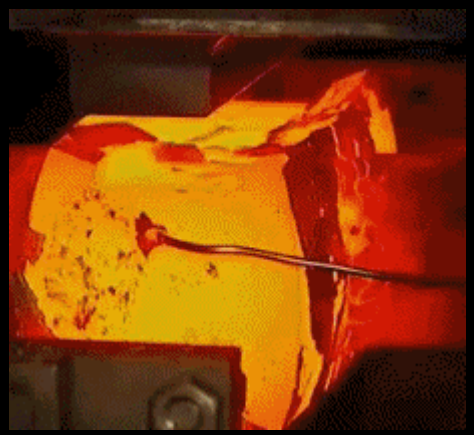
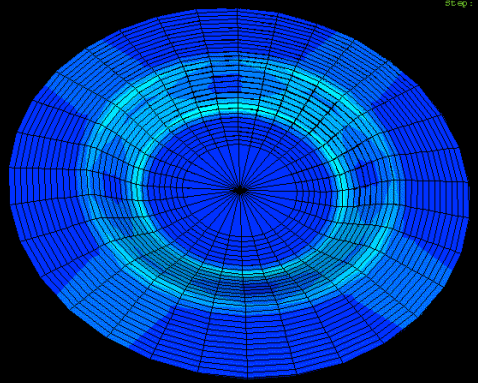
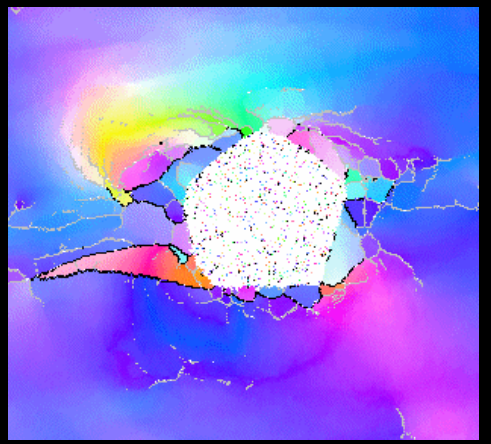
Max-Planck-Institut für Eisenforschung GmbH

Grain boundary mechanics in Crystal Plasticity Finite Element Modeling

Dierk Raabe, Franz Roters, Anxin Ma







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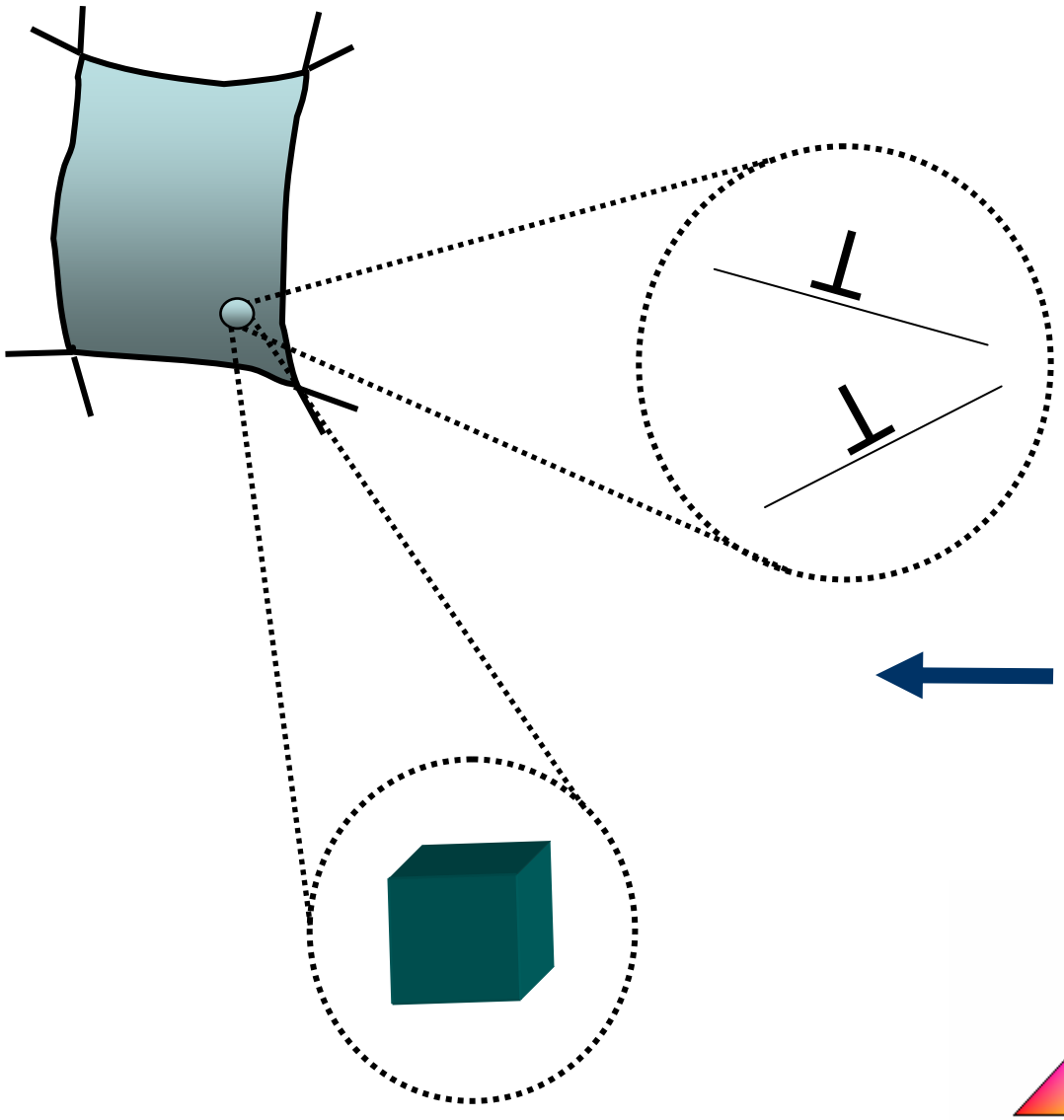
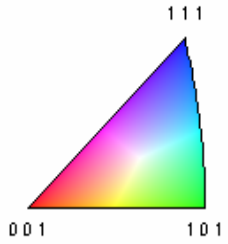
overview

- Crystal mechanics-FEM
- 3D EBSD
- Materials science of arthropods: lobster

crystal plasticity FEM





70.00 µm = 70 steps

crystal kinematics and dynamics

multiplicative decomposition of the deformation gradient

F* : "elastic" deformation gradient
F : total deformation gradient
Fp : plastic deformation gradient
Lp : plastic velocity gradient
Le : elastic velocity gradient

flow law

DOF:

$$\tilde{\mathbf{L}}_\mathrm{p} = \sum_{\alpha=1}^{24} \dot{\gamma}_\alpha \tilde{\mathbf{d}}_\alpha \otimes \tilde{\mathbf{n}}_\alpha$$

$\dot{\gamma}_\alpha(\tau_\alpha, \tau_{c\alpha}, \theta)$ ⟶ phenomenological

$\dot{\gamma}_\alpha(\tau_\alpha, \boldsymbol{\rho}, \theta)$ ⟶ dislocation rate formulations

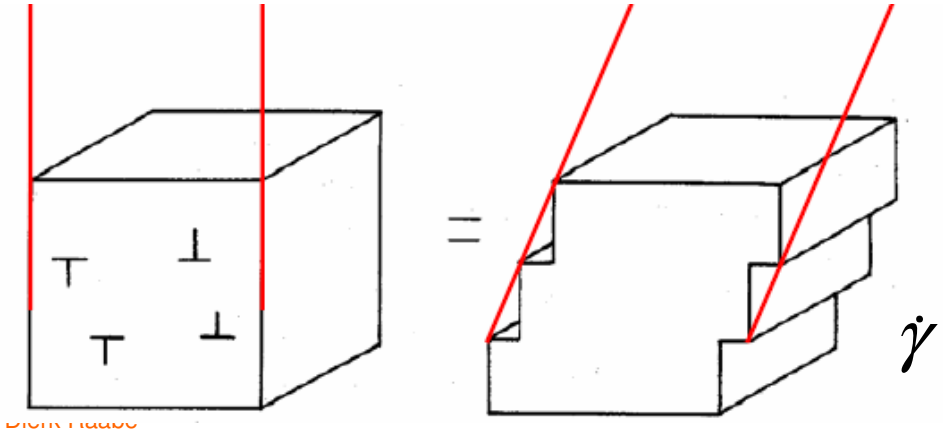
Definitions:

$$\mathbf{L} := \dot{\mathbf{F}}\mathbf{F}^{-1}$$

$$\mathbf{L}_\mathbf{e} := \dot{\mathbf{F}}_\mathrm{e}\mathbf{F}_\mathrm{e}^{-1}$$

$$\tilde{\mathbf{L}}_\mathrm{p} := \dot{\mathbf{F}}_\mathrm{p}\mathbf{F}_\mathrm{p}^{-1}$$

$$\mathbf{L}_\mathrm{p} := \mathbf{F}_\mathrm{e}\tilde{\mathbf{L}}_\mathrm{p}\mathbf{F}_\mathrm{e}^{-1}$$



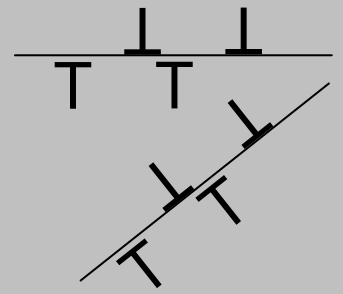
$$\dot{\gamma} = \frac{\mathrm{d}\gamma}{\mathrm{d}t} = n\frac{\mathrm{d}x}{X}\frac{b}{Z}\frac{1}{\mathrm{d}t} = \rho_\mathrm{m} b v$$

physics-based constitutive laws

1

1. set internal variables

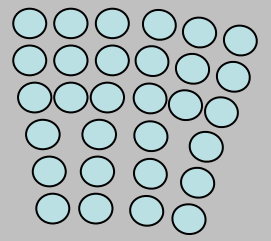
dyadic flow law based on dislocation mechanics



2

2. set internal variables

plastic gradients,
size scale and orientation gradients (implicit)

