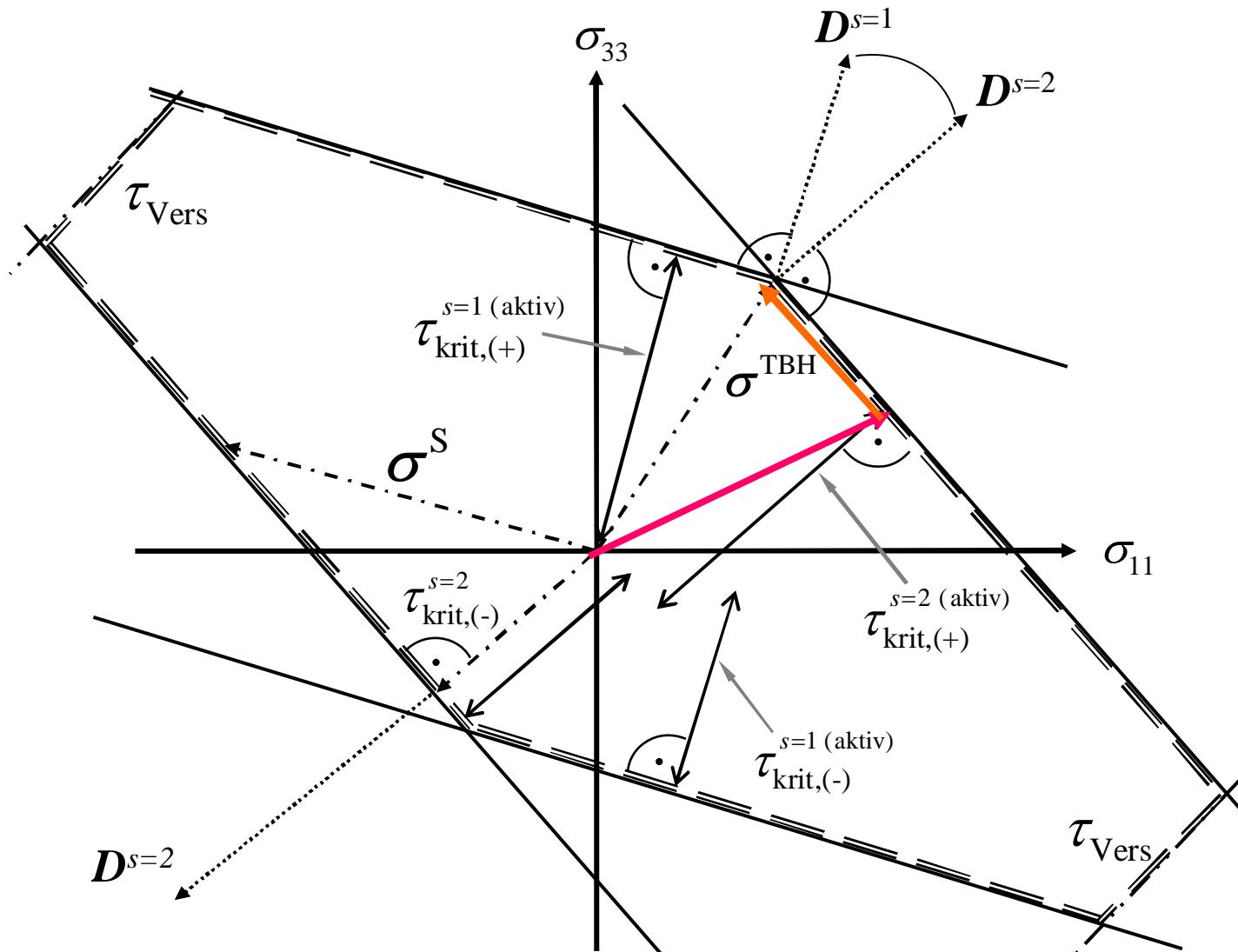


polycrystal: strain homogenization ?





polycrystal : strain homogenization



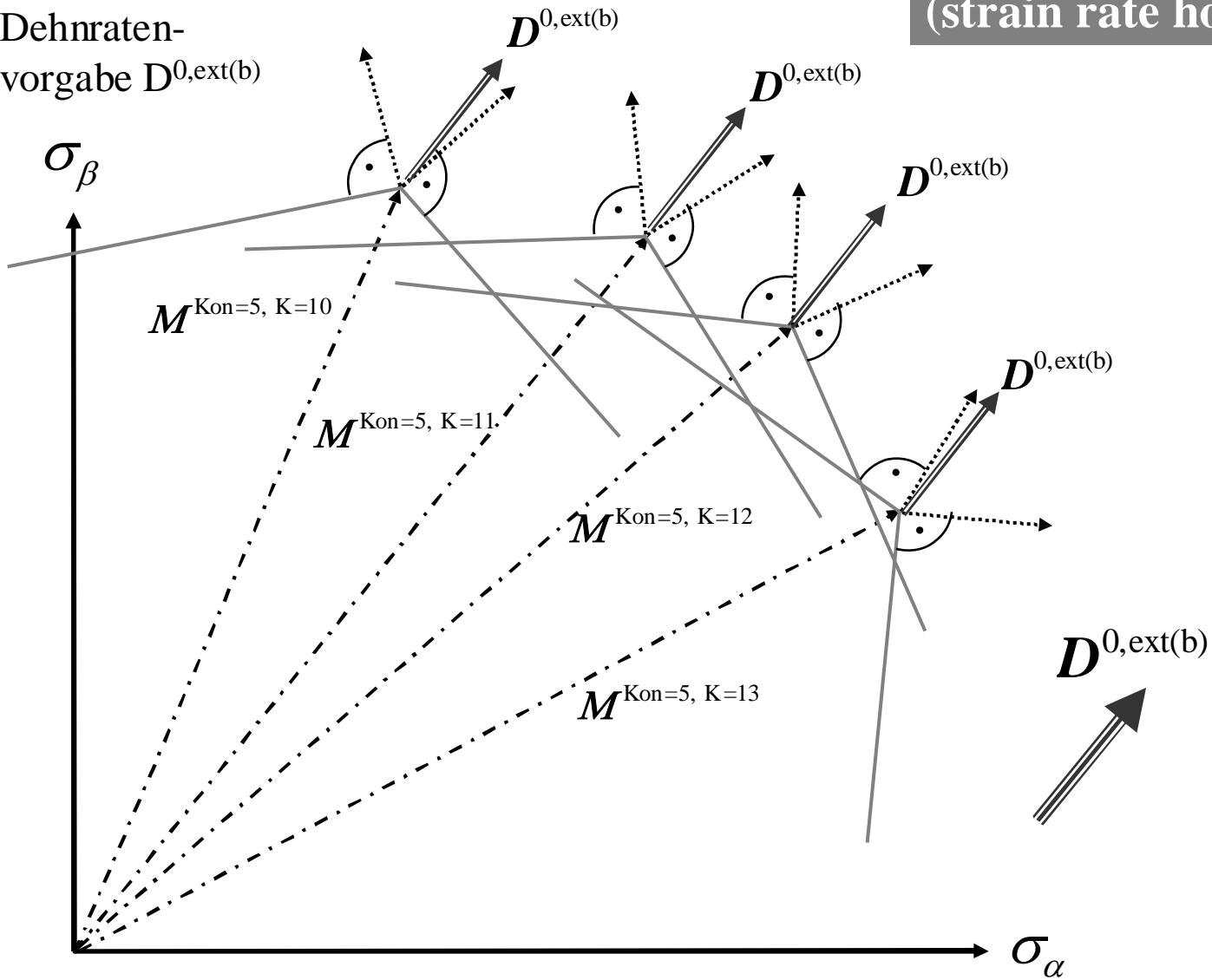
1 grain, many systems (stress space)



polycrystal: strain homogenization

Dehnrate-vorgabe $D^{0,\text{ext(b)}}$

many grains, 2 systems
(strain rate homogenization)





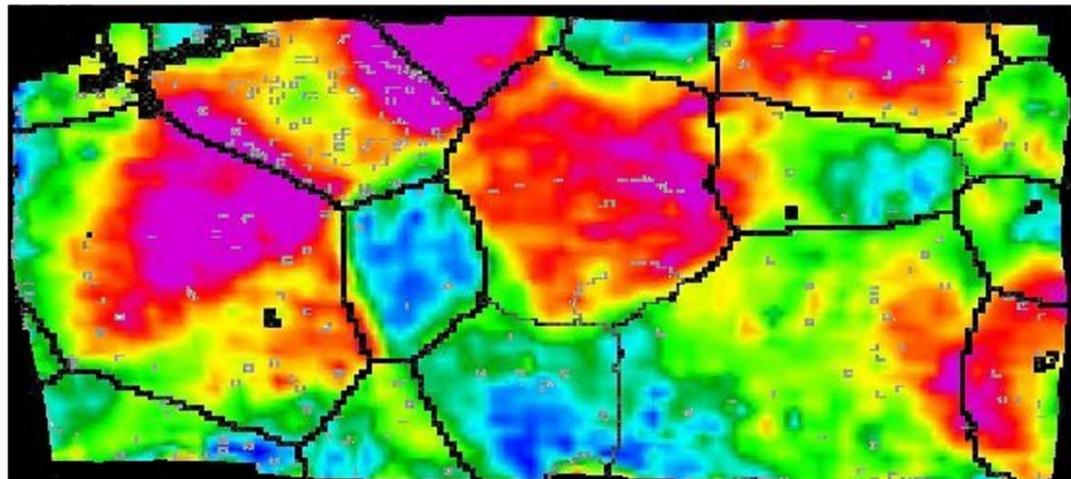
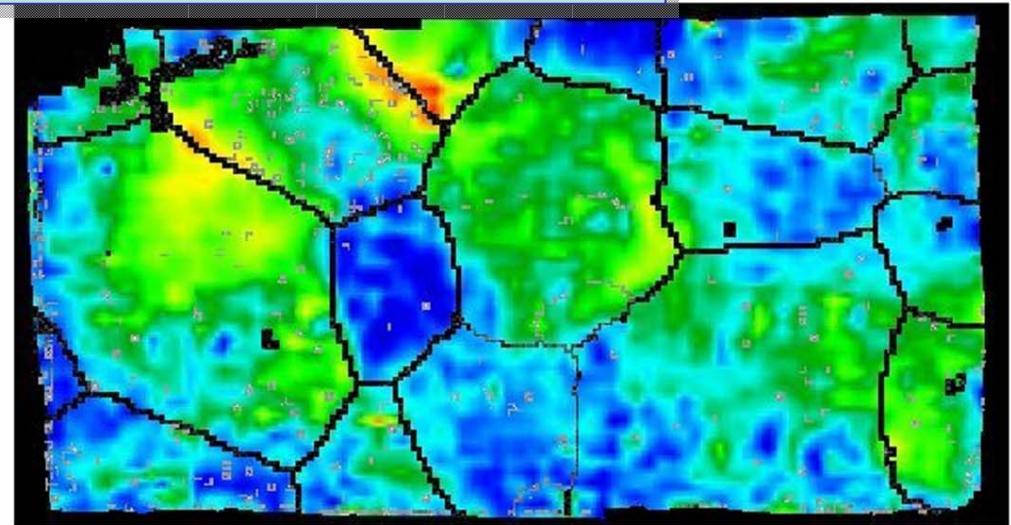
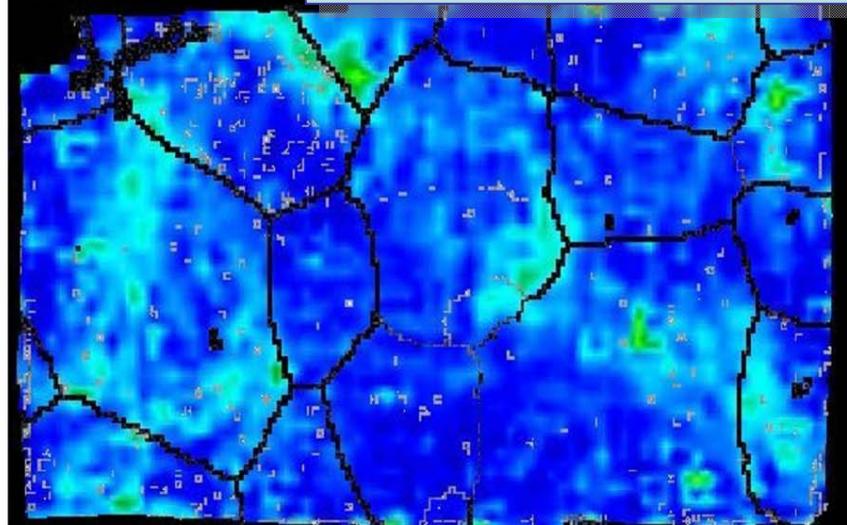
polycrystal reality