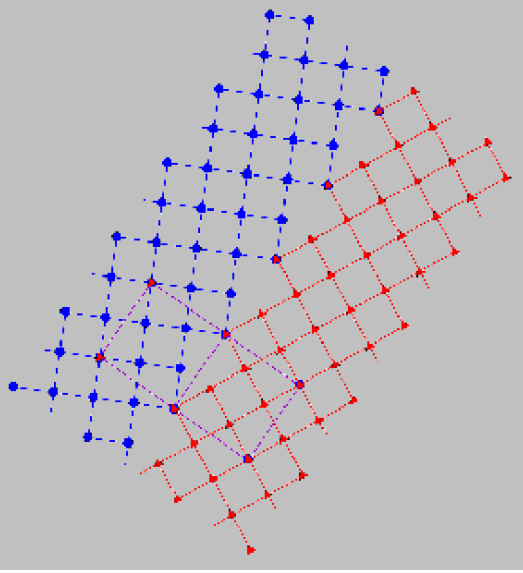


3

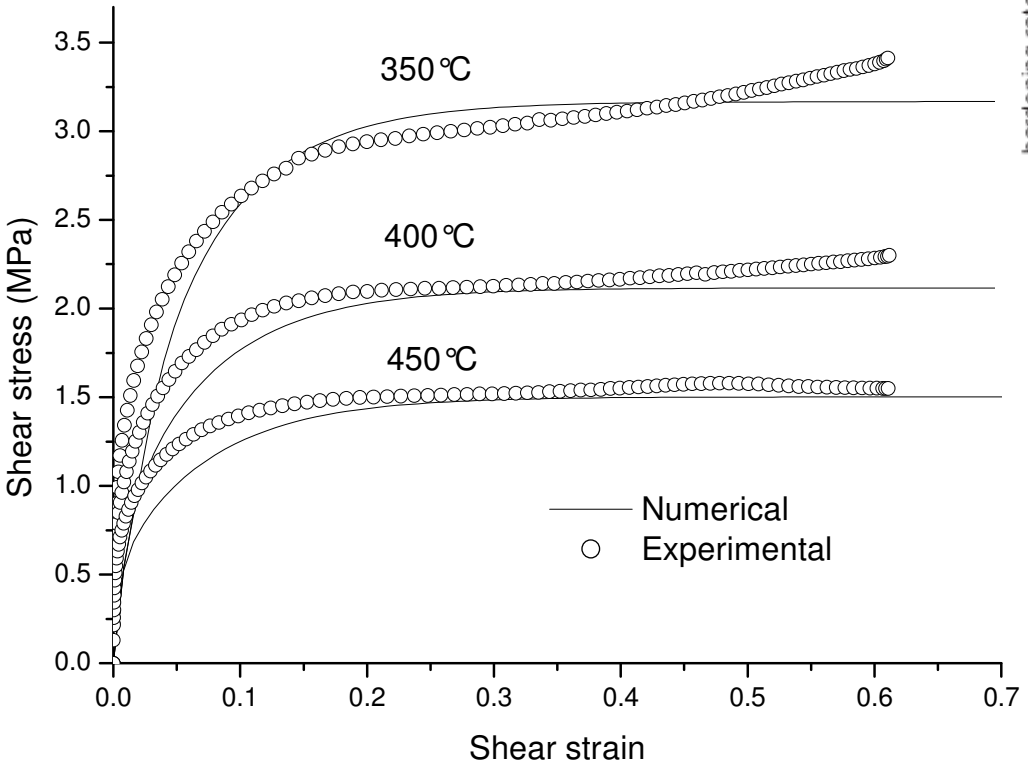
3. set internal variables

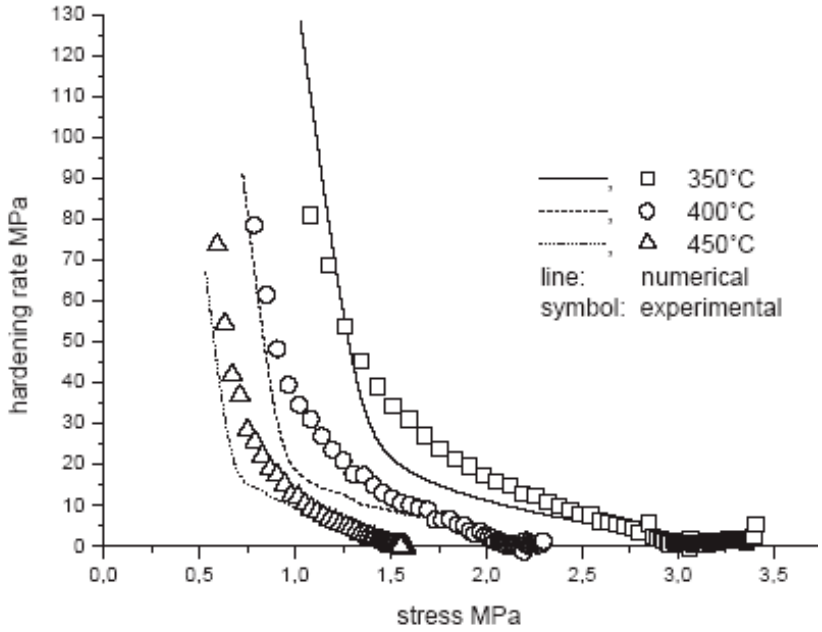
interfaces

activation concept



uniaxial compression of Al single crystals

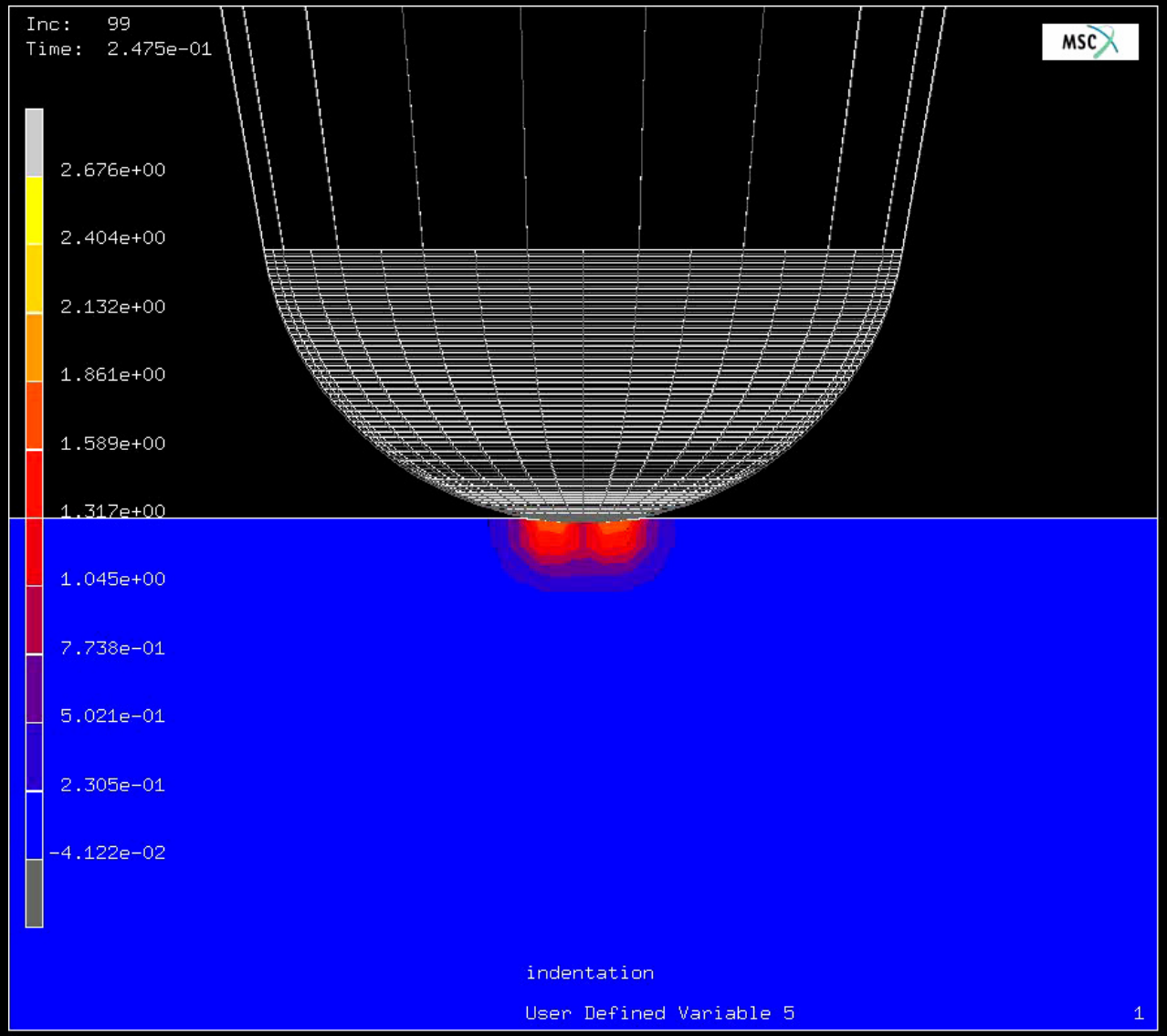




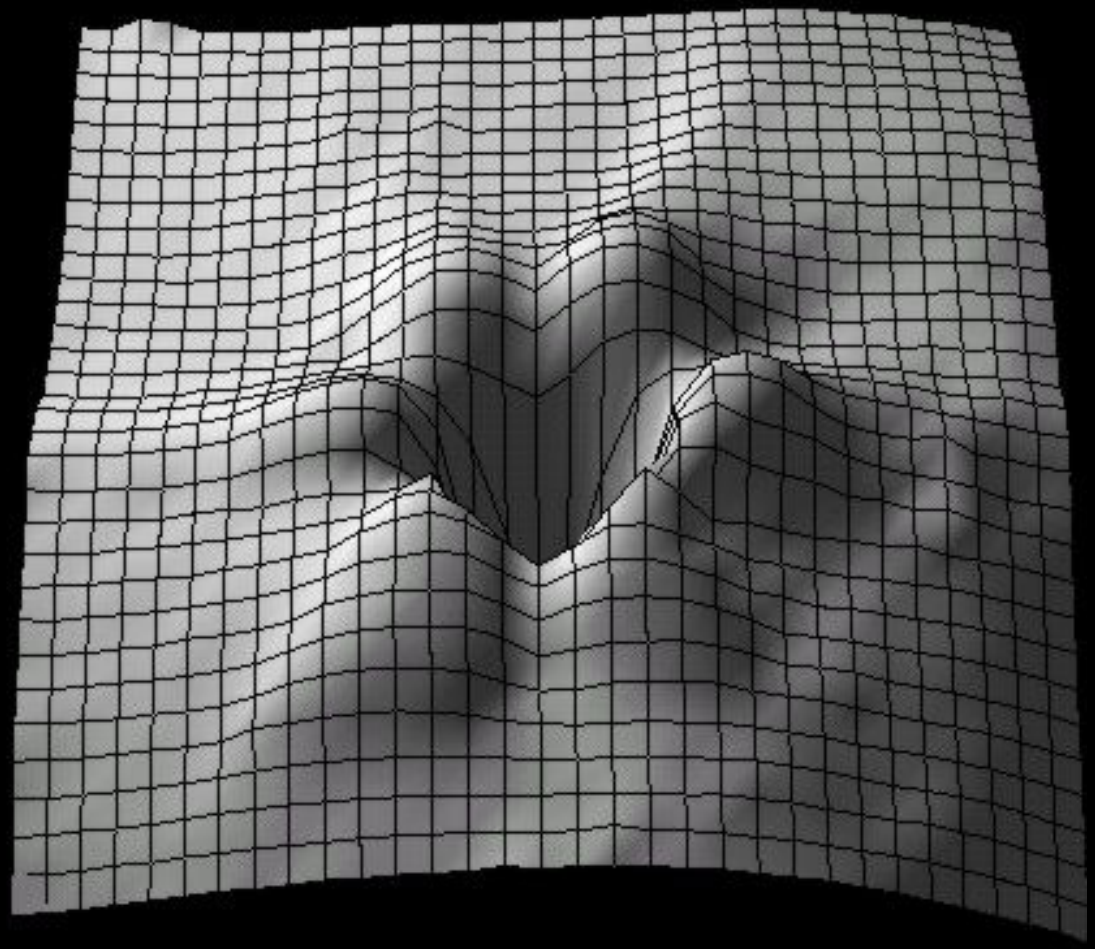
uniaxial compression along [110]

force rate = 0.2 N/s, average strain rate: 0.0001 1/s

indentation

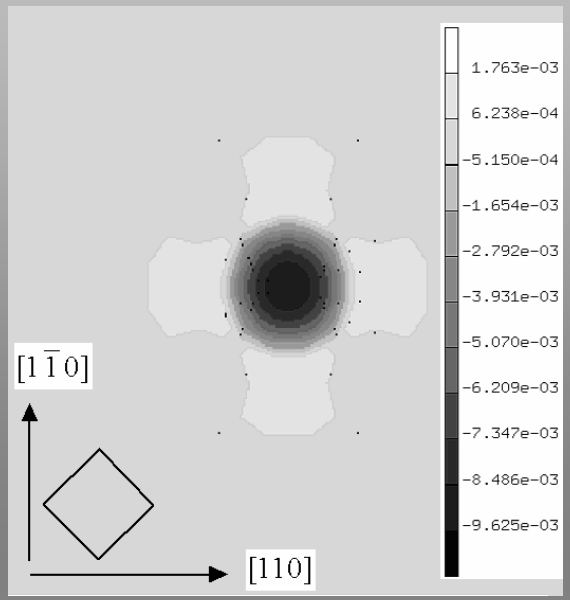


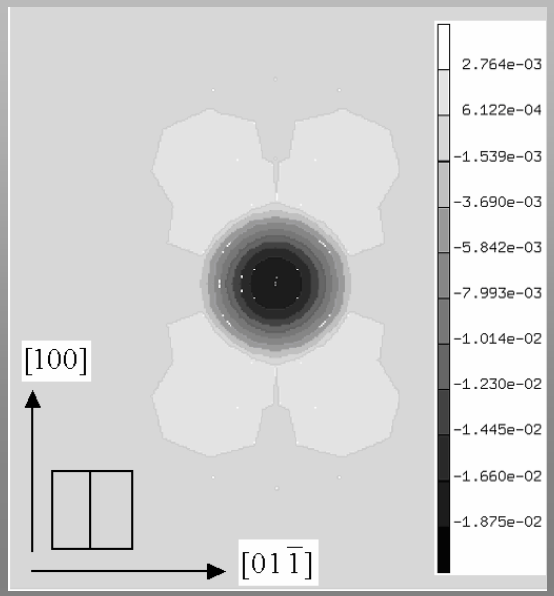
crystal plasticity FEM at small scales

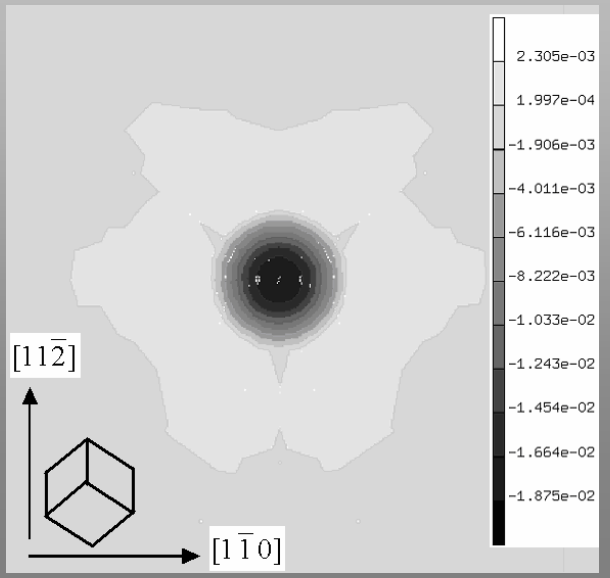


small scales – single crystals

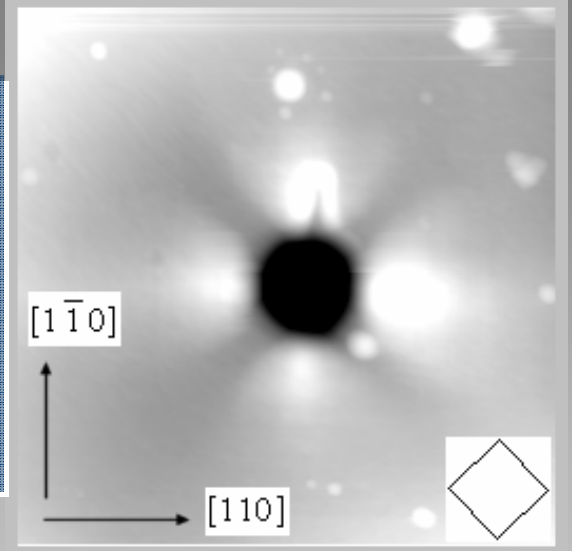
simulation

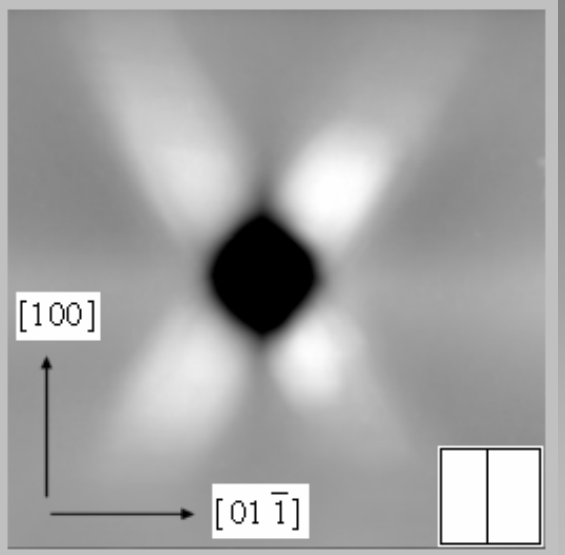


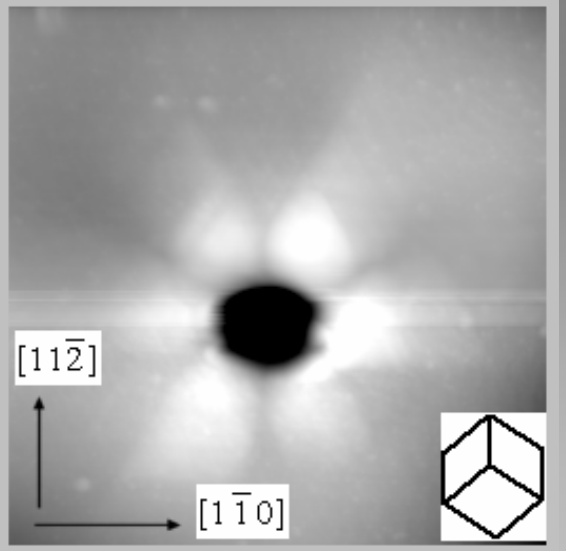




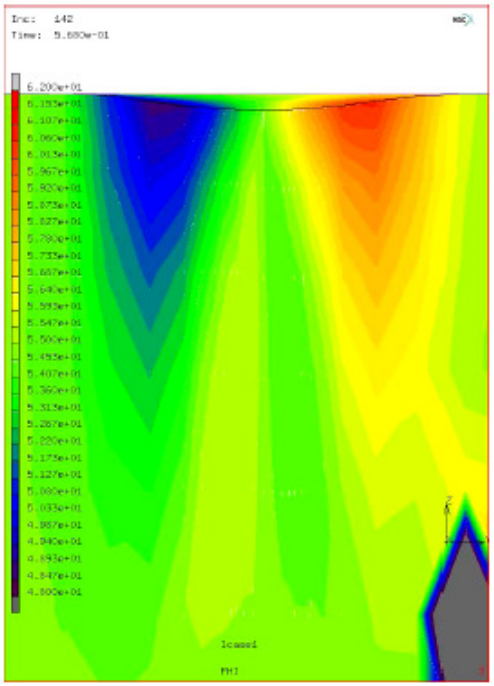
experiment



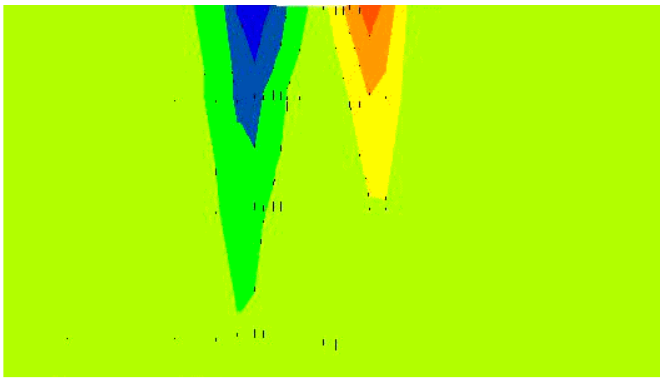




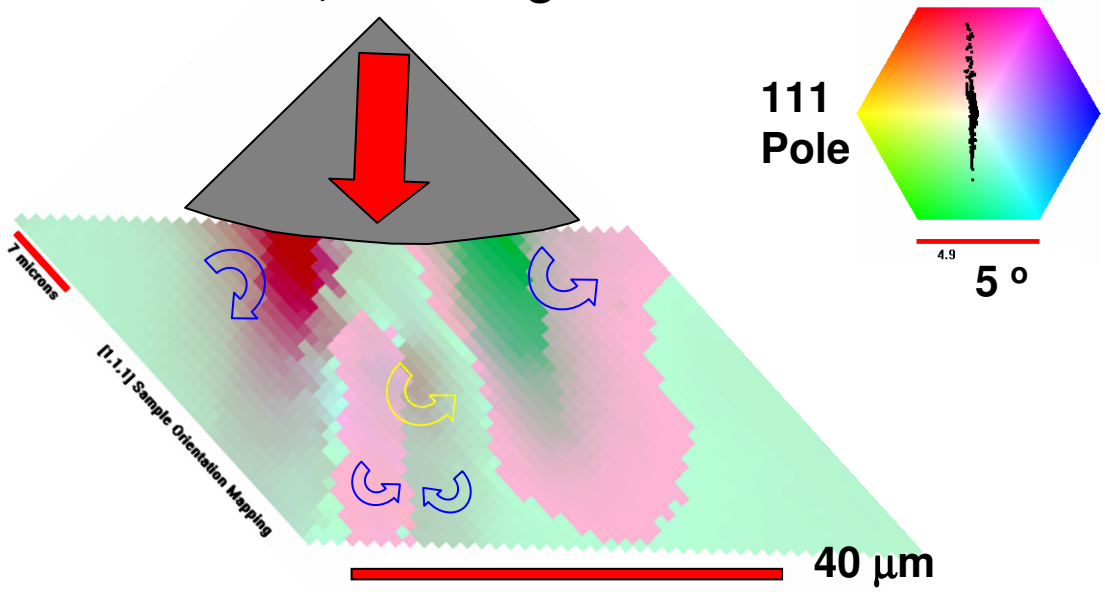
small scales – single crystals



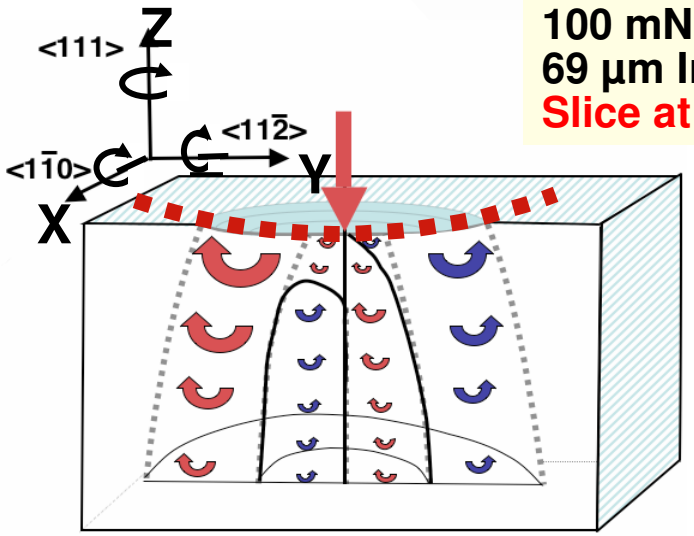
<111> Al (Calculated)
100 mN Indent Force
70 µm Indent Radius
Slice at Center of Indent



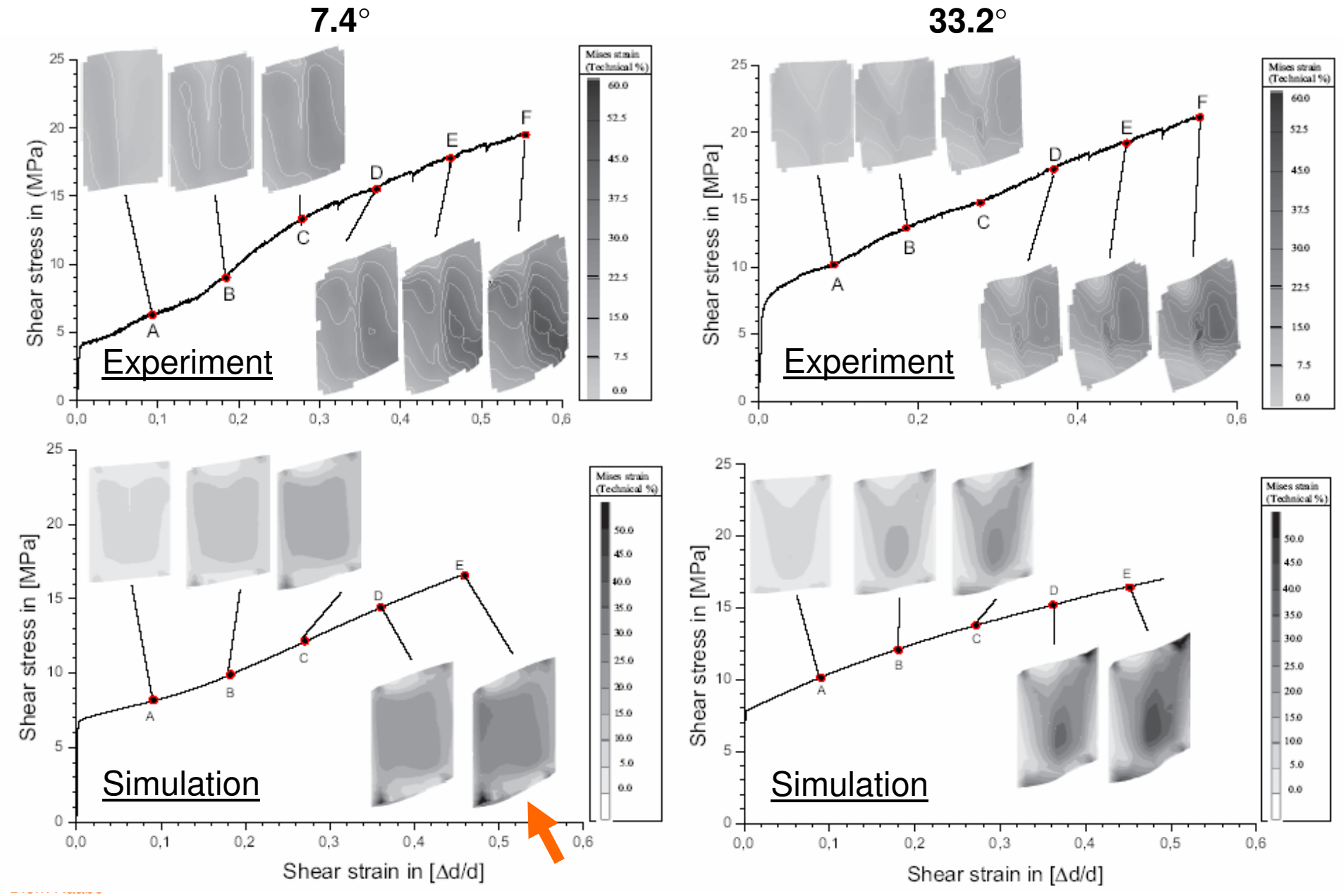
Bennett Larson, Oak Ridge Nat. Lab.



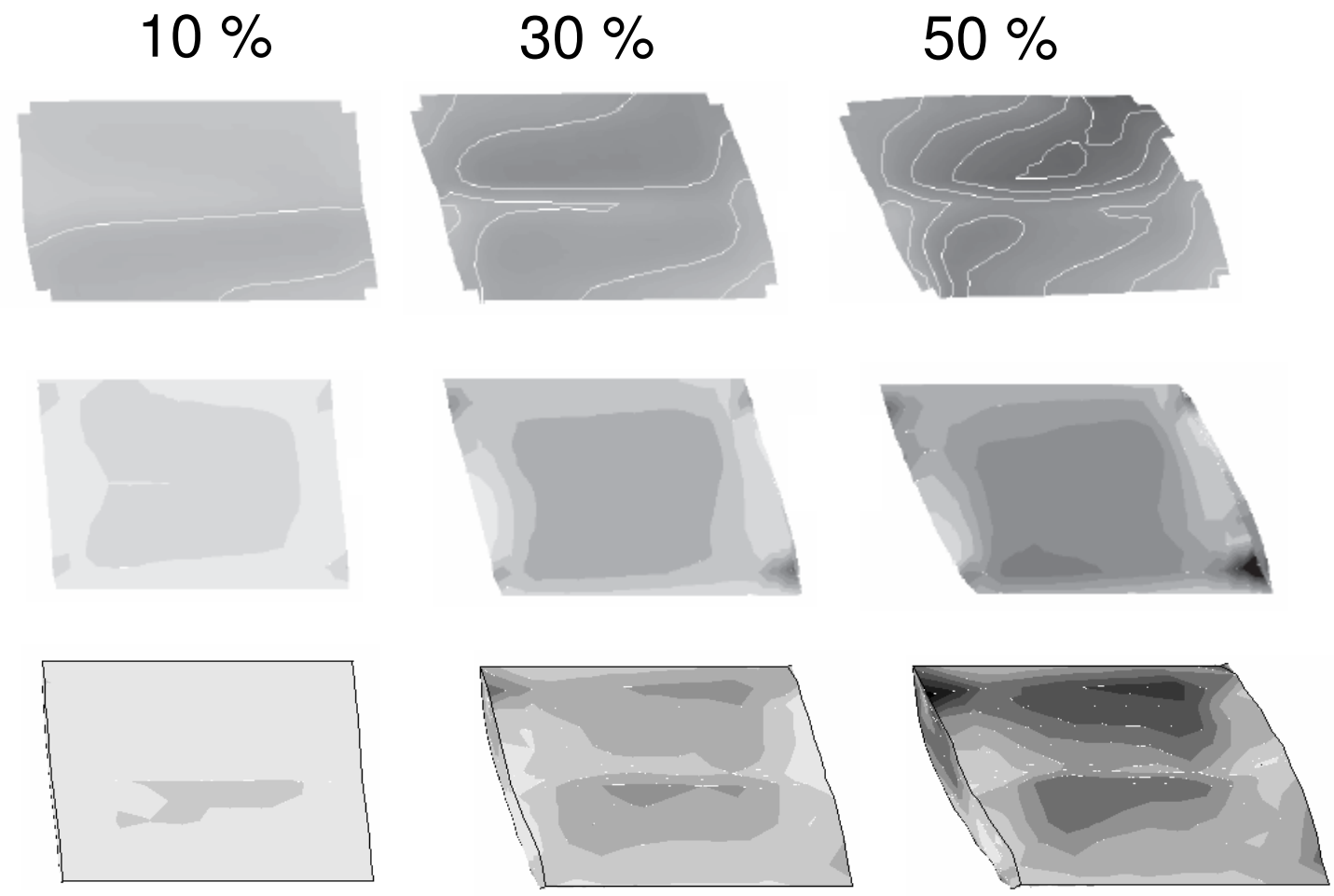
<111> Cu (Measured)
100 mN Indent Force
69 µm Indent Radius
Slice at Center of Indent