Crystal-scale homogeneity does not exist

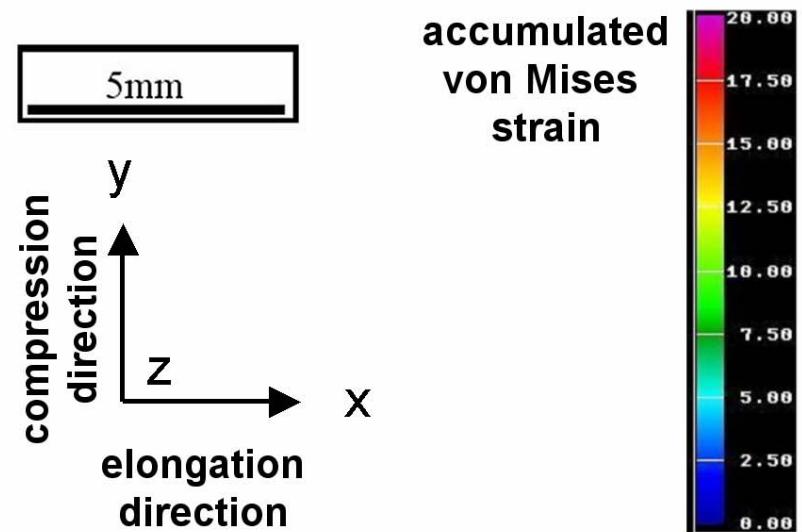
Control of boundary conditions essential

3%

8%



15%





polycrystal: homogenization

averages

$$\langle \sigma_{ij} \rangle = \frac{1}{V} \int_V \sigma_{ij}(x, g) dV \quad \langle D_{ij} \rangle = \frac{1}{V} \int_V D_{ij}(x, g) dV$$

typical boundary conditions

$$D_{ij}^{\text{ext}} = \langle D_{ij} \rangle = \frac{1}{V} \int_V D_{ij}^K(x, g) dV, \quad \text{problem: } D_{ij}^K(x, g) \quad \sigma_{ij}^K(x, g)$$

$$D_{ij}^{\text{ext}} = \frac{1}{V} \int_V D_{ij}^K(x, g) dV$$

$$\sum_{\text{Komp}} D_{ij}^K(g) \frac{V^{\text{Komp}}}{V} \approx D_{ij}^K(g)$$

less typical boundary conditions

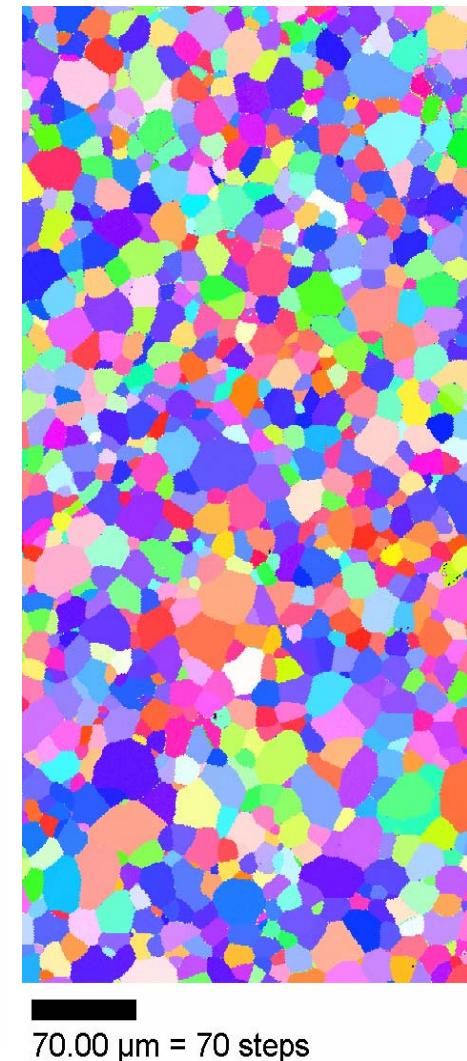
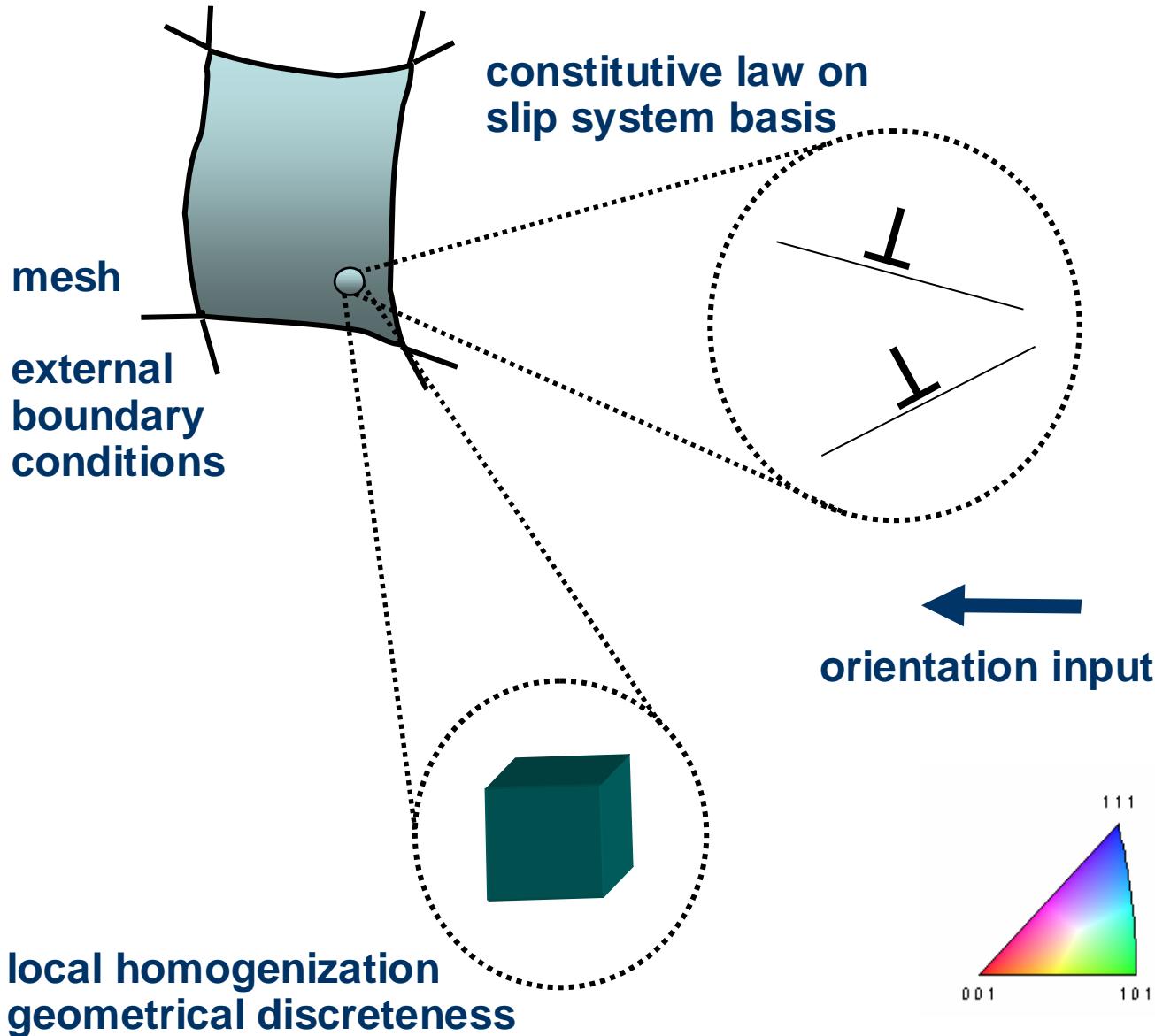
$$\sigma_{ij}^{\text{ext}} = \langle \sigma_{ij} \rangle = \frac{1}{V} \int_V \sigma_{ij}^K(x, g) dV, \quad \text{Problem: } \sigma_{ij}^K(x, g)$$

- 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”