small scales – bicrystals - conventional theory

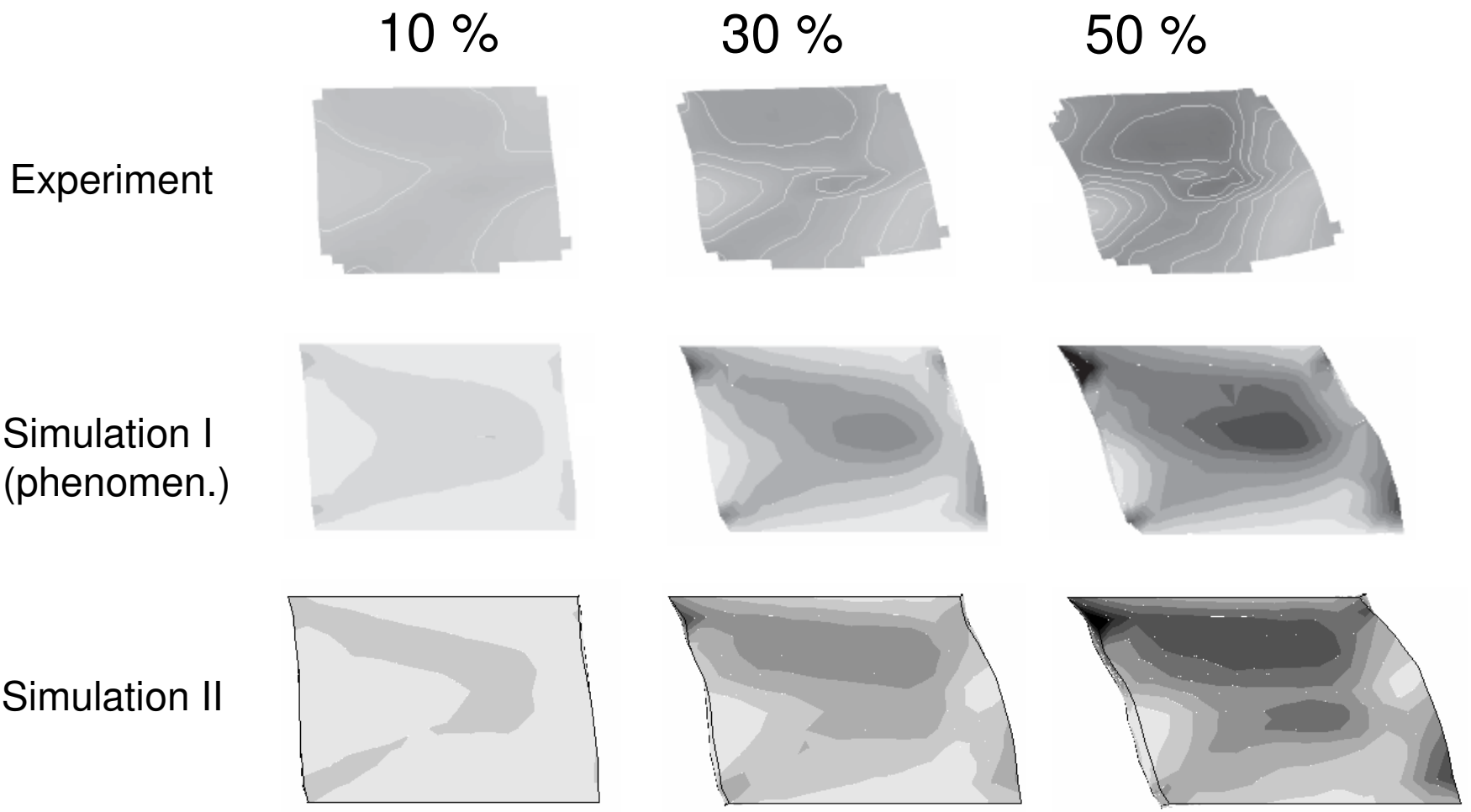


small scales – bicrystals

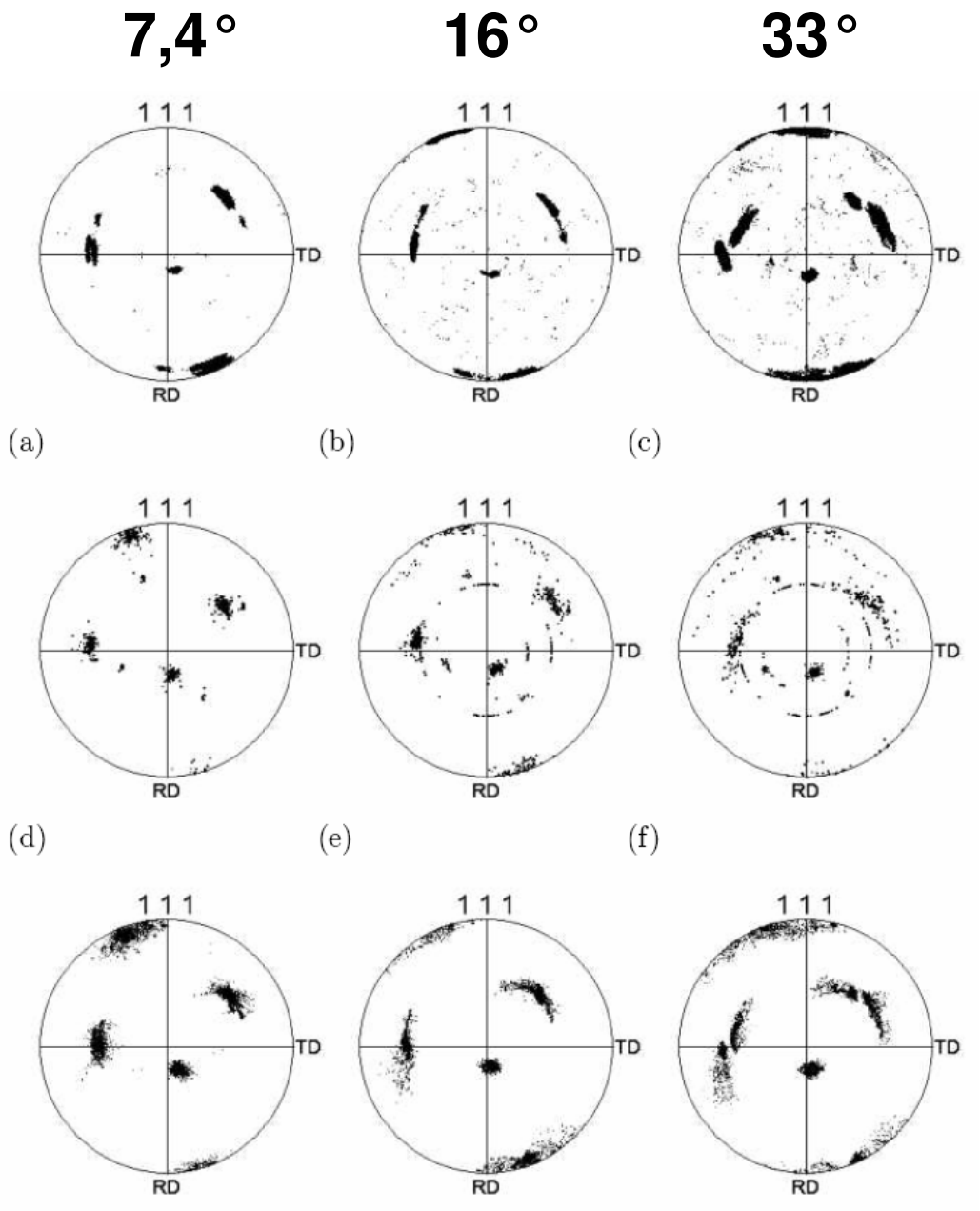


7.4°

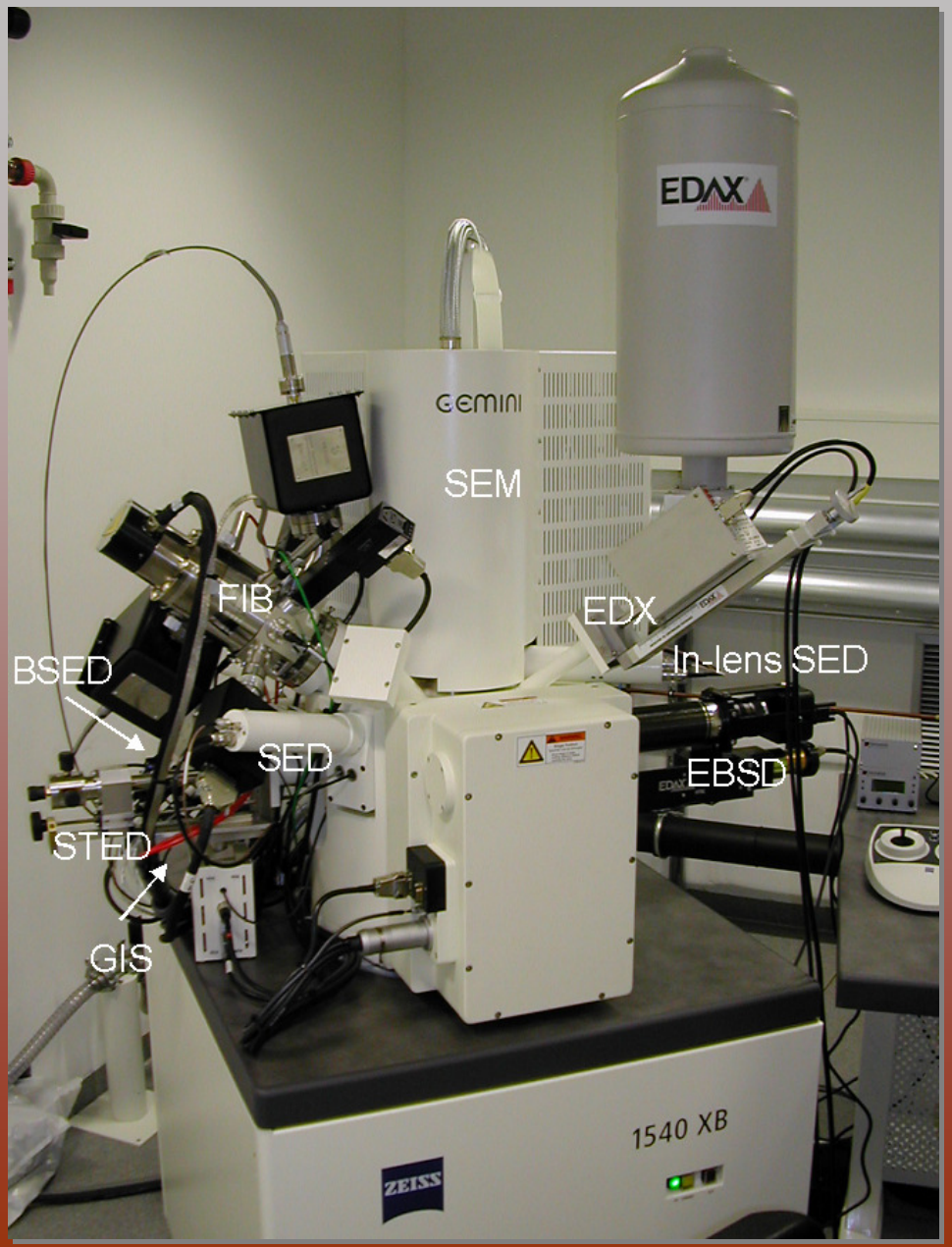
small scales – bicrystals



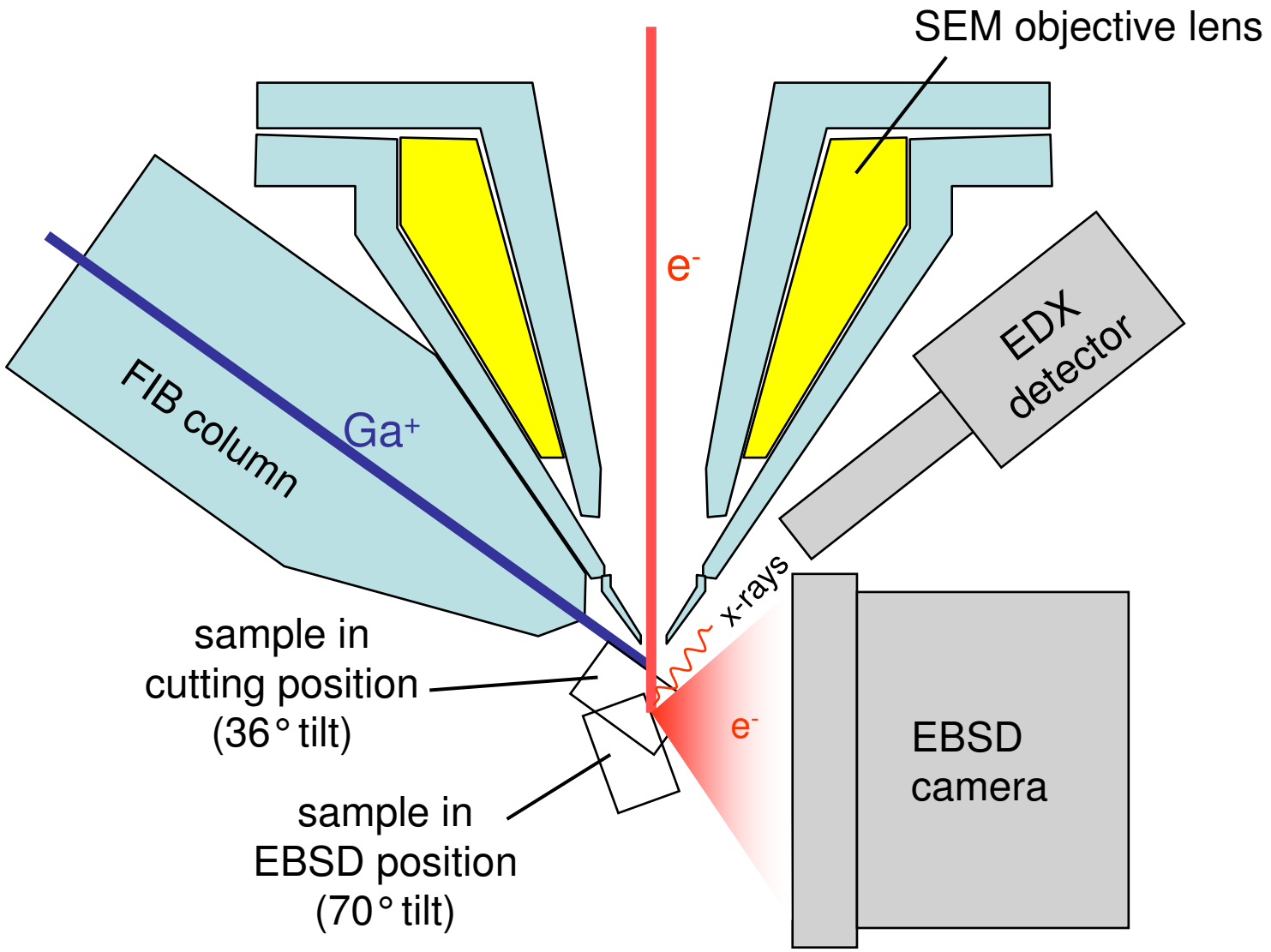
small scales – bicrystals



3D electron microscopy



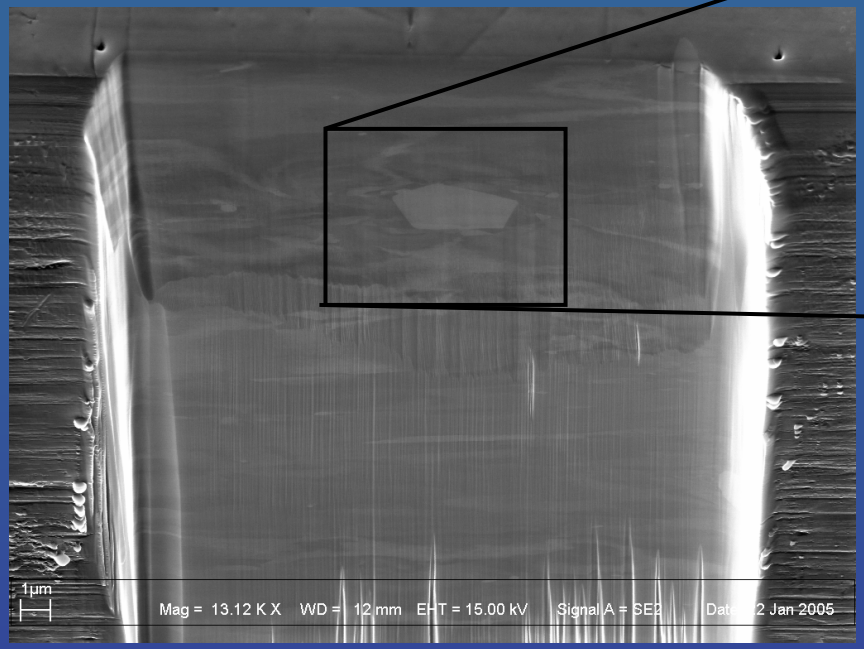
schematics of serial sectioning set-up



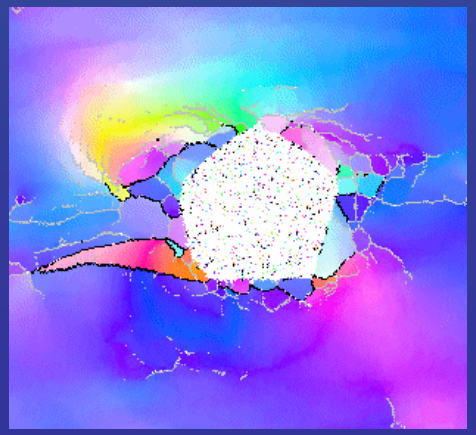
⇨ easy and precise change between cutting and analysing positions

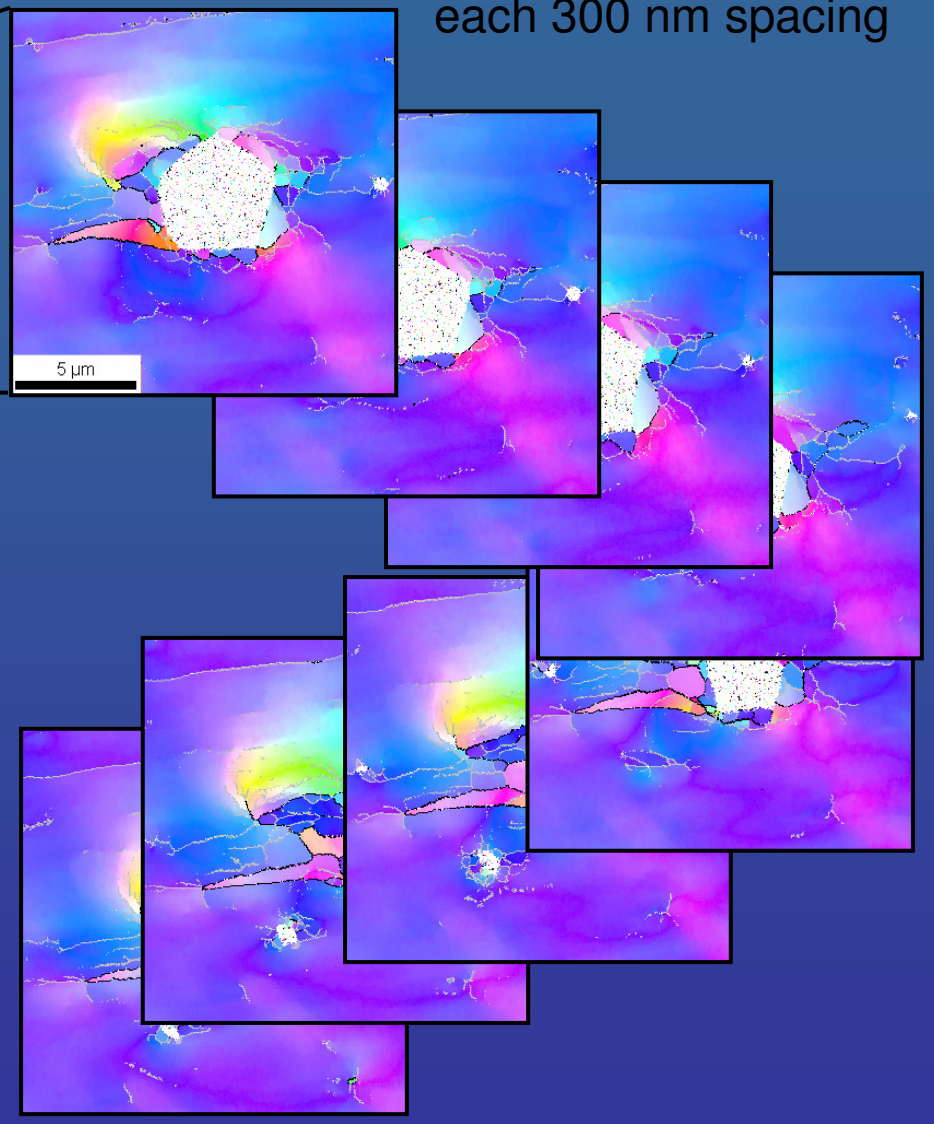
3D EBSD by serial FIB sectioning

each 300 nm spacing

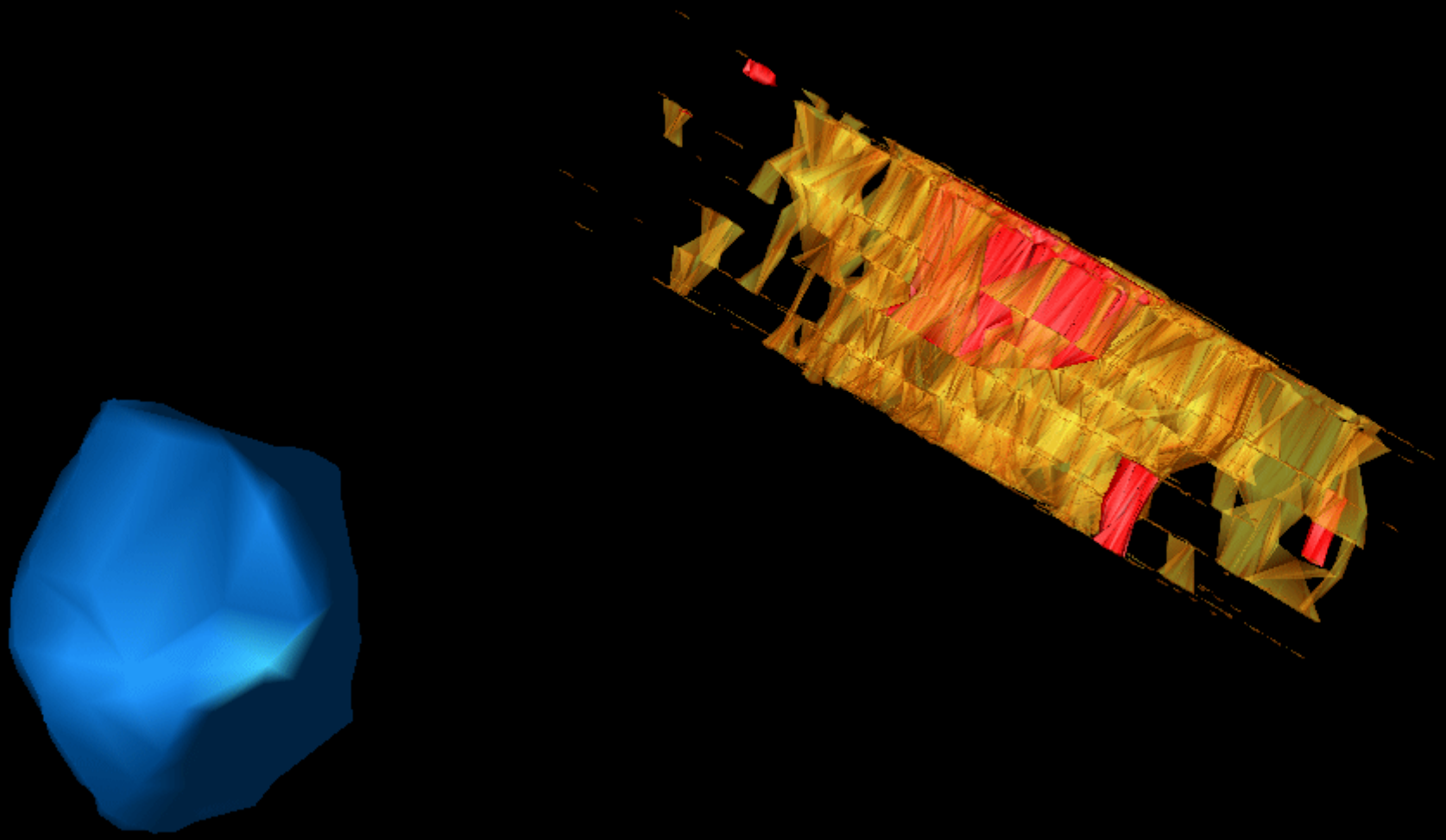


SE-image



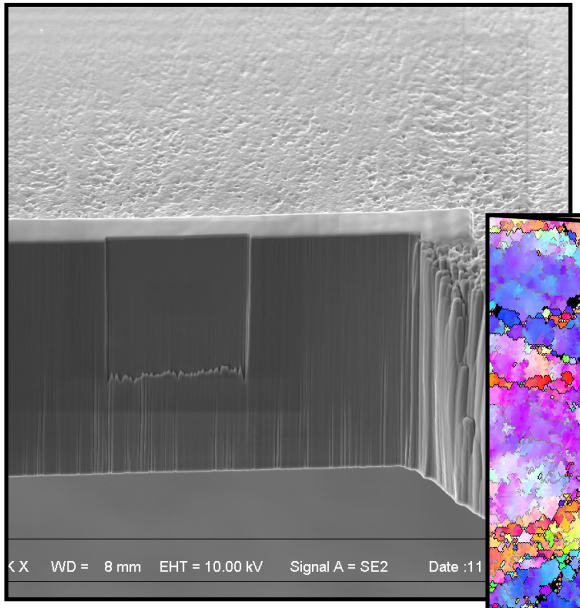


3D rendering of EBSD sections

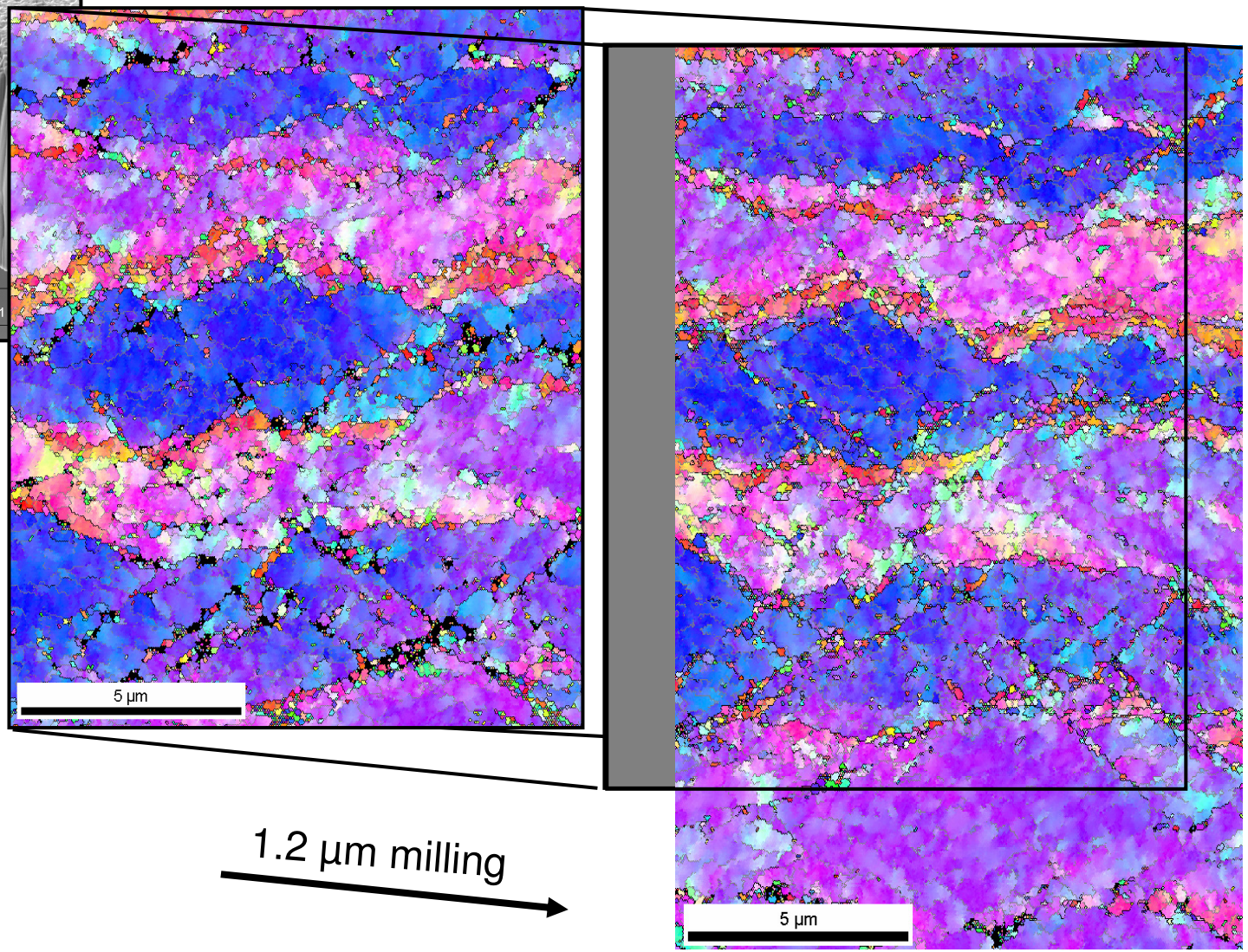


IMOD: public domain software, Boulder Laboratory for 3D Electron Microscopy of Cells, University of Colorado, Ref.: J. Struct. Biol. 116 (1996), 71-76

guided preparation

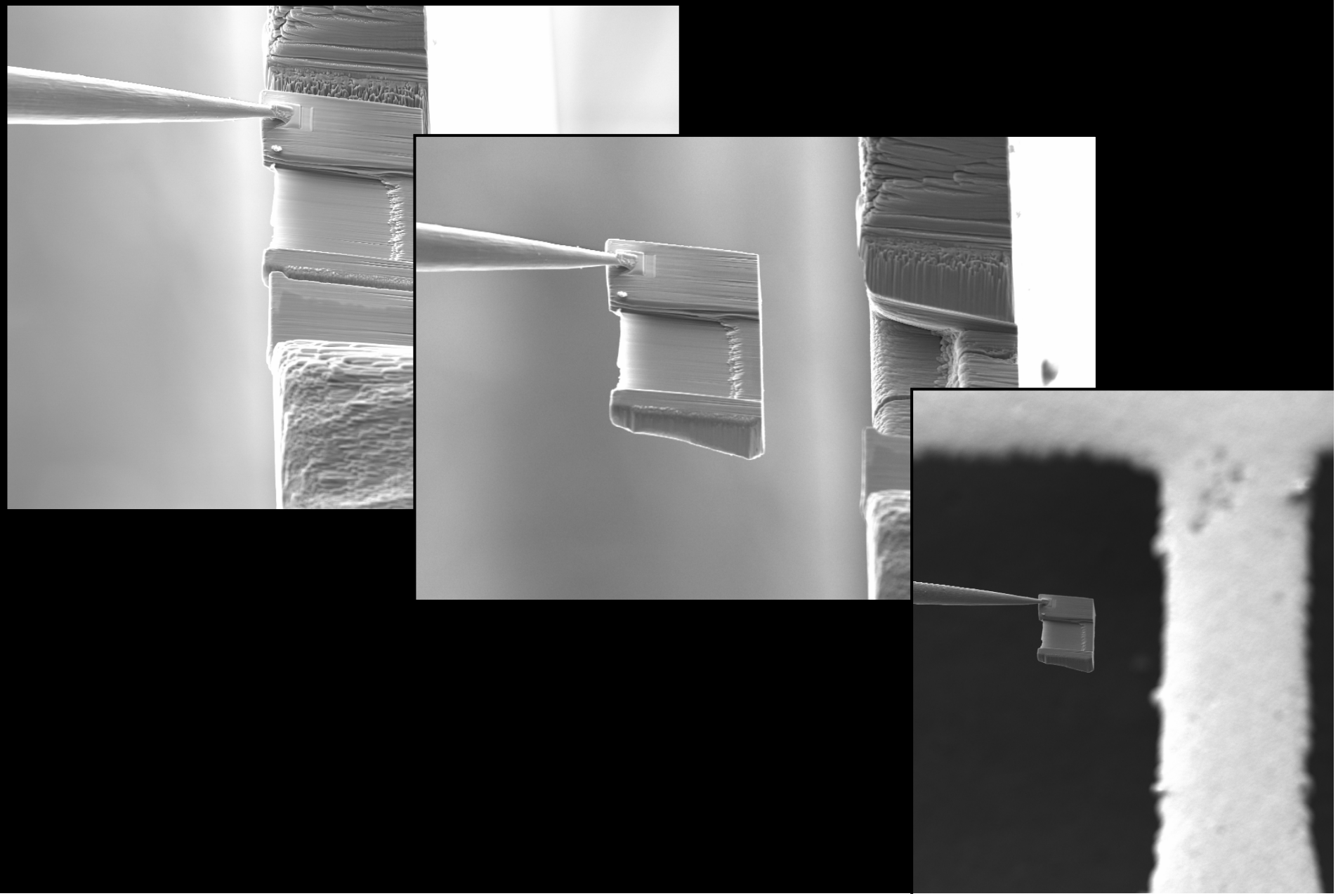


colour code: RD

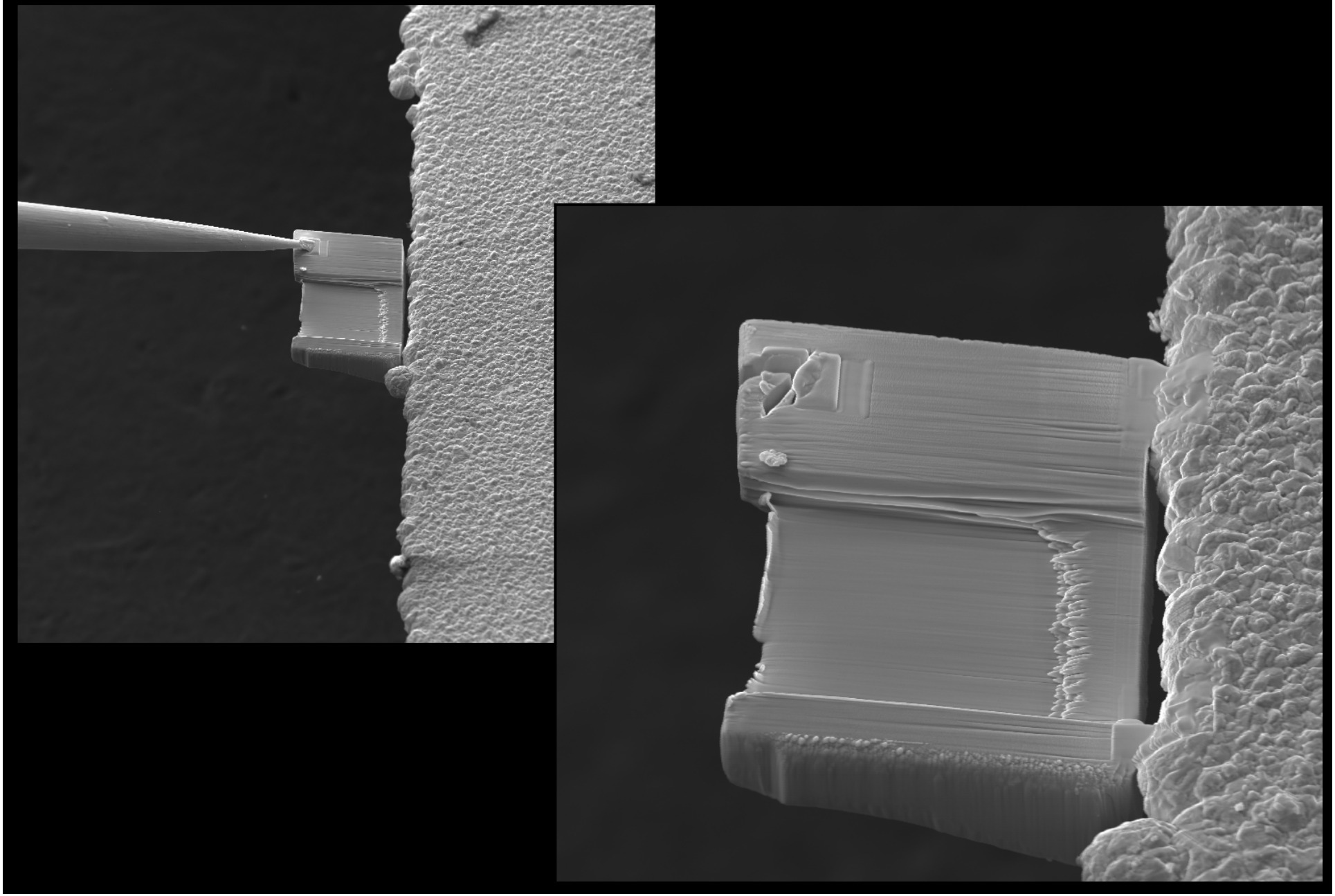


1.2 µm milling

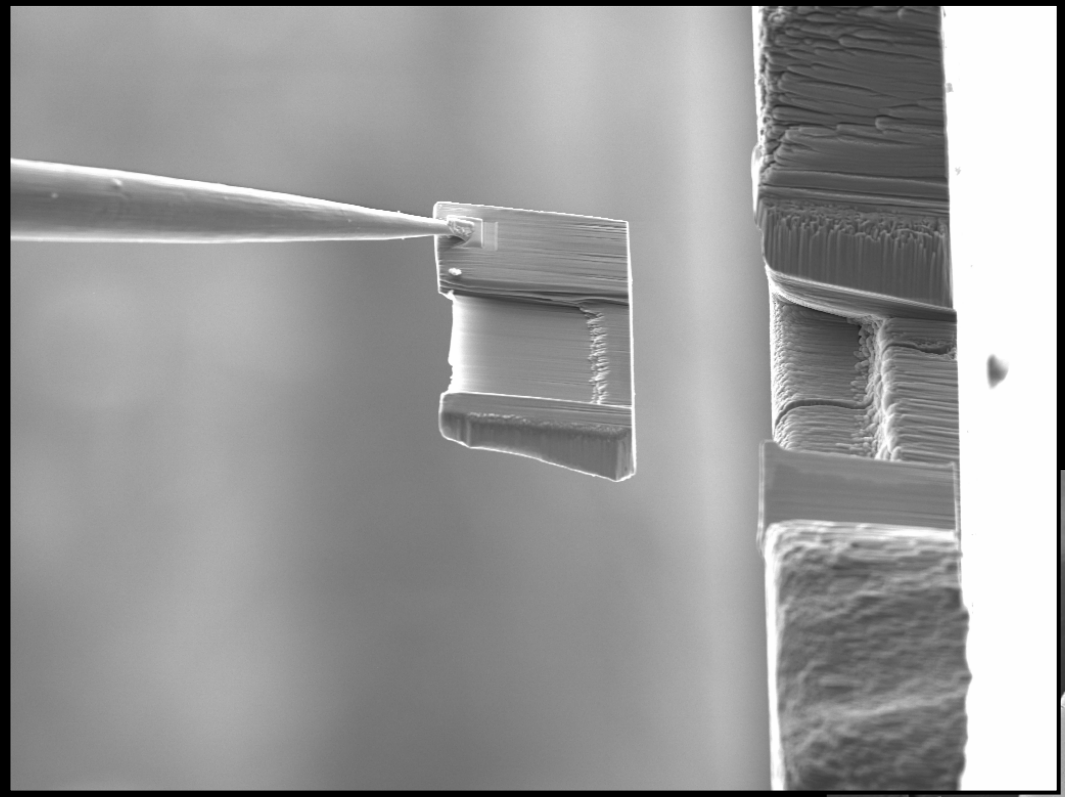
guided preparation



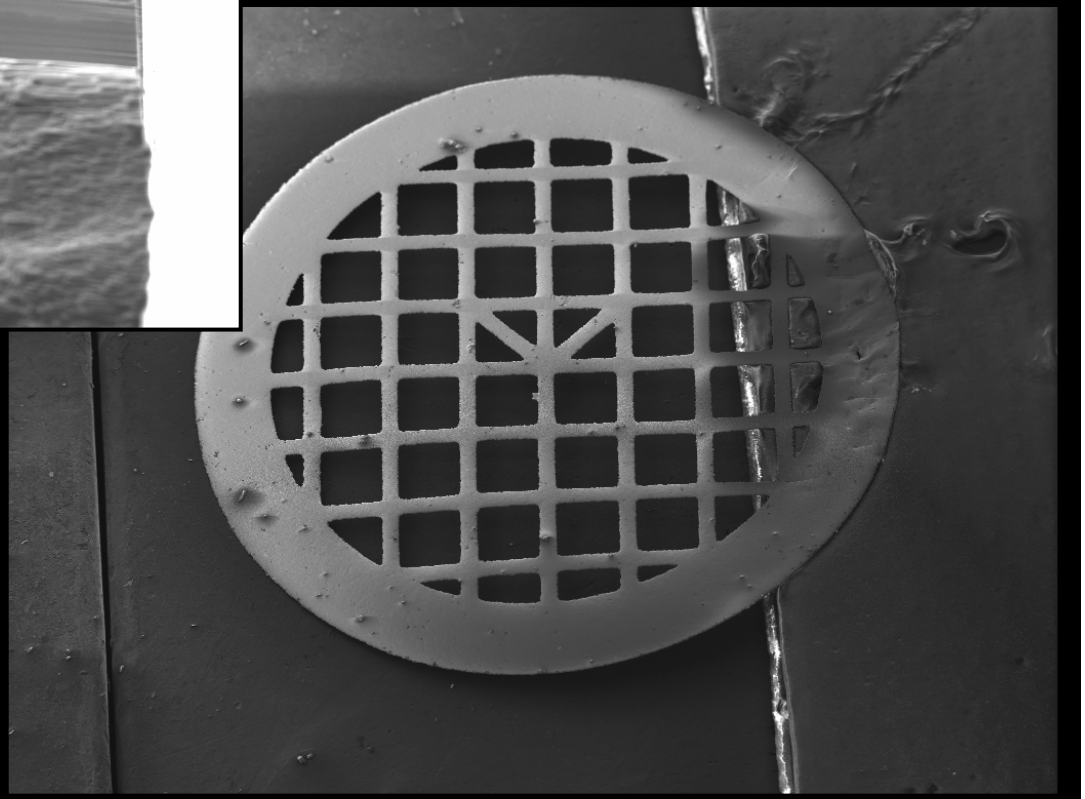
guided preparation



extracting and mounting TEM samples



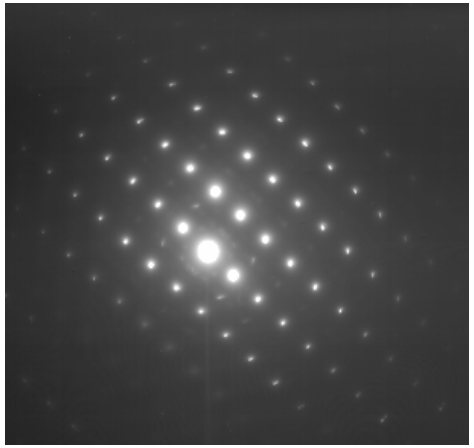
extraction of thin foil with nano-manipulator