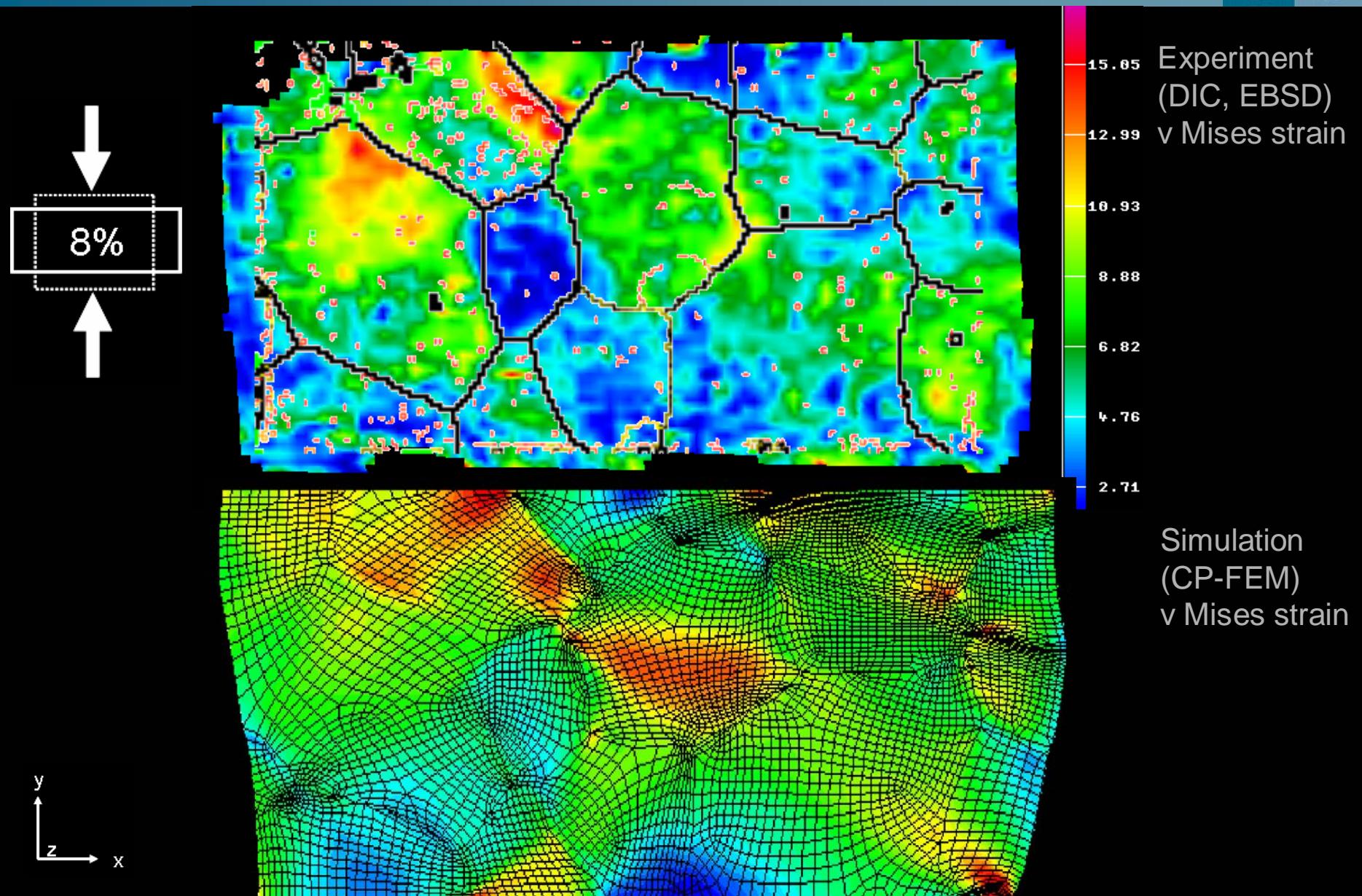


Crystal Mechanics FEM (General)

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



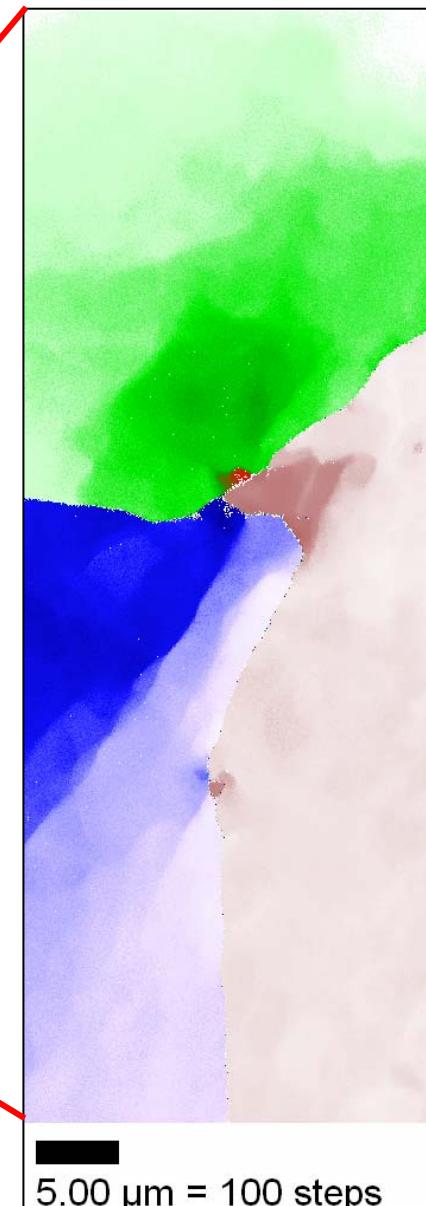
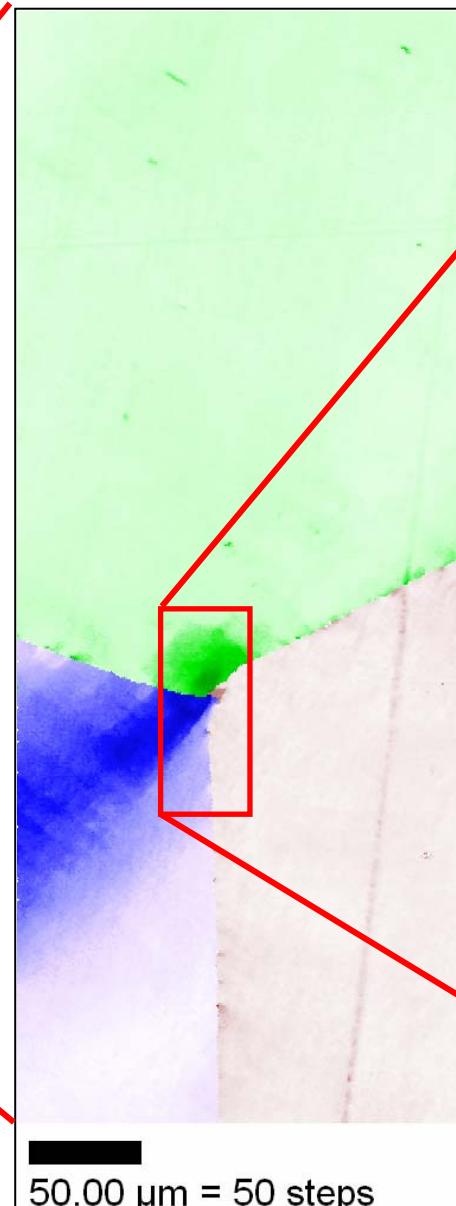
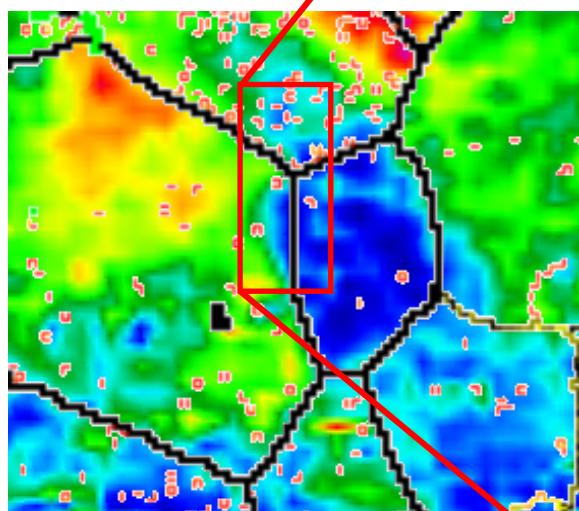
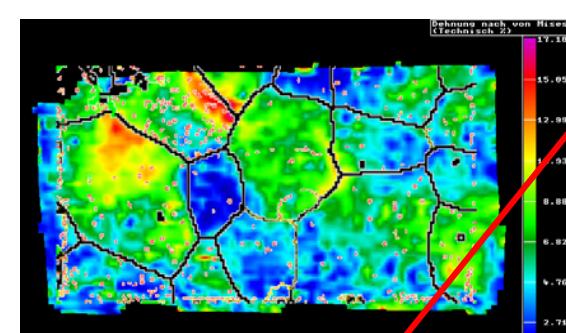
Crystal Mechanics FEM, grain scale mechanics (2D)



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”

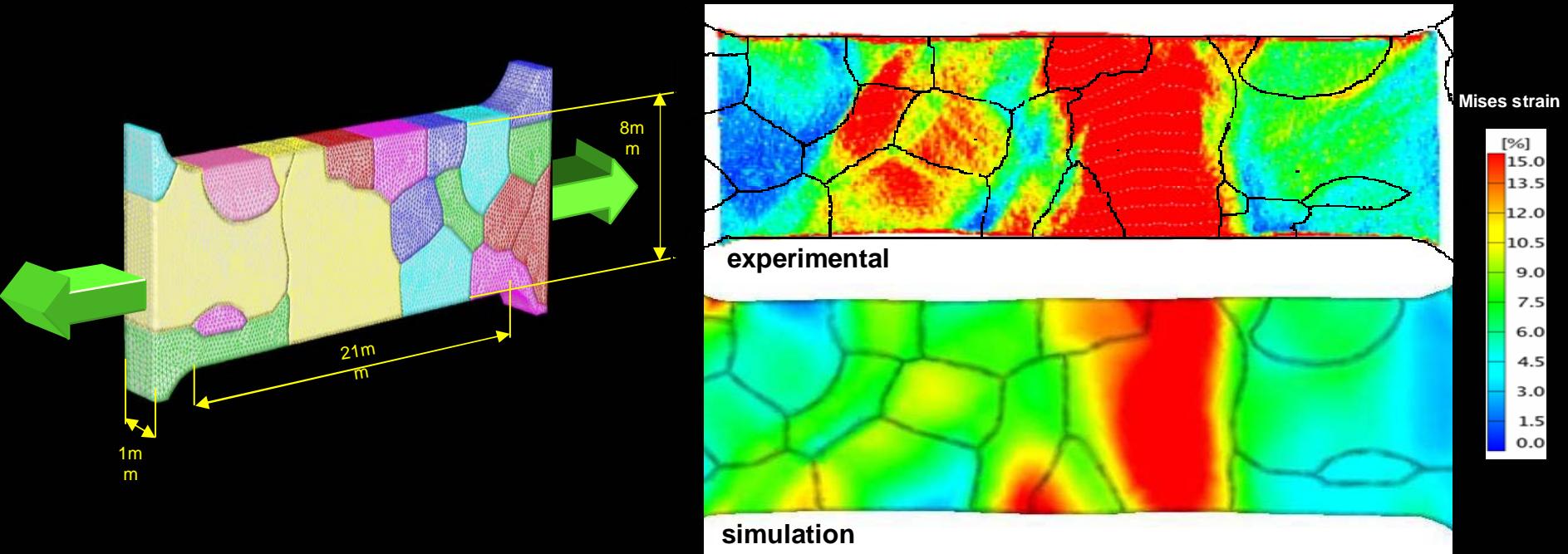
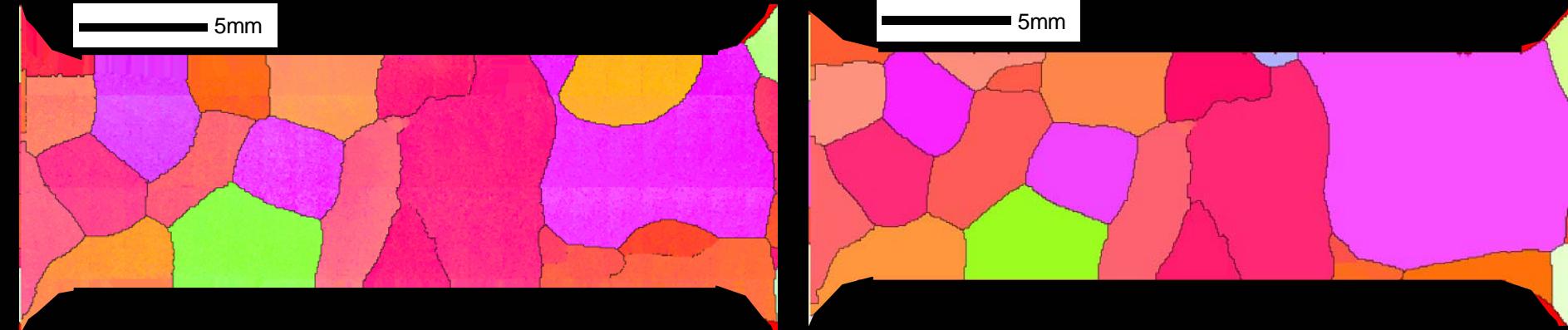