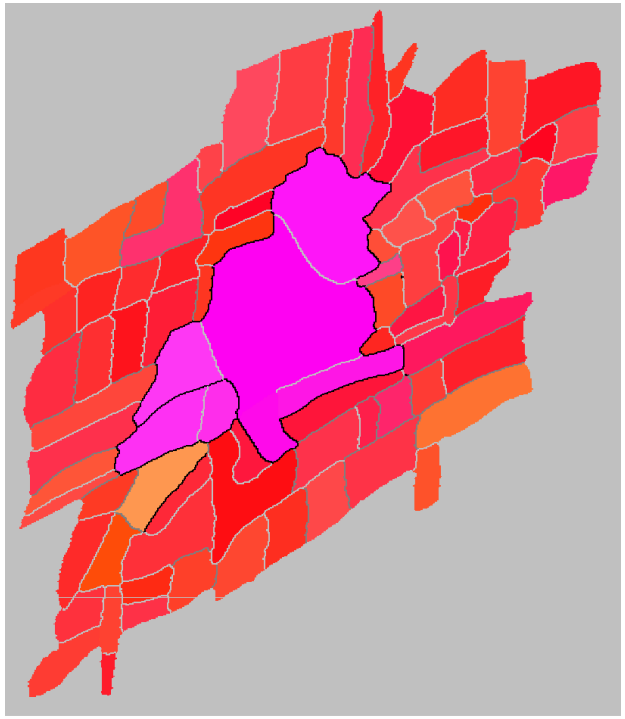


TEM sample fixed to a 3-mm TEM grid

TEM

Hellfeld





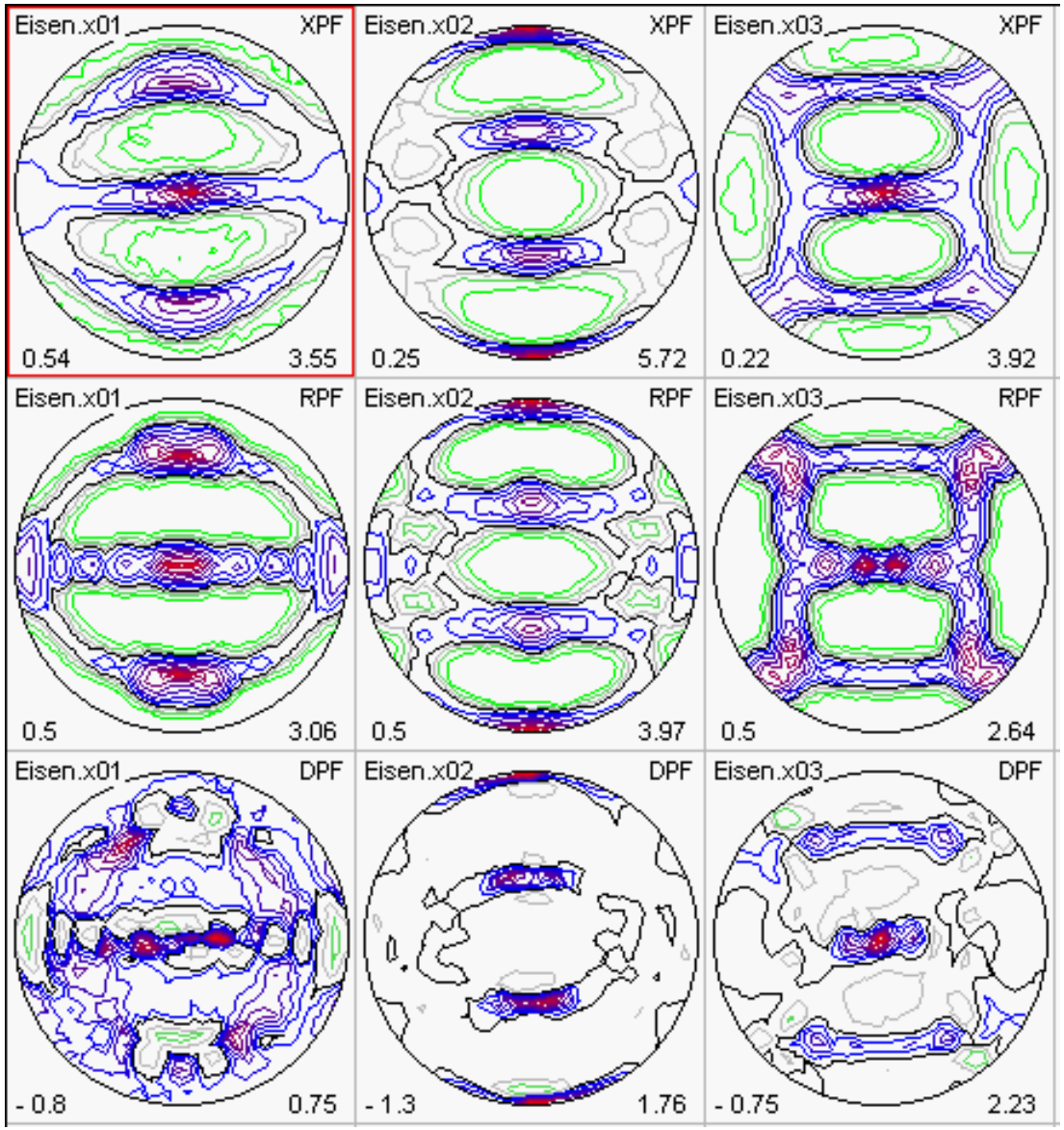
Orientierung

Extract components and background from experiments

Exp. input

Backcalculation

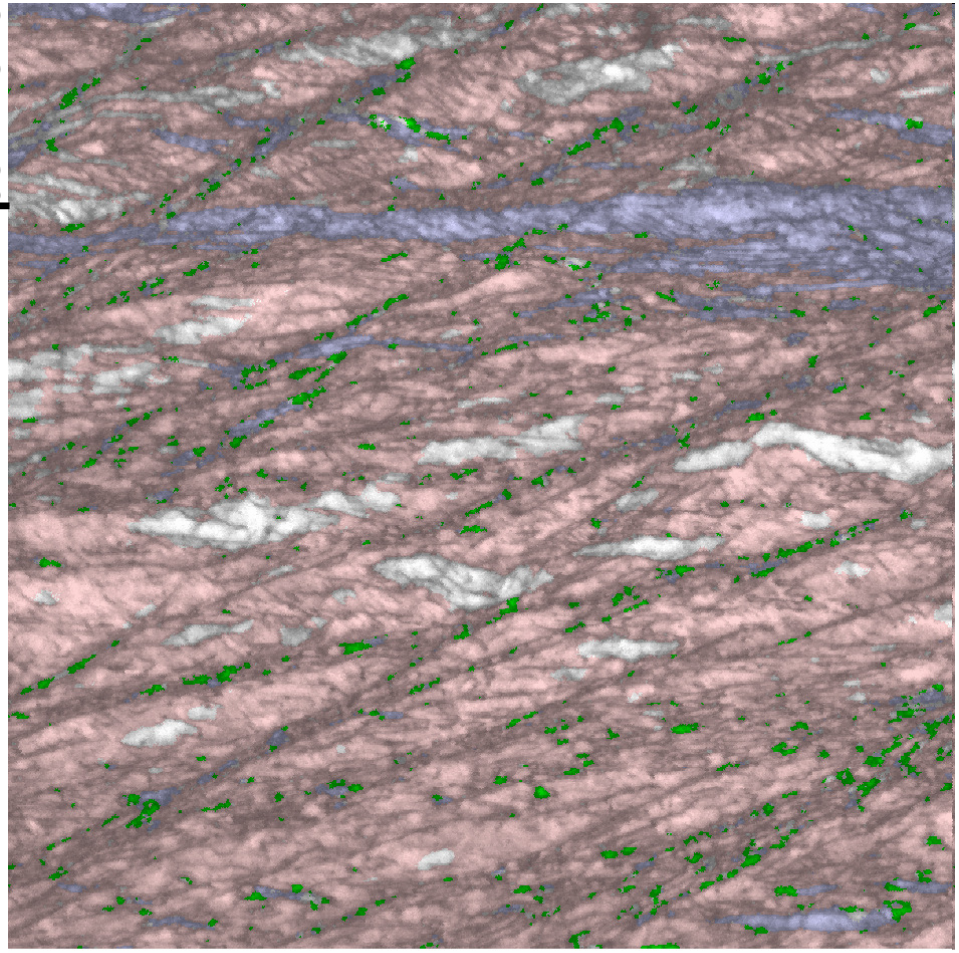
Difference



MulTex 2.0 K. Helming

Fließfelddivergenz und intrinsische Orientierungsgradienten

Experiment



NR

WR

5.00 µm = 100 steps IQ -14.348...76.6936, Orientation

(011)[100]: 0° - 15° Misorientierung

(111)[11-2]: 0° - 20° Misorientierung

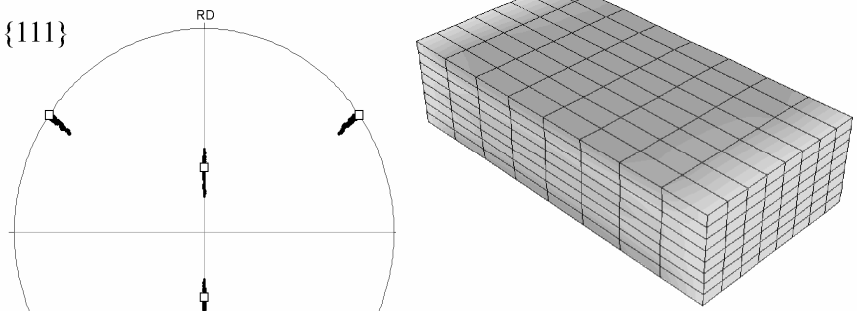
(111)[-1-12]: 0° - 20° Misorientierung

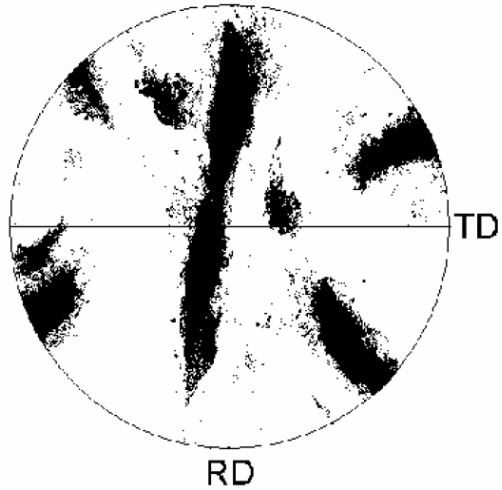
EBSD pattern quality:

low high

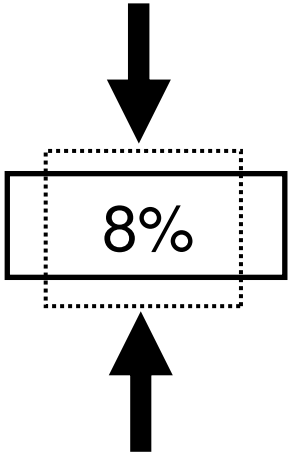
89 % plane strain
Orientation and band contrast

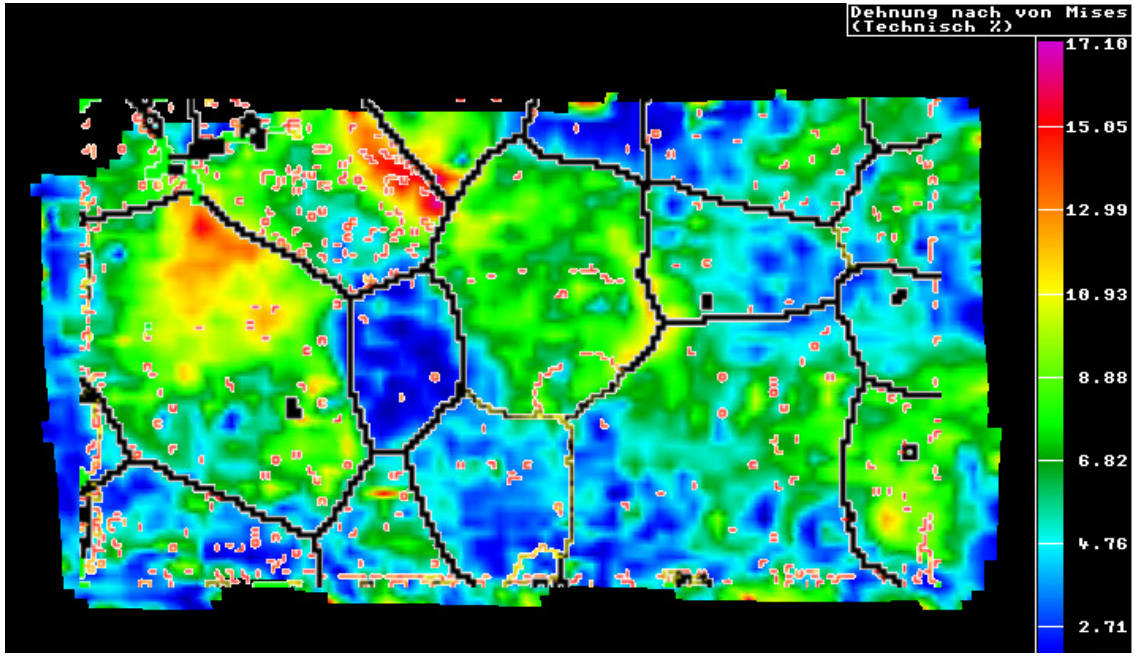
Simulation



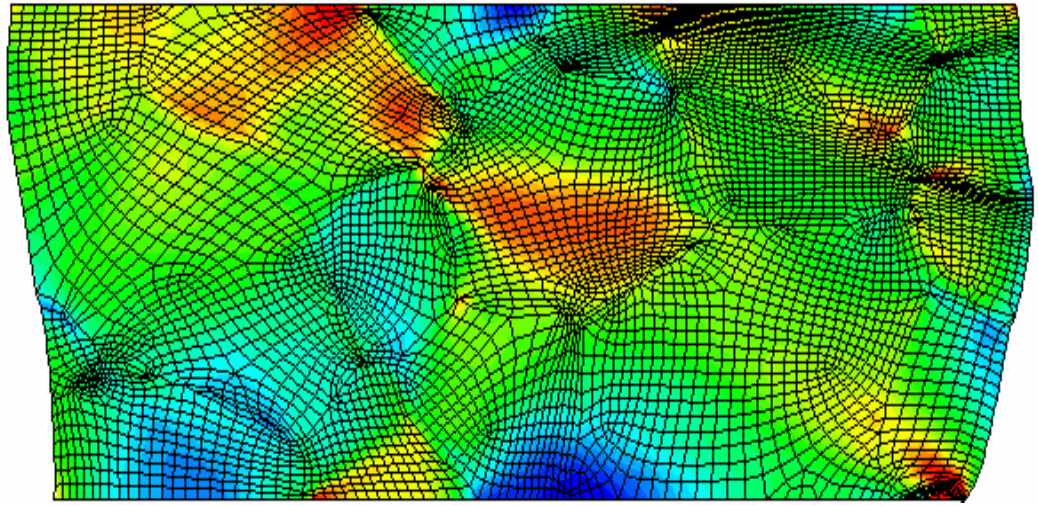


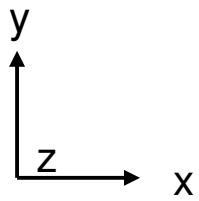
Kleine Skalen: Oligokristalle, Al, ebene Dehnung



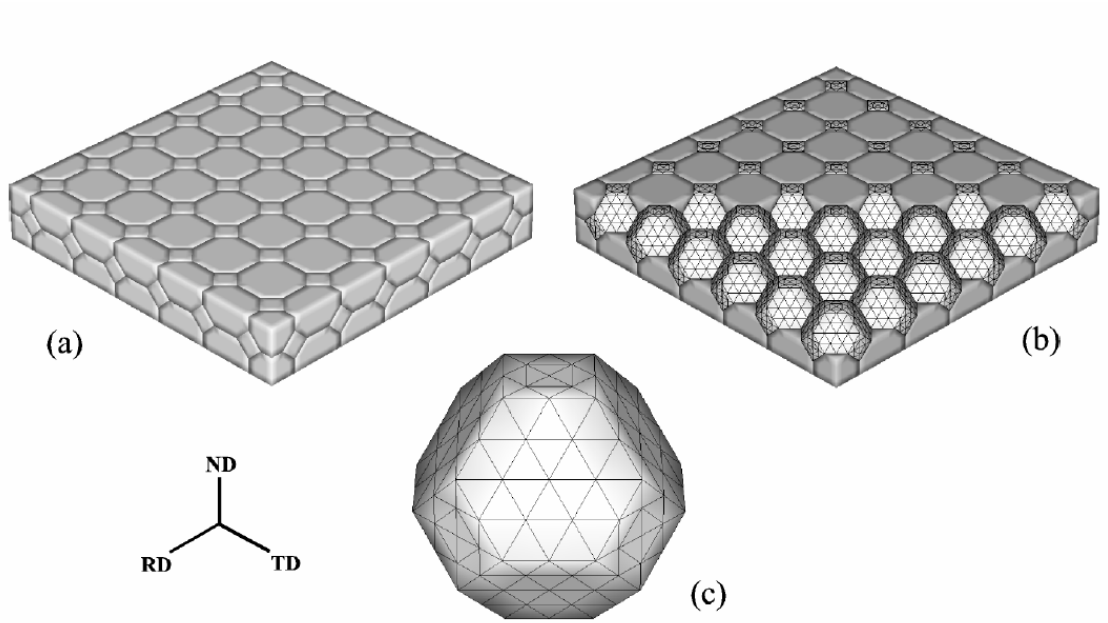


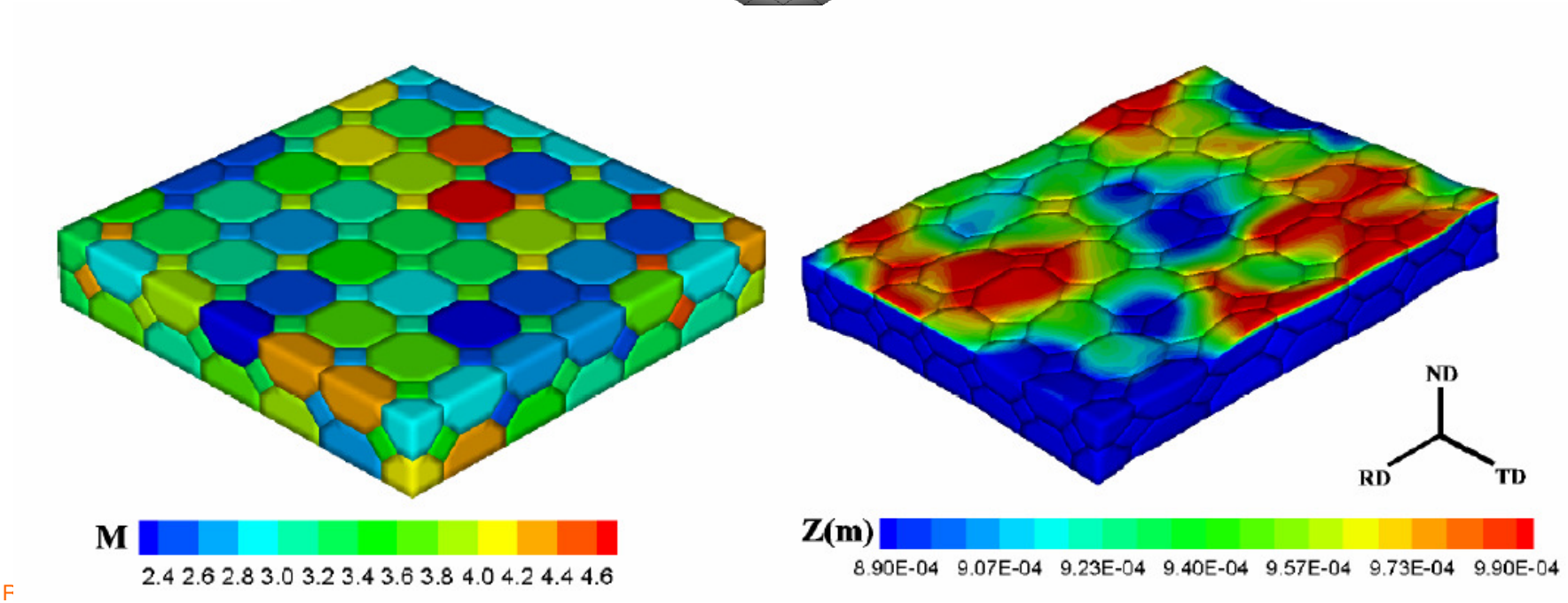
von-Mises strain



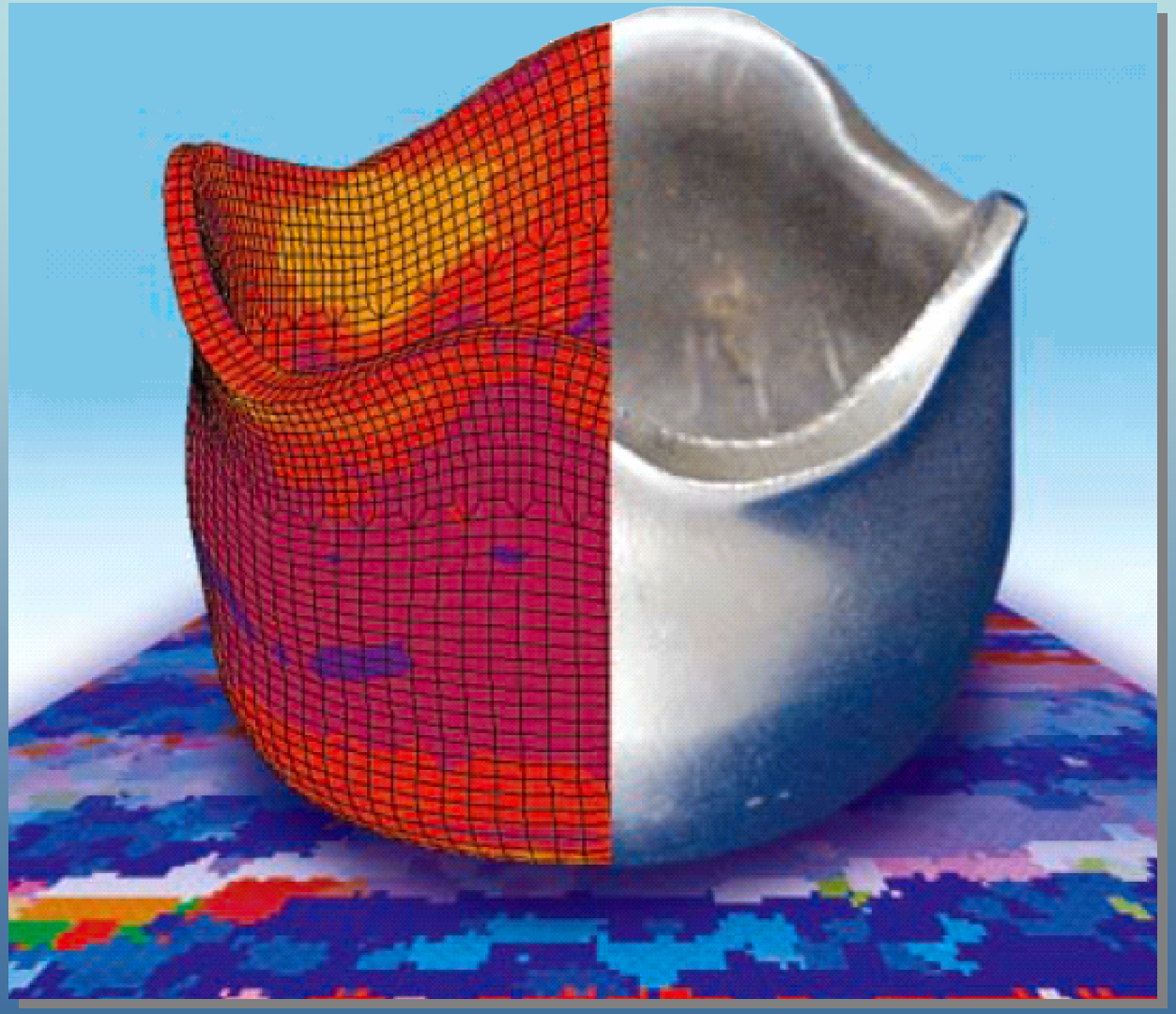


Vielkristallmechanik, große Skalen





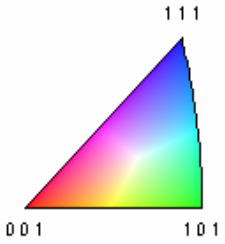
crystal plasticity FEM at large scales



TCCP-FEM: the texture component crystal plasticity FEM

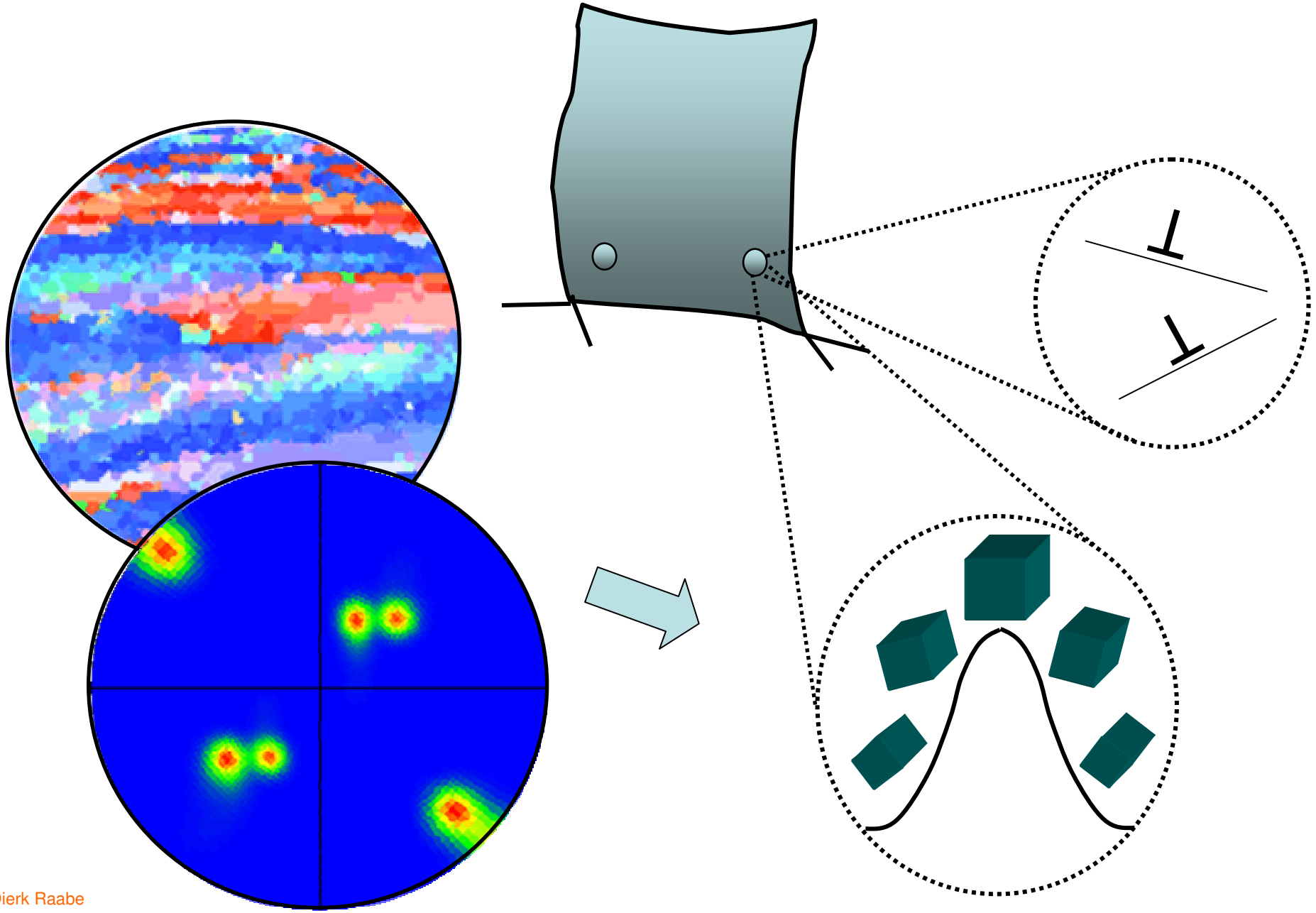
1-billion grain scale

a car contains more than 50 billion grains !



70.00 µm = 70 steps

components for mapping the start texture



Textur-Komponenten für Abbildung der Starttextur

$$f(g) = F + \sum_{c=1}^{C} w^c f^c(g) = \sum_{c=0}^{C} w^c f^c(g)$$

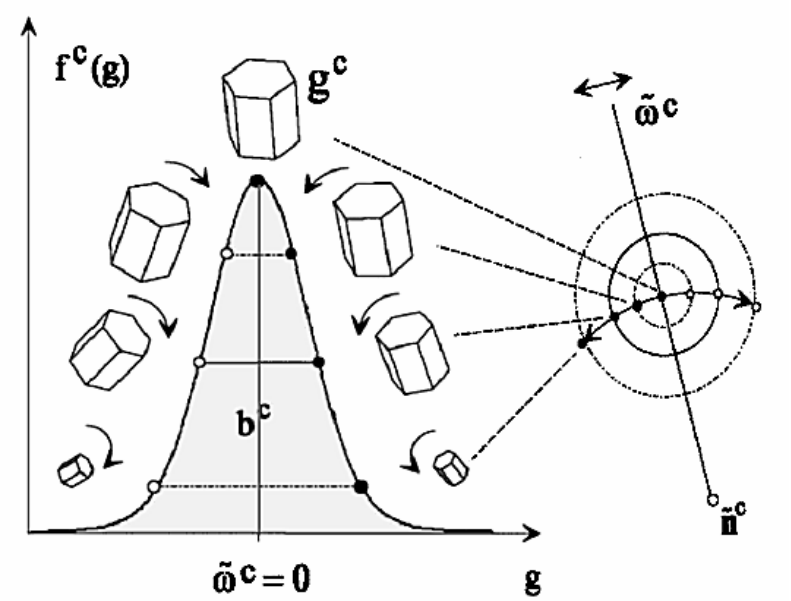
$$w^0 = F,\ f^0(g) = 1$$

g	orientation
$f(g)$	ODF
F	random-texture component
w^c	volume fraction of all crystals belonging to texture component c

Use texture components for mapping

$$\tilde{\omega}^c = \tilde{\omega}(g^c, g) \qquad f^c(g) = N^c \exp\left(S^c \cos\tilde{\omega}\right)$$

$$S^c = \frac{\ln 2}{1-\cos(b^c/2)} \quad \text{and} \quad N^c = \frac{1}{I_0(S^c) - I_1(S^c)}$$



$I_l(x)$ **generalized Bessel functions**

b^c **value is the halfwidth (mean diameter of a spherical component in orientation space)**

Lücke, Pospiech, Virnich, Jura: Acta metall. 29 (1980) p. 167

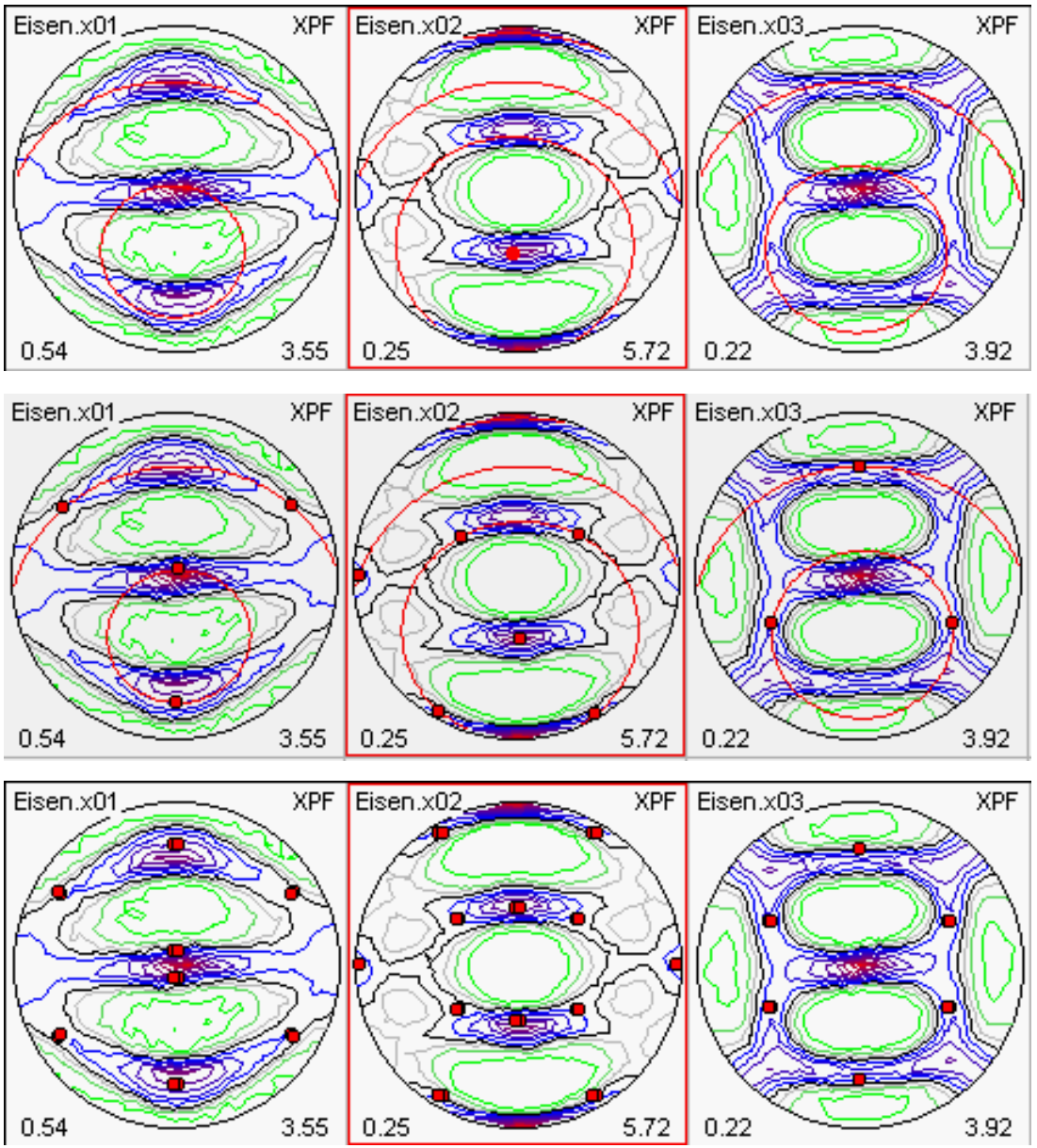
Helming, Schwarzer, Rauschenbach, Geier, Leiss, Wenk, Ullemeier, Heinitz: Z. Metallkd. 85 (1994) p. 545/554