Inhomogeneity





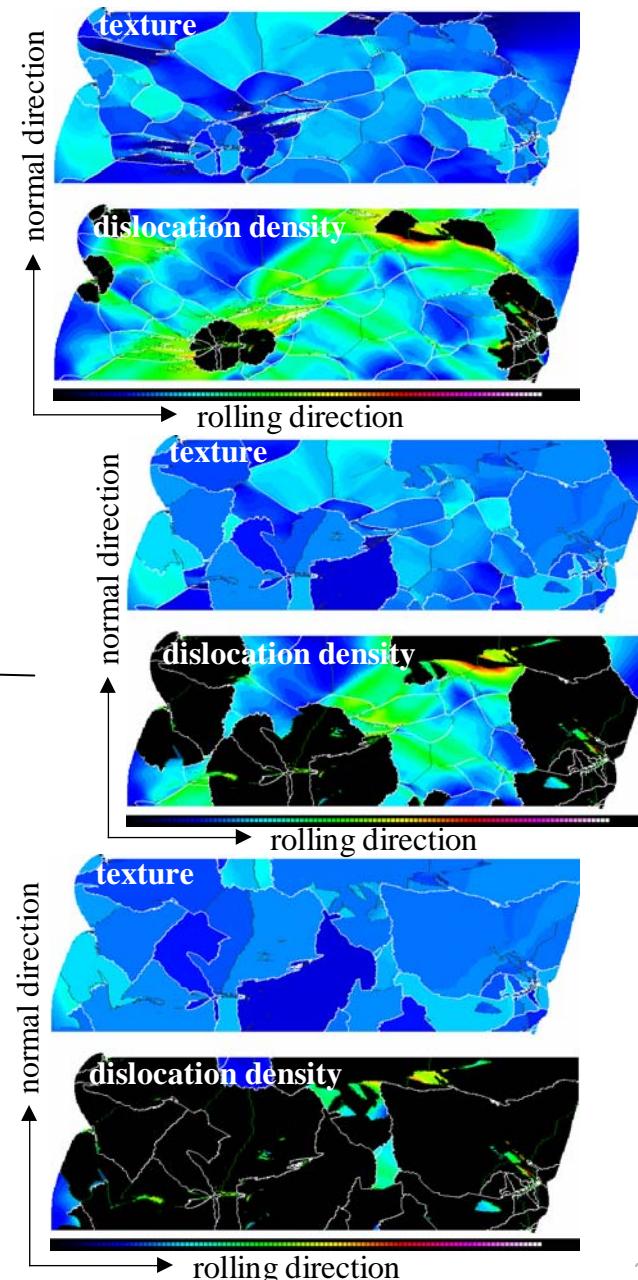
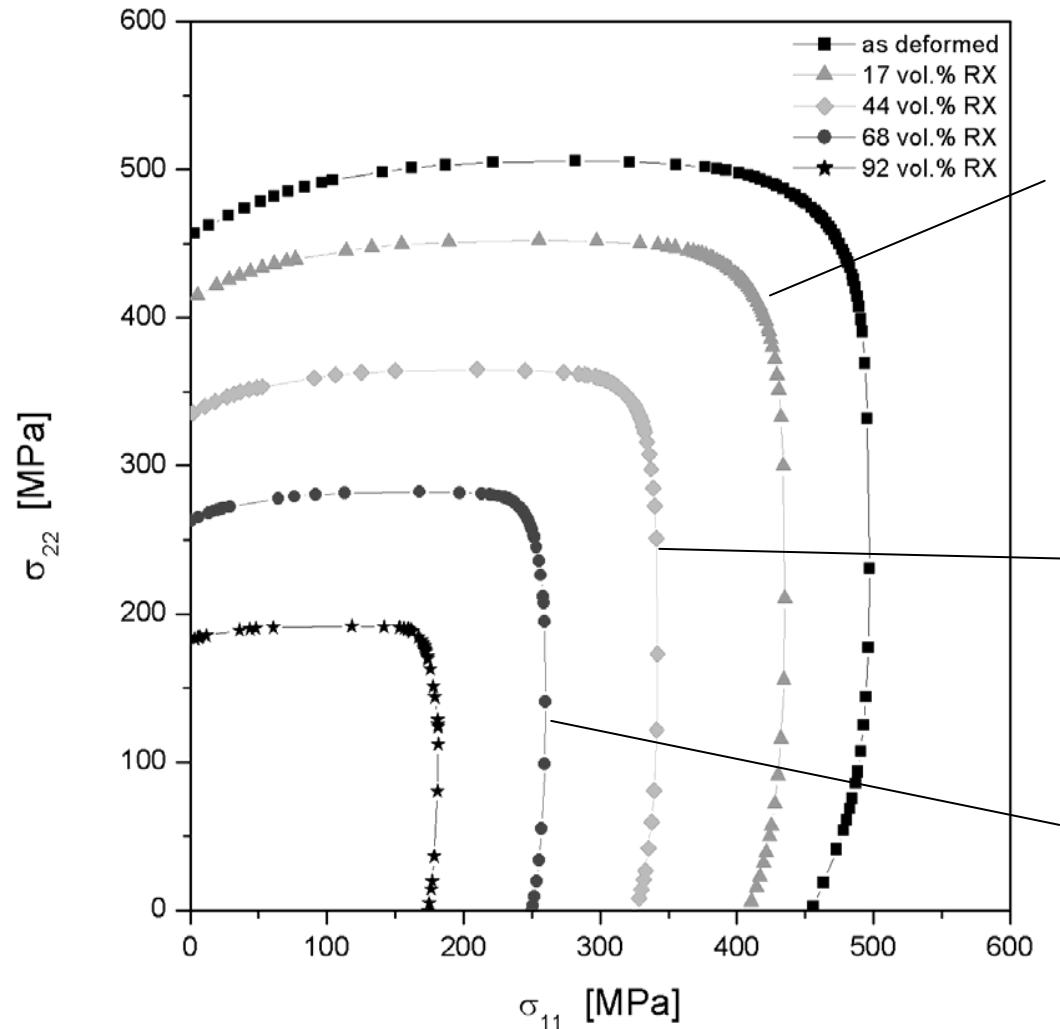
Crystal Mechanics FEM, grain scale mechanics (3D)



Crystal Mechanics FEM + transformation (recrystallization)

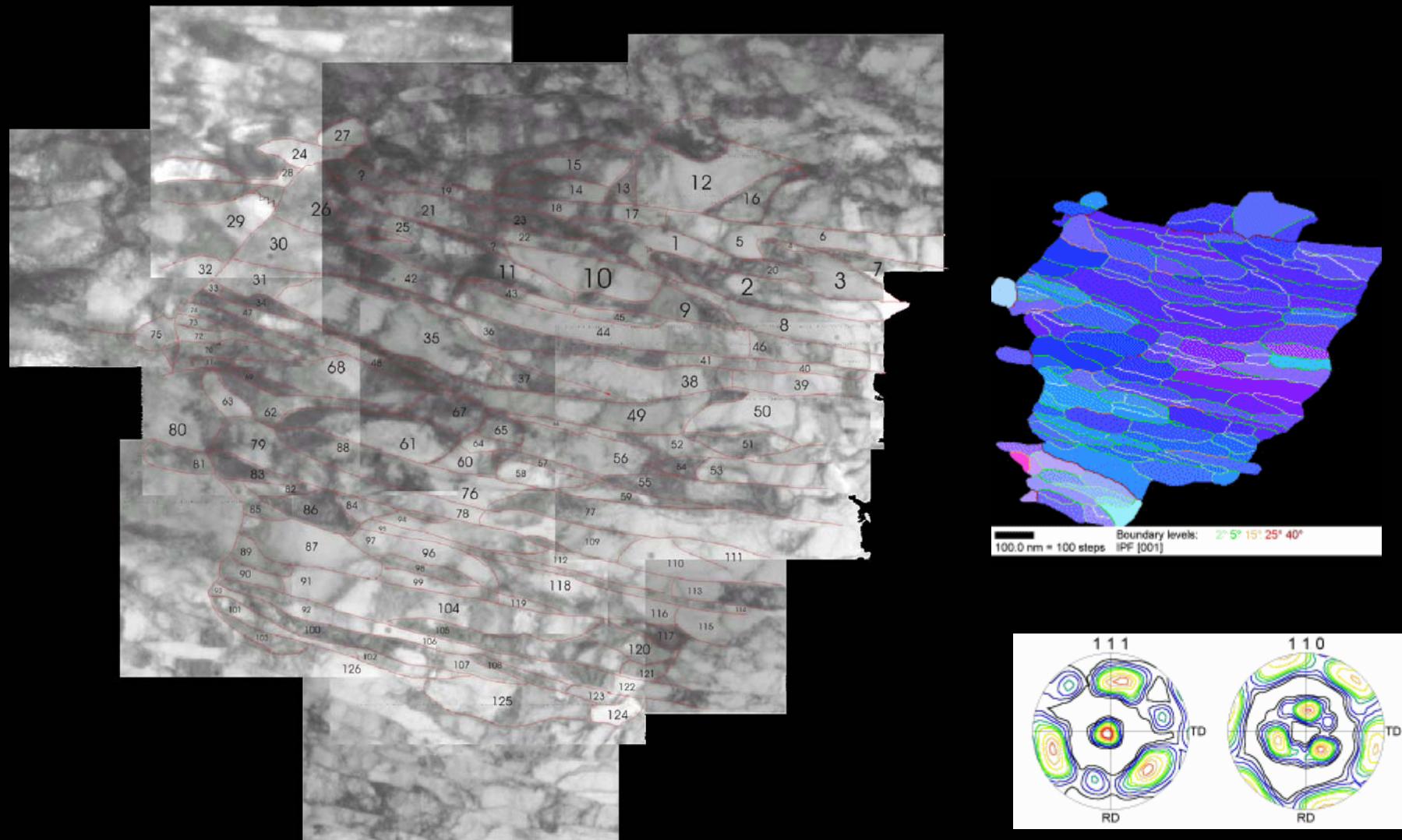


D. Raabe, R. Becker: Modelling and Simulation in Materials Science and Engineering 8 (2000) 445-462
 „Coupling of a crystal plasticity finite element model with a probabilistic cellular automaton for simulating primary static recrystallization in aluminum“





Nucleation in transformation (recrystallization)

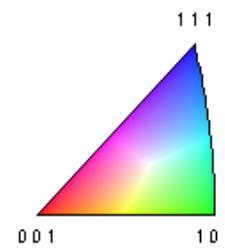


source: Stefan Zaefferer

10 billion grains



too many
grains



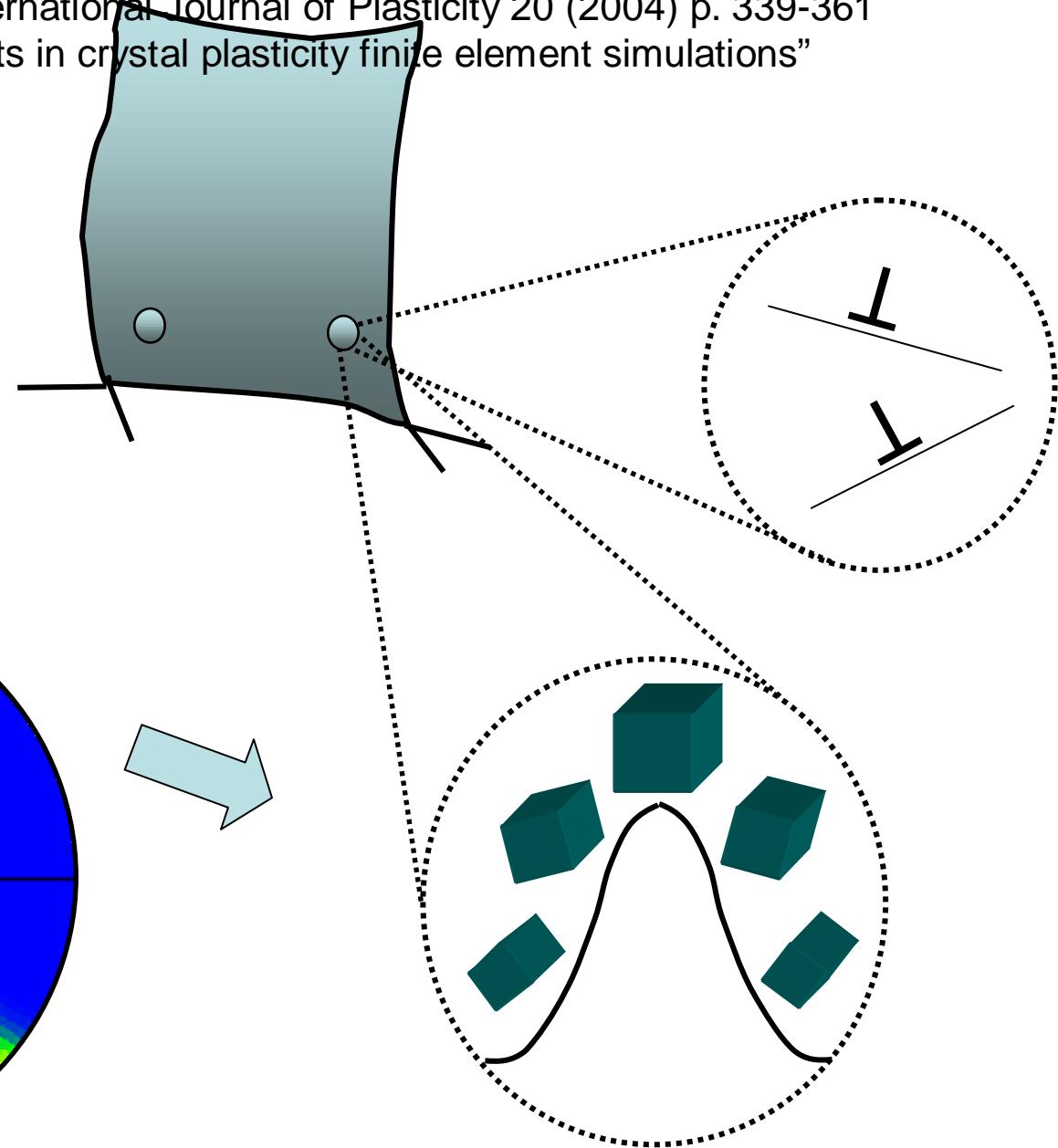
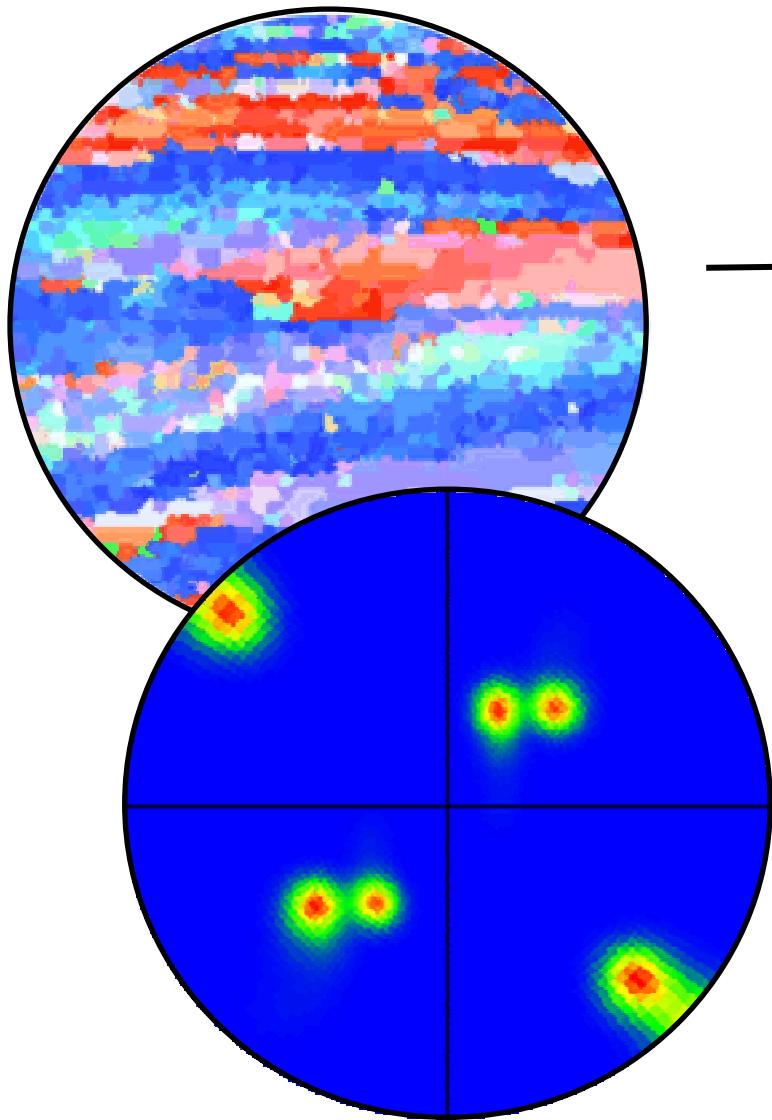
70.00 μm = 70 steps



map texture functions into FEM

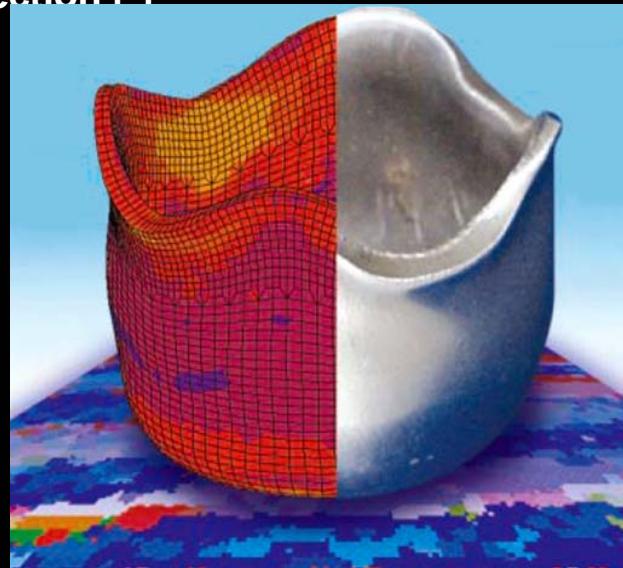
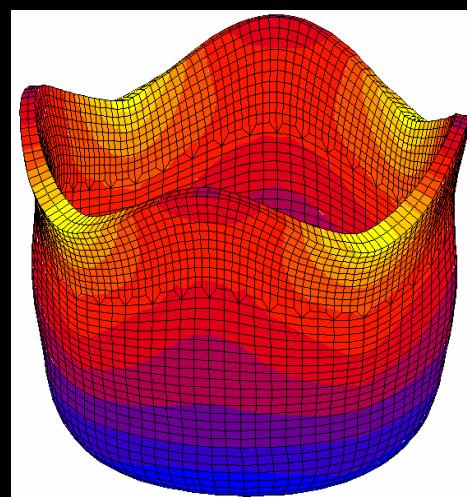
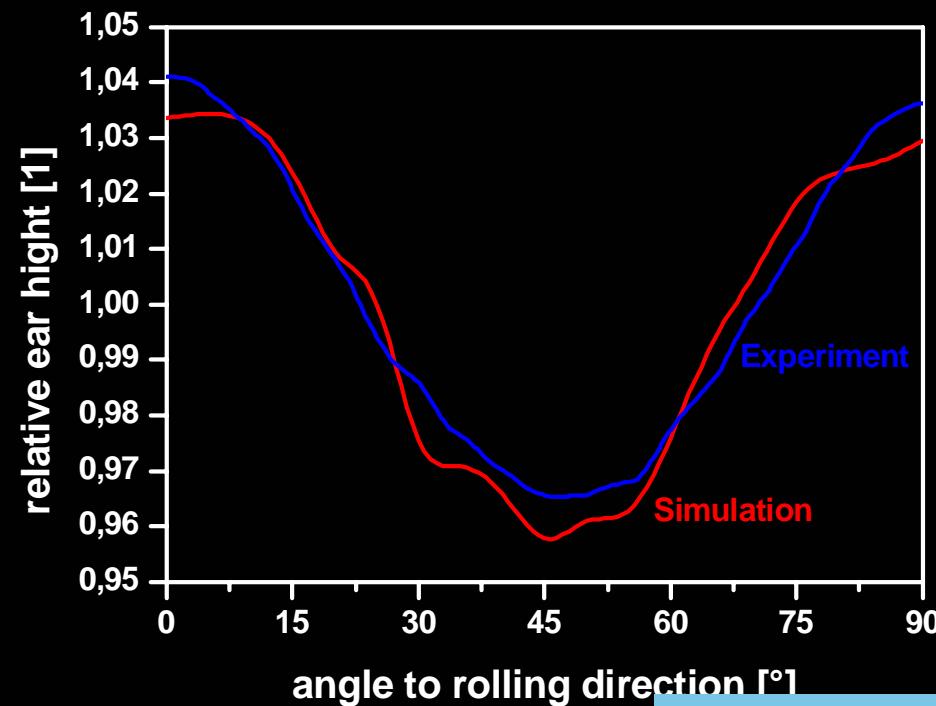


D. Raabe and F. Roters: International Journal of Plasticity 20 (2004) p. 339-361
„Using texture components in crystal plasticity finite element simulations”