Extract components and background from experiments

Sample reference

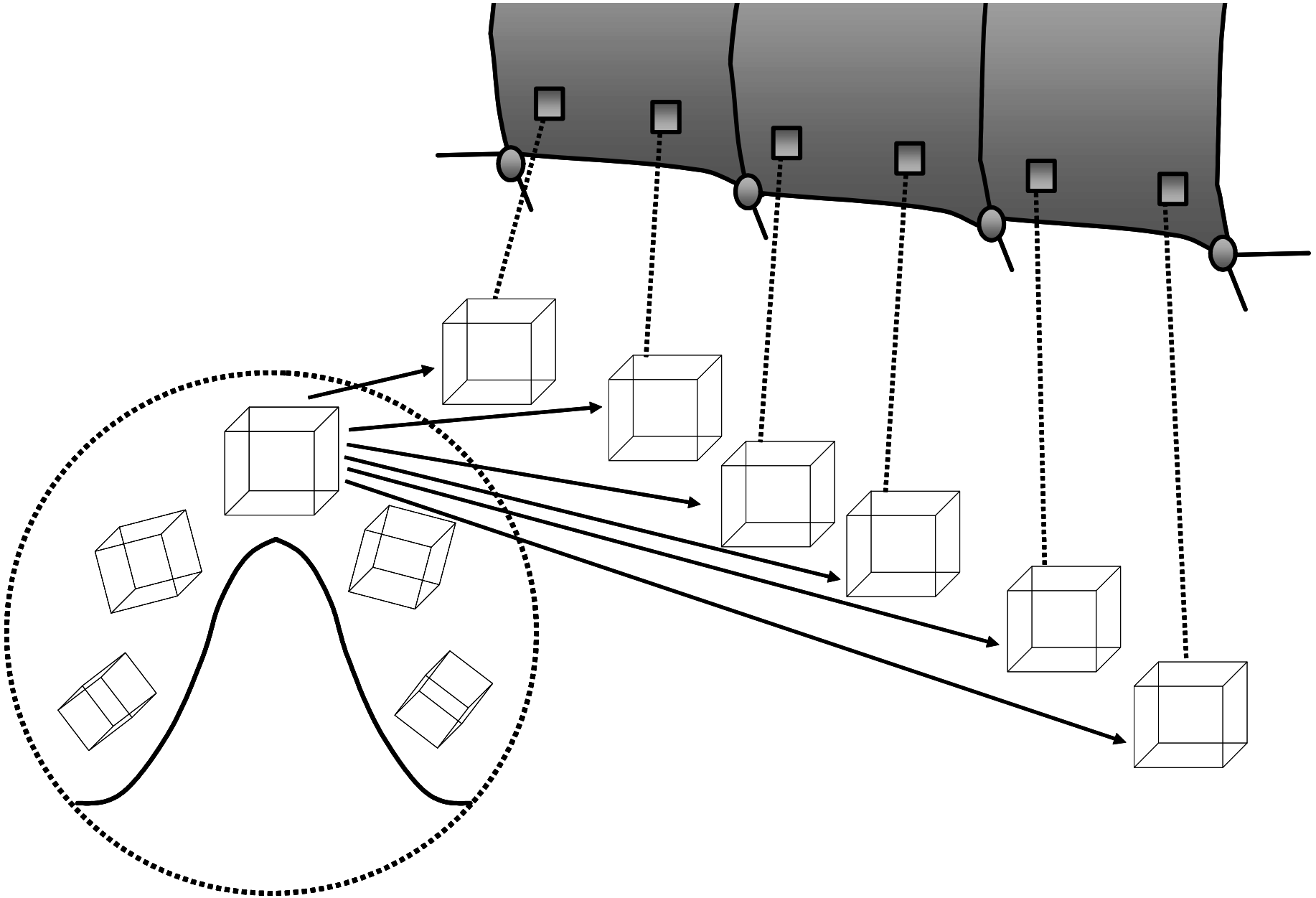
Main texture components

Symmetry

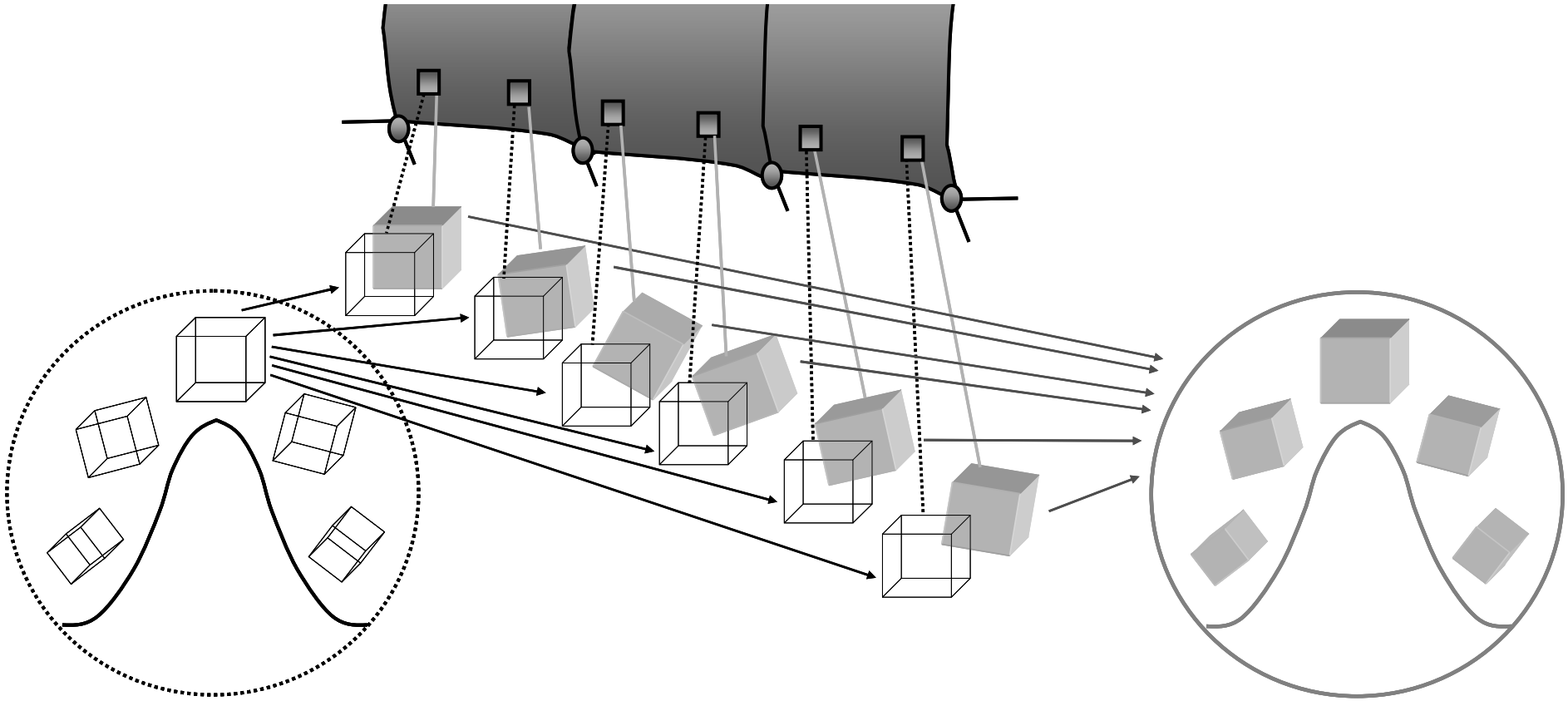


MulTex 2.0 K. Helming

components for mapping the start texture

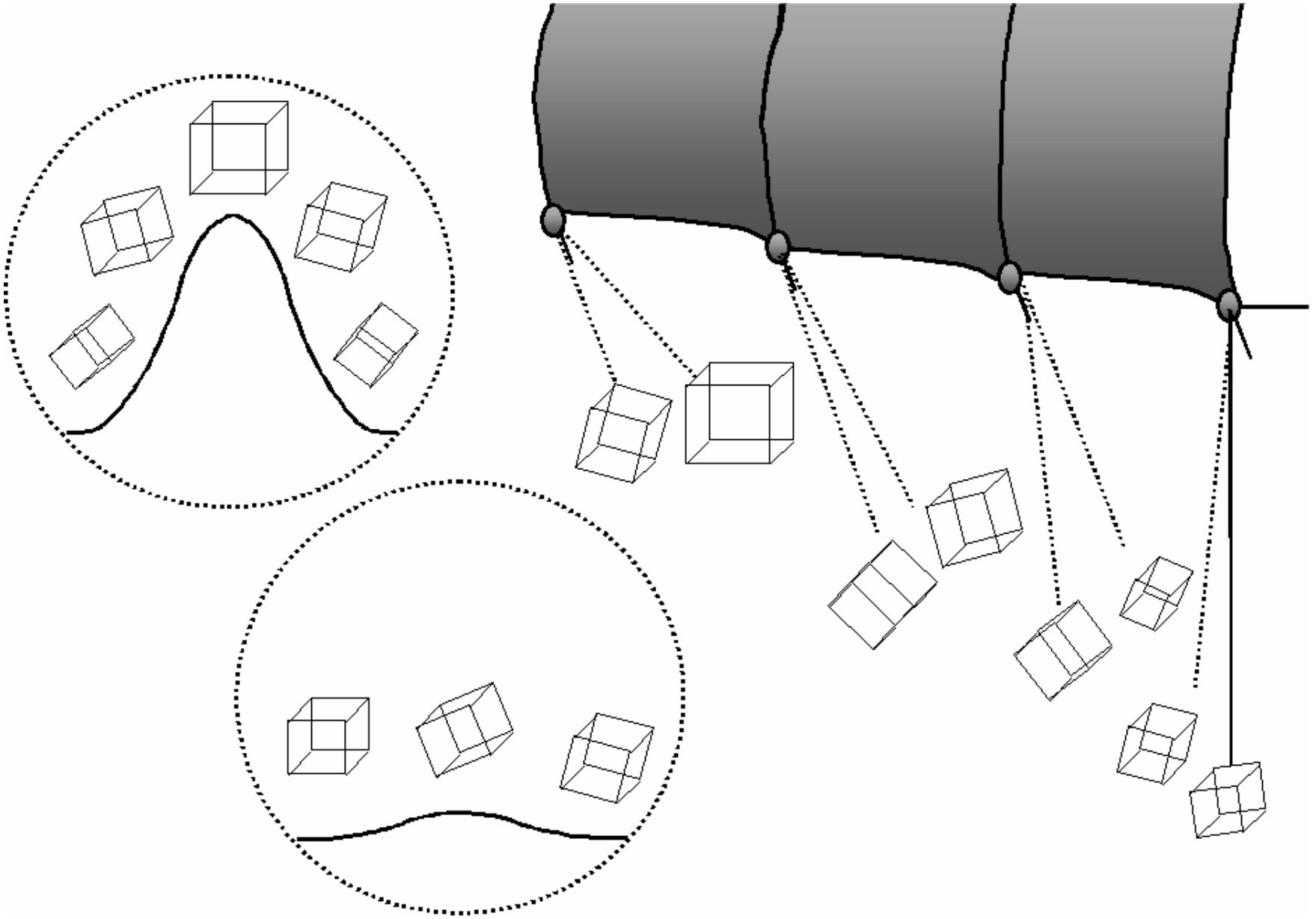


components for mapping the start texture

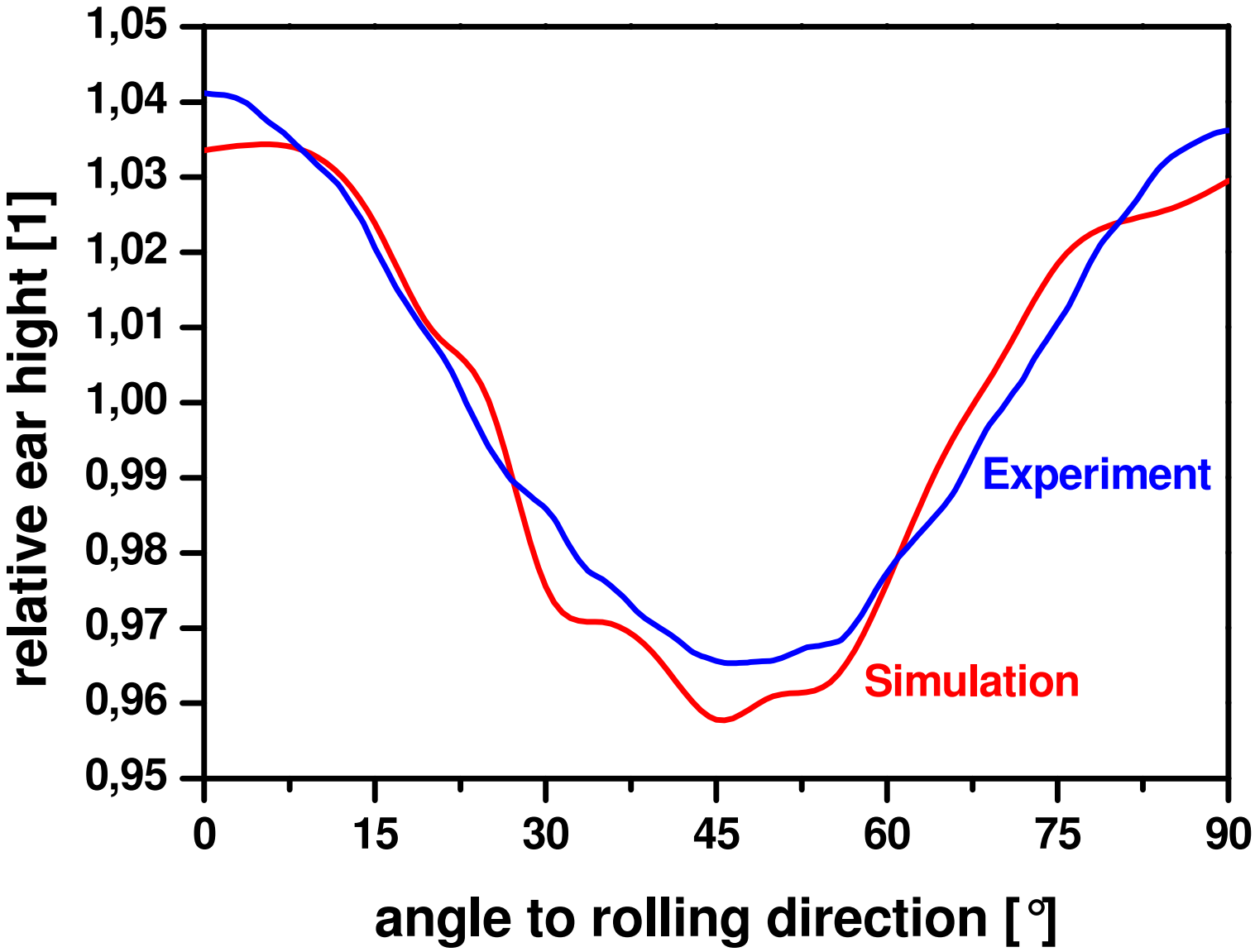


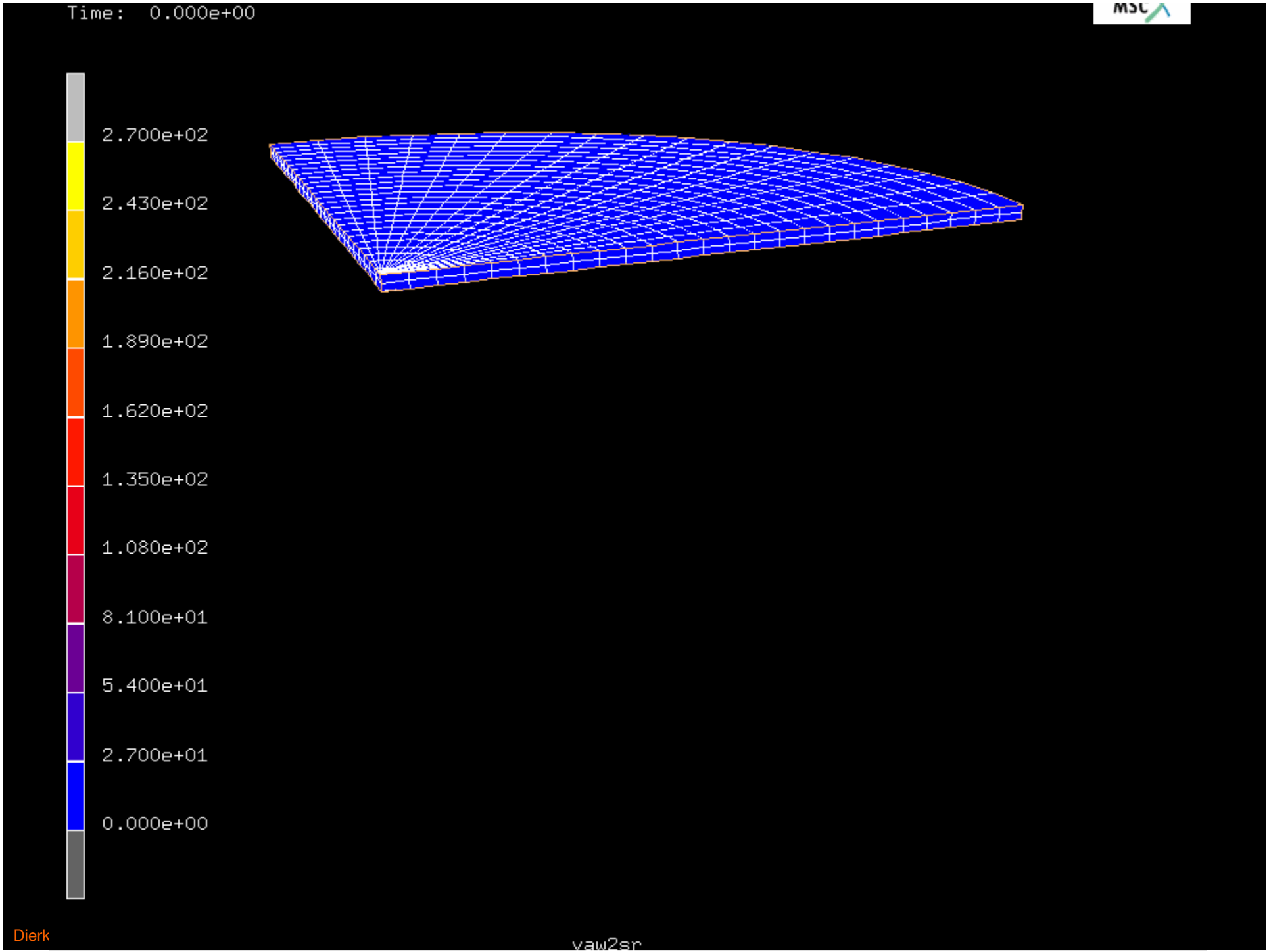
local stress homogenization of more than one component possible

local homogenization



Beispiel, Al, Vielkristall, Würfeltextur+"random"




Time: 0.000e+00
2.700e+02
2.430e+02
2.160e+02
1.890e+02
1.620e+02
1.350e+02
1.080e+02
8.100e+01
5.400e+01
2.700e+01
0.000e+00
Dierk
yaw2sr

Large scale anisotropy: TCCP-FEM

Procedure

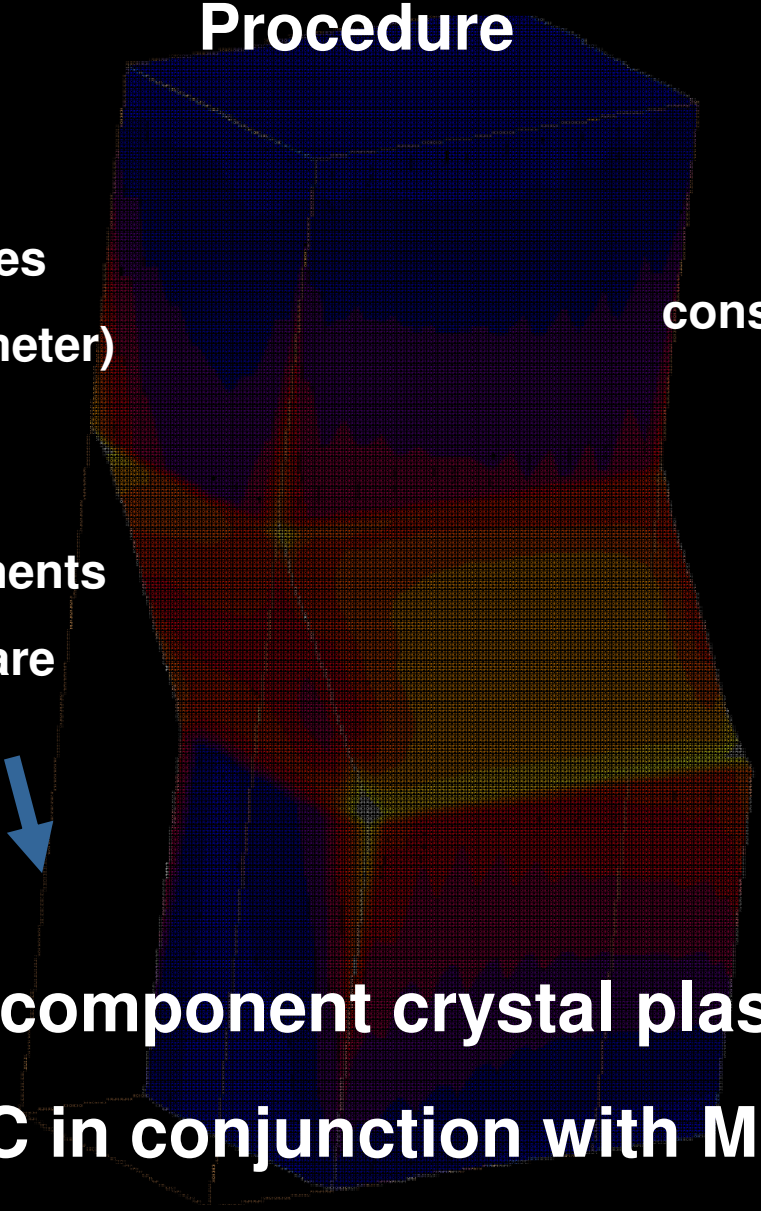
3 Pole figures

(Textur goniometer)

Texture components

(Multex Software - freeware)

constitutive parameter



texture component crystal plasticity FEM

(ABQ or MARC in conjunction with MPI - Subroutines)

The team

F. Roters (MPI)	CP-FEM
A. Ma (MPI)	CP-FEM
S. Zaefferer (MPI)	experimental

DFG, MPG