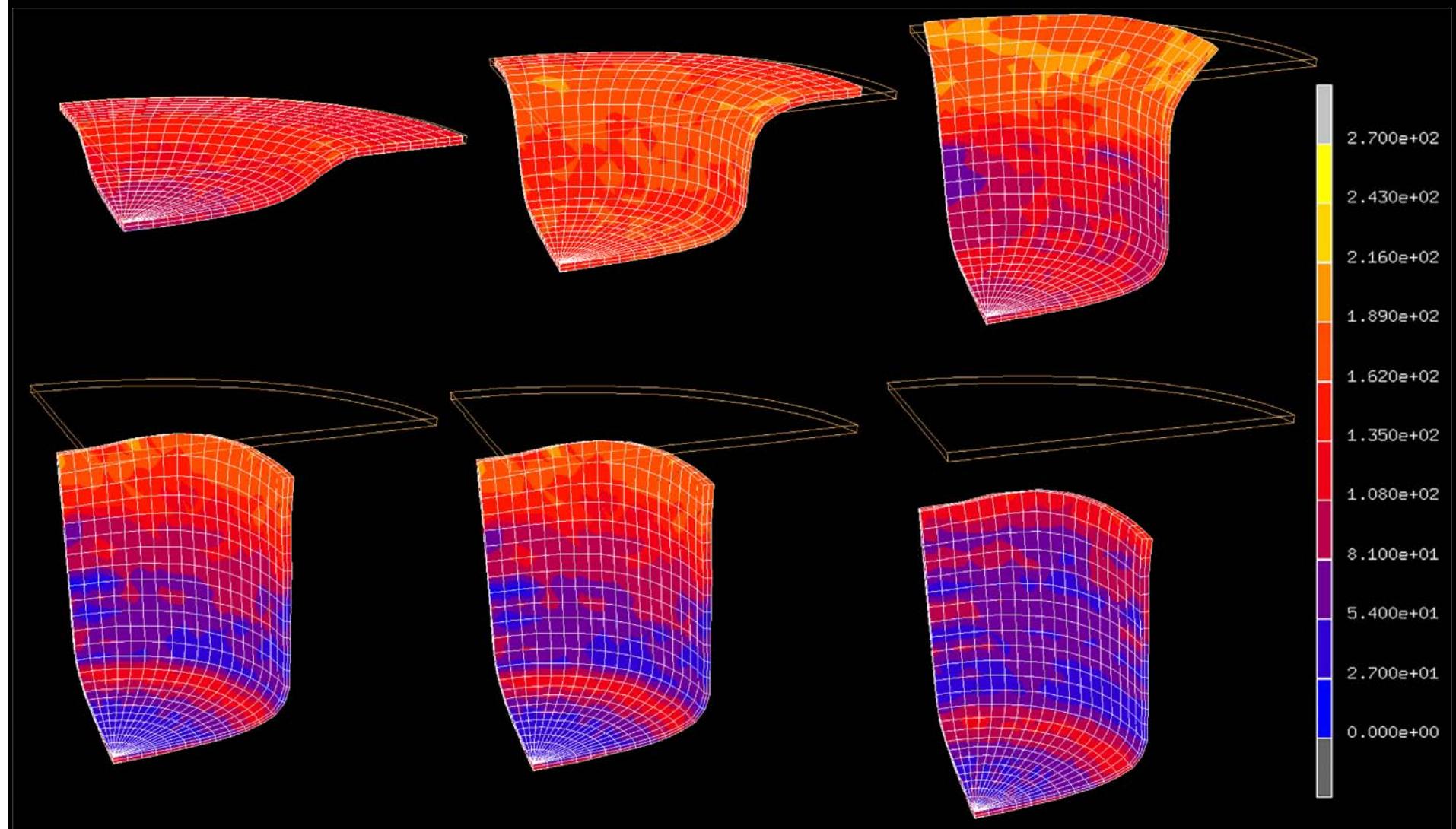


Crystal Plasticity FEM





Crystal Plasticity FEM





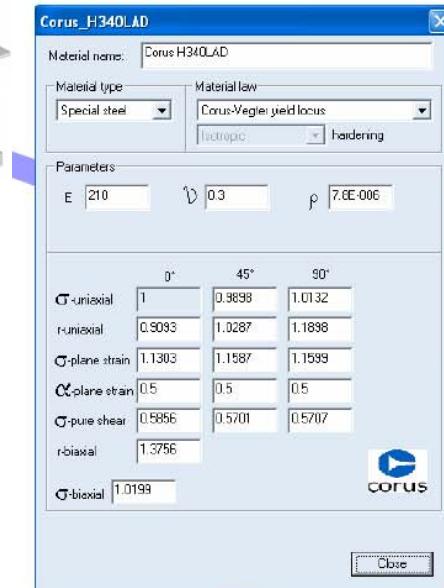
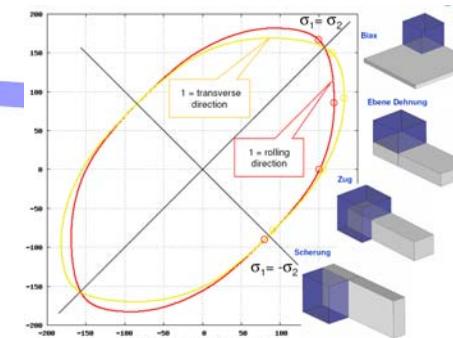
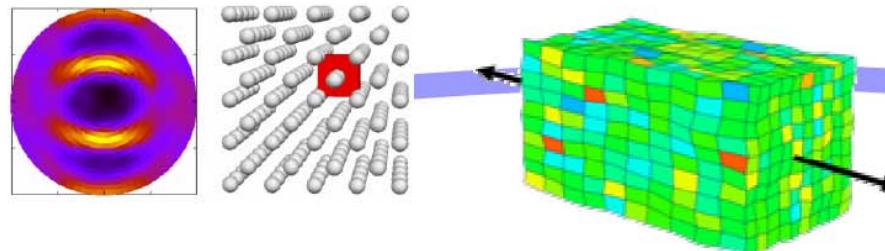
Example: Automobile (Coarse graining, Parametertransfer)

Numerical Laboratory

From Crystal Plasticity to Deep Drawing



inpro



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

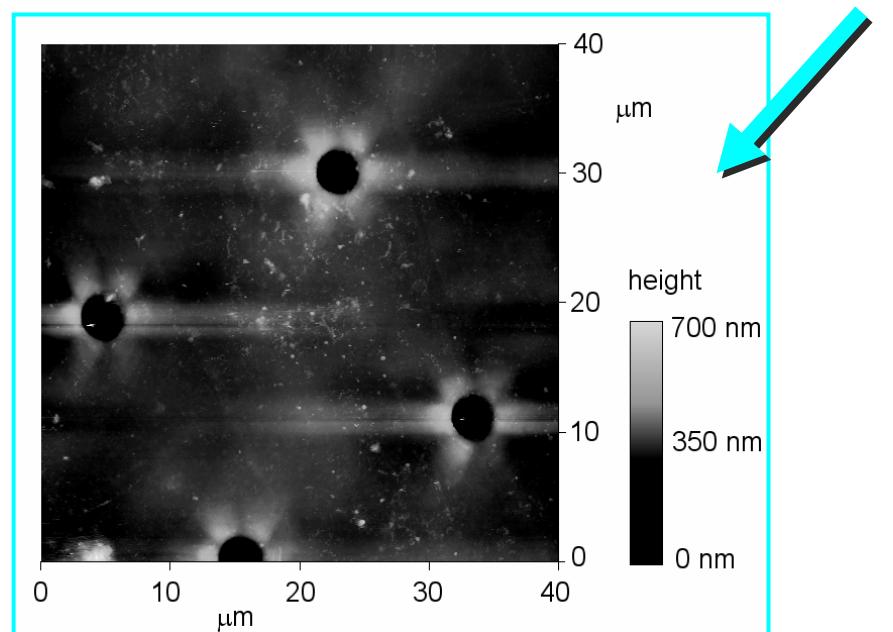
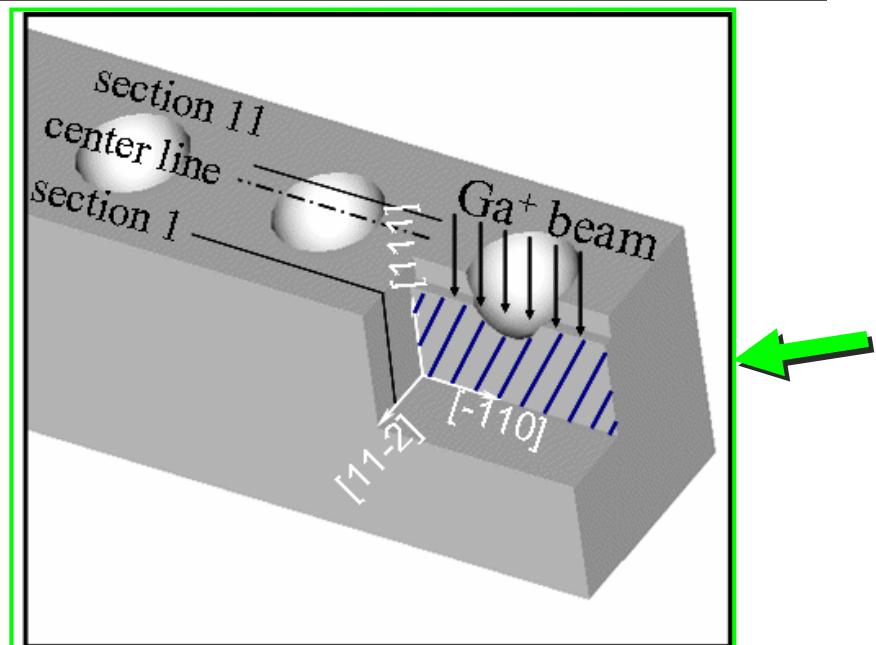
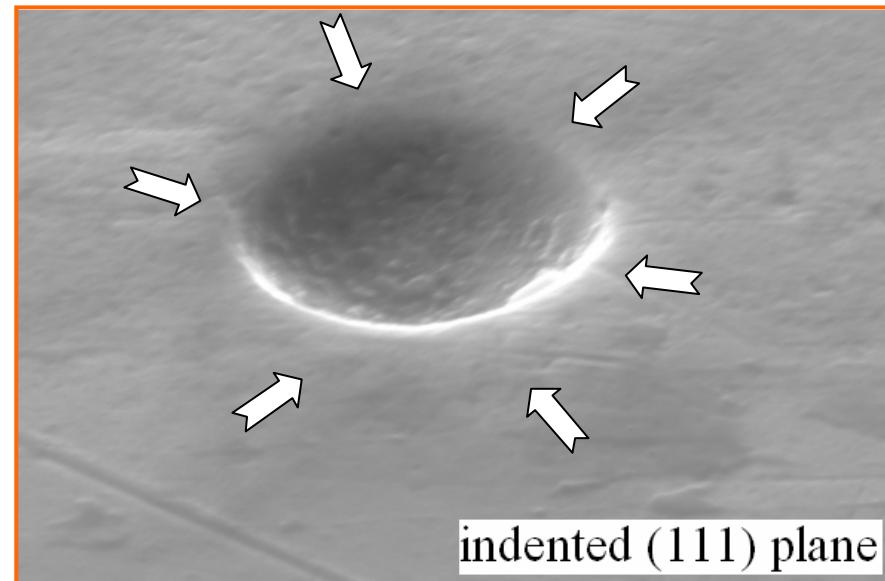
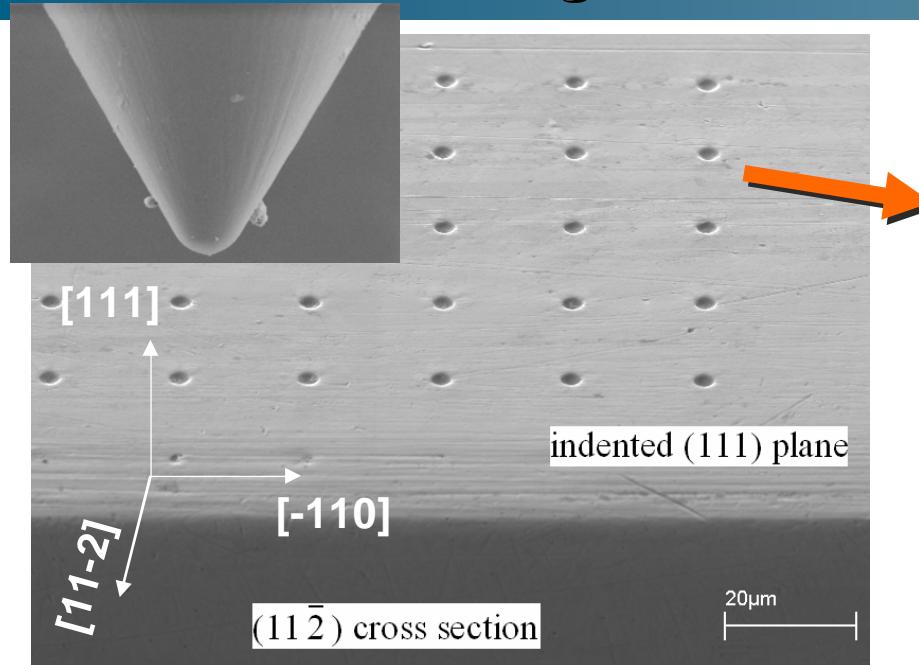


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- **Limits in plasticity continuum models (small
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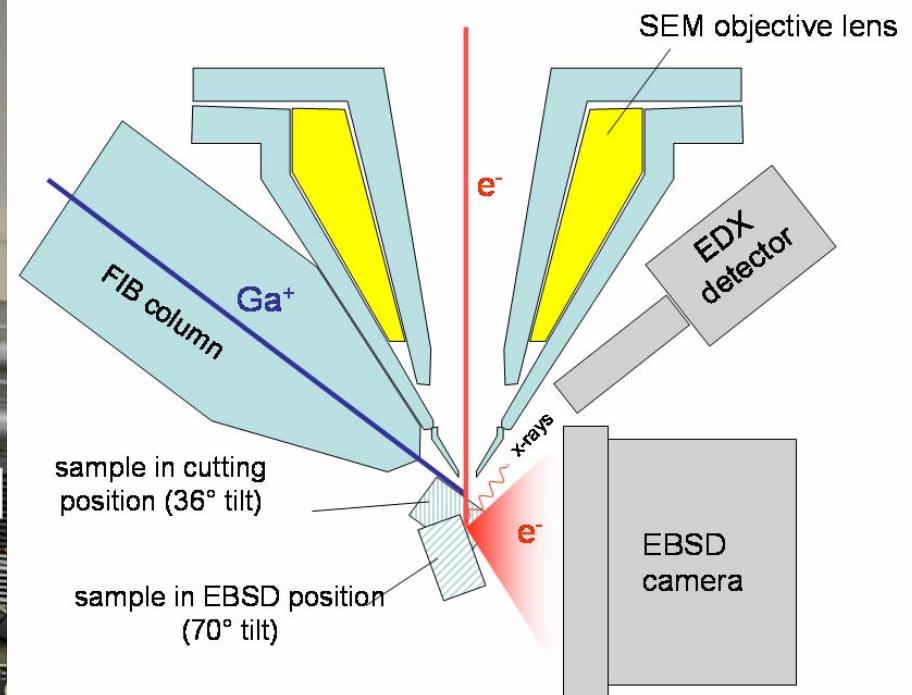
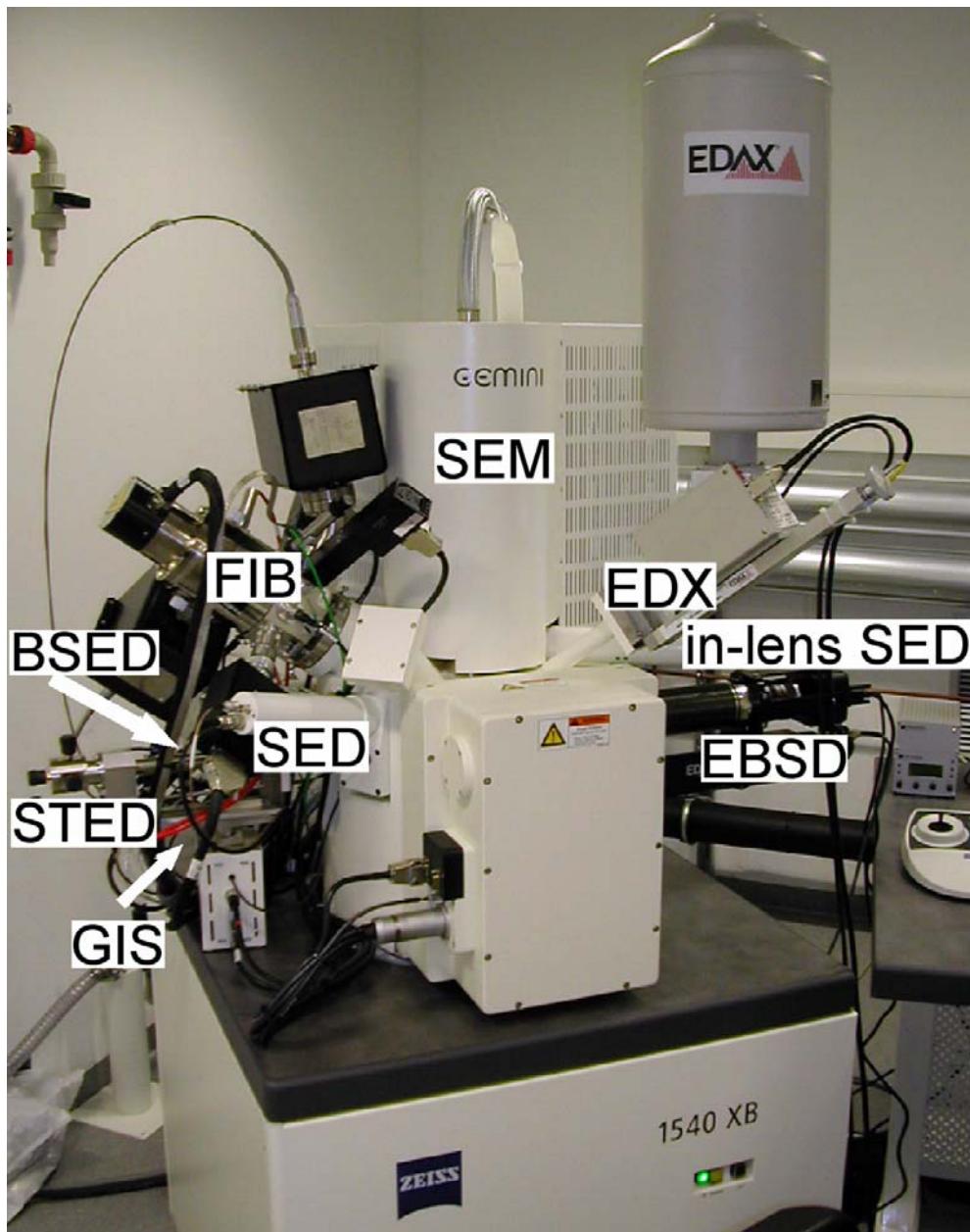


Nanoindentierung





3D electron - microscopy

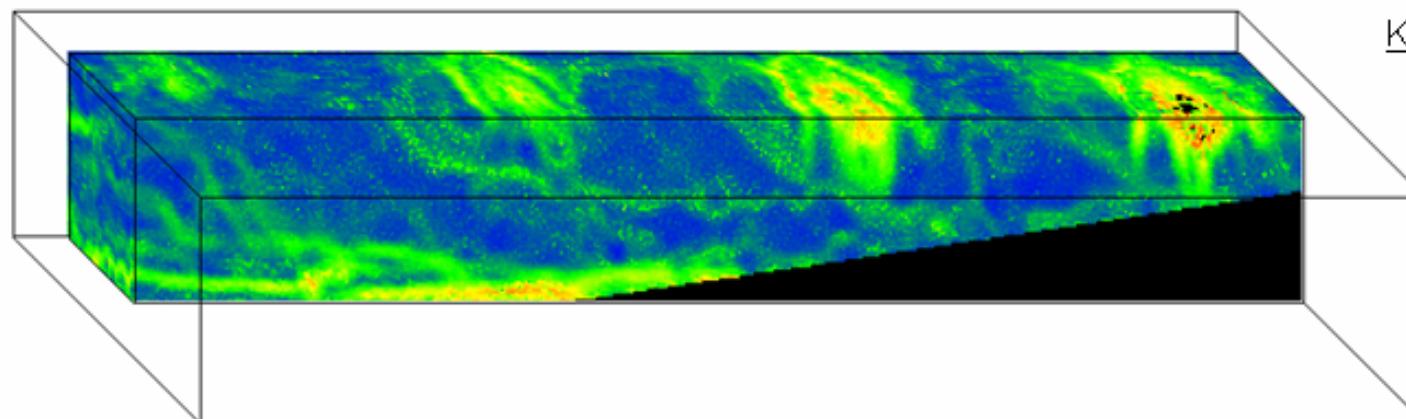
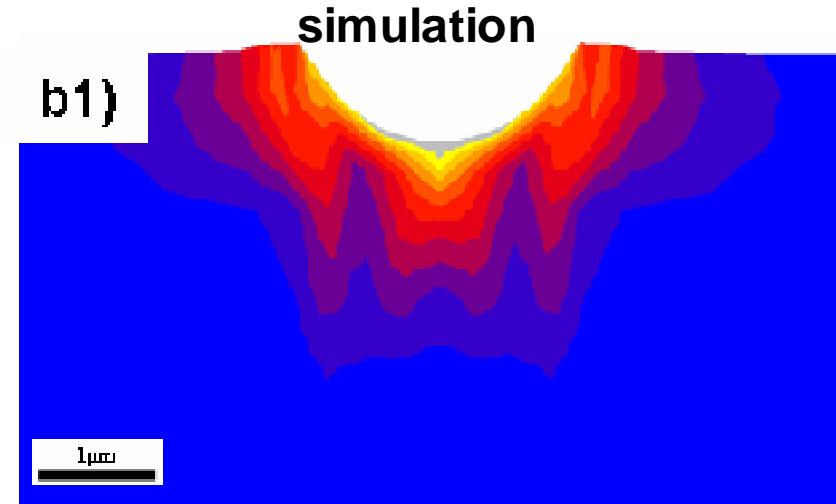
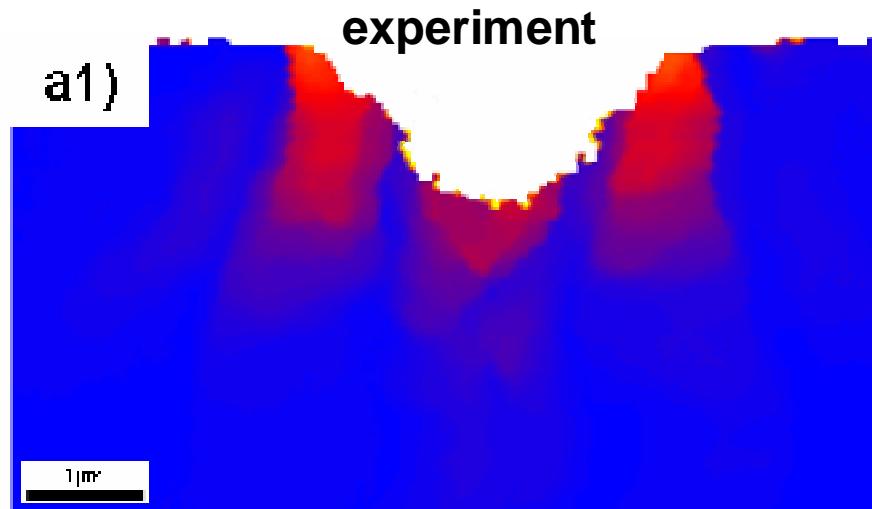




Misorientation map

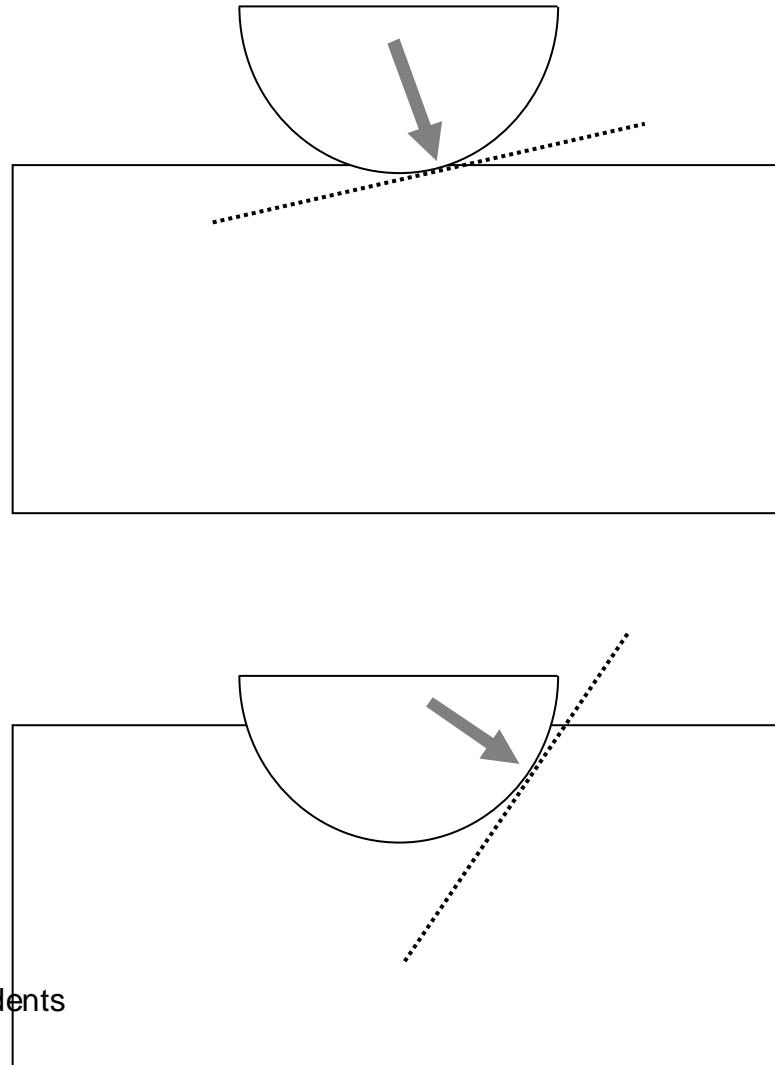
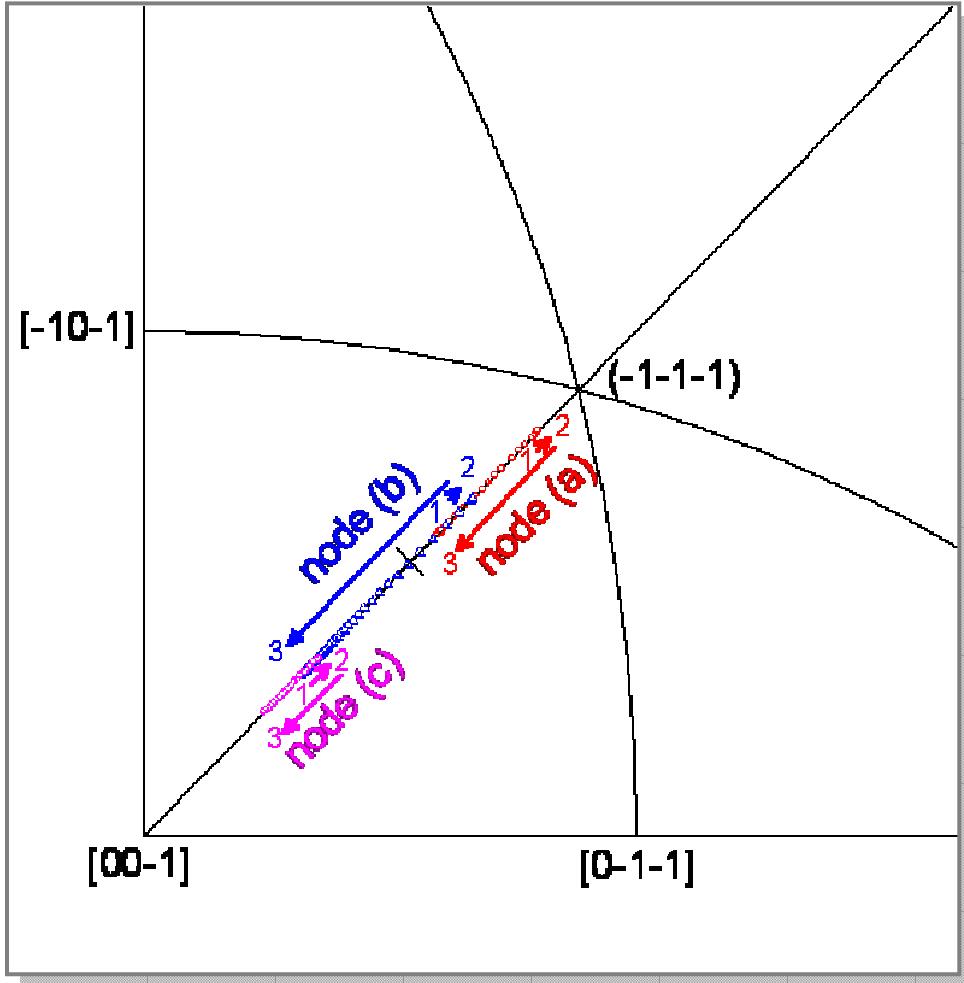
N. Zaafarani D. Raabe, R. N. Singh, F. Roters, S. Zaefferer,
Acta Materialia, Volume 54, Issue 7, Pages 1707-1994 (April 2006)

"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

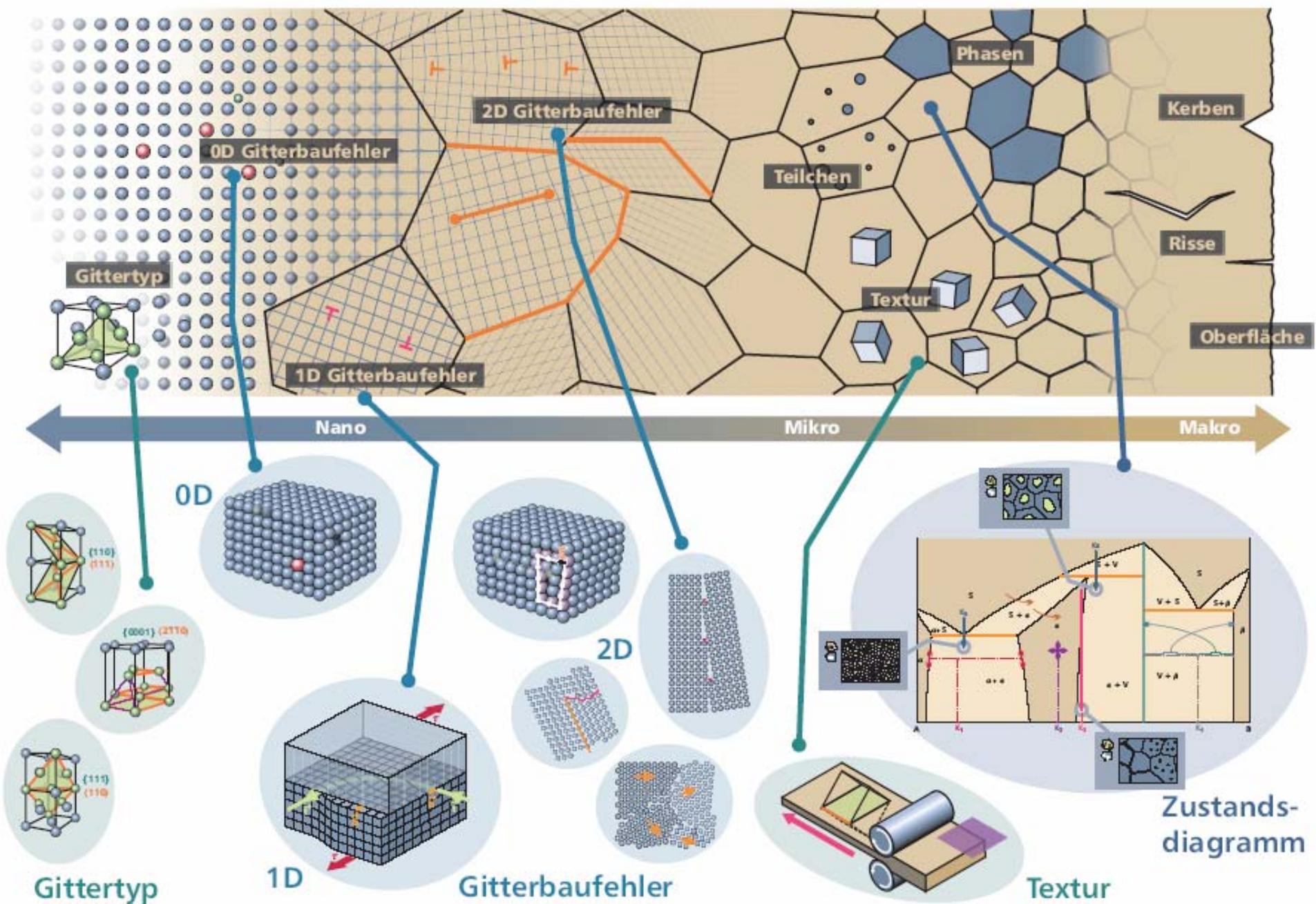
Simplify



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**