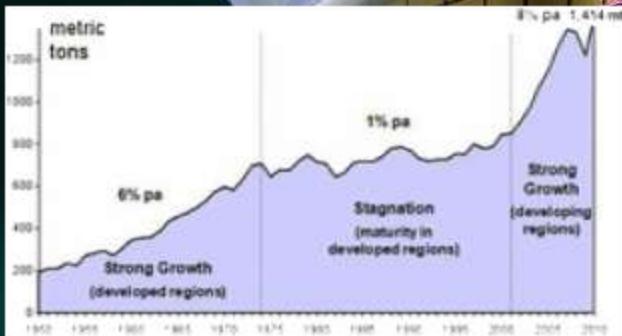


Nanostructuring 1 Billion Tons: Combining Rapid Alloy Prototyping, Multiscale Models, and Characterization for Advanced Manufacturing

D. Raabe, H. Springer, P. Eisenlohr, C. Tasan, I. Gutierrez , P. Choi, F. Roters, S. Zaefferer, N. Koyama, R. Kirchheim, Y. Li, J. Neugebauer

Max-Planck Institut für Eisenforschung
Düsseldorf, Germany





Complex Alloys occupy key roles
(energy, transportation, health, safety, infrastructure)

Materials-related industries account for 46% of all EU manufacturing value
and 11% of its domestic product

3.5 billion € per day in the EU

World Trade Organisation

Mission: Integrate Models, Experiments, Properties, and Processing for
Bringing Nanostructured Steels into Manufacturing Practise

Images: courtesy Porsche

Maturation of Advanced High Strength Auto Steels

What's new ?



Processing

Bulk Combinatorial Synthesis

Combinatorial Thermomechanical Treatment

Combinatorial Welding

High Throughput Thin Film Synthesis

Thin Strip Casting

.....

Structure

TEM Tomography

Atom Probe Tomography

Electron Channeling Contrast Imaging

3D EBSD

.....

Properties

Nanomechanics

Cluster Mechanics by DIC

In-Situ Testing

Testing under Hydrogen

High-throughput Tensile Testing

.....

Simulation

Ab Initio

Dislocation Dynamics

Cluster Homogenization

Crystal Plasticity FEM / Spectral Solver

Virtual Forming Lab

.....



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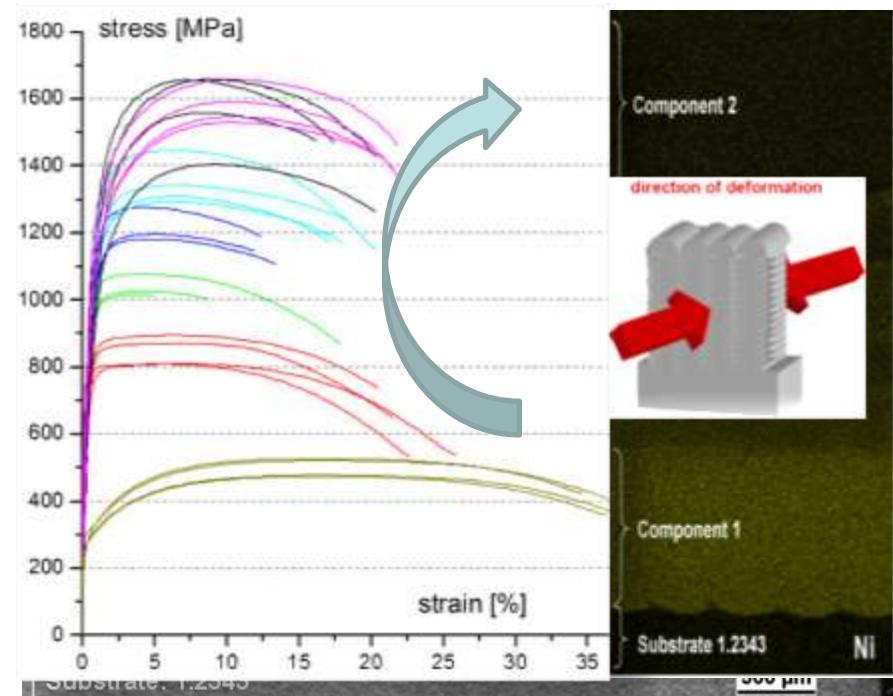
Cluster Homogenization

Crystal Plasticity FEM / Spectral Solver

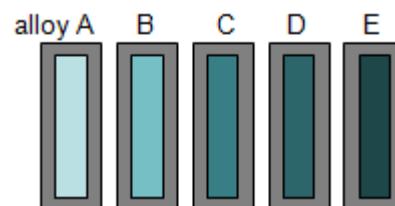
Virtual Forming Lab

Laser-Plasma-Synthesis

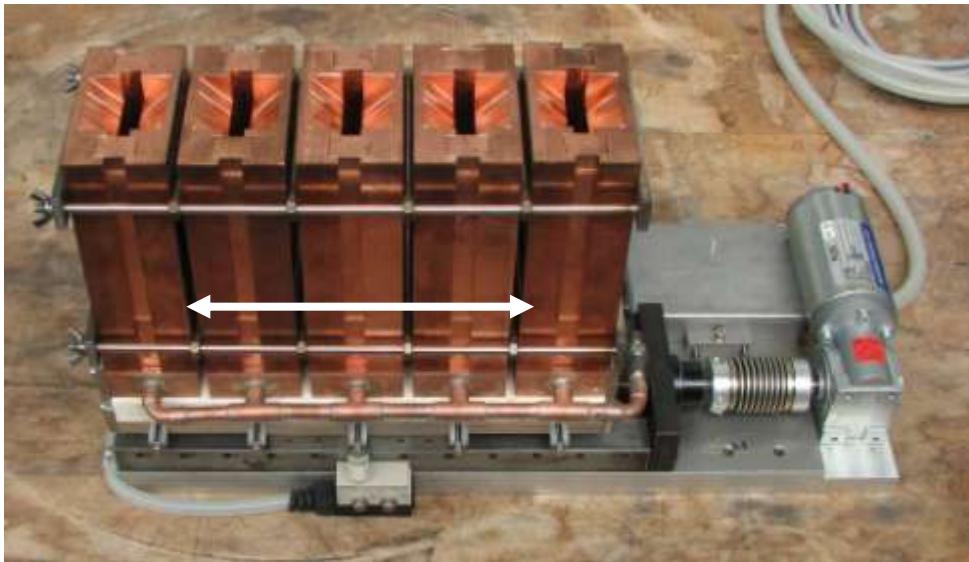
Combinatorial strip casting



RAP: Steel-plant-in-a-box

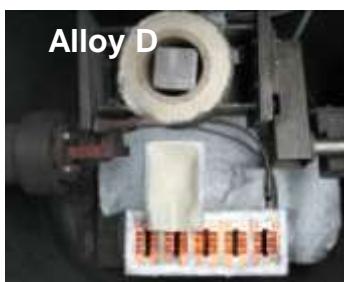
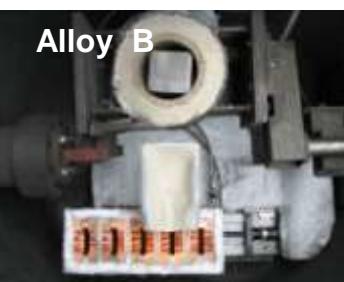


Rapid alloy prototyping: multiple ingot casting and in-line TMT



5 Cu-moulds, 60 kW vacuum induction furnace (vacuum, Ar, air)

10 x 50 x 150 mm³



Alloys [wt.%] "TRIPLEX steels"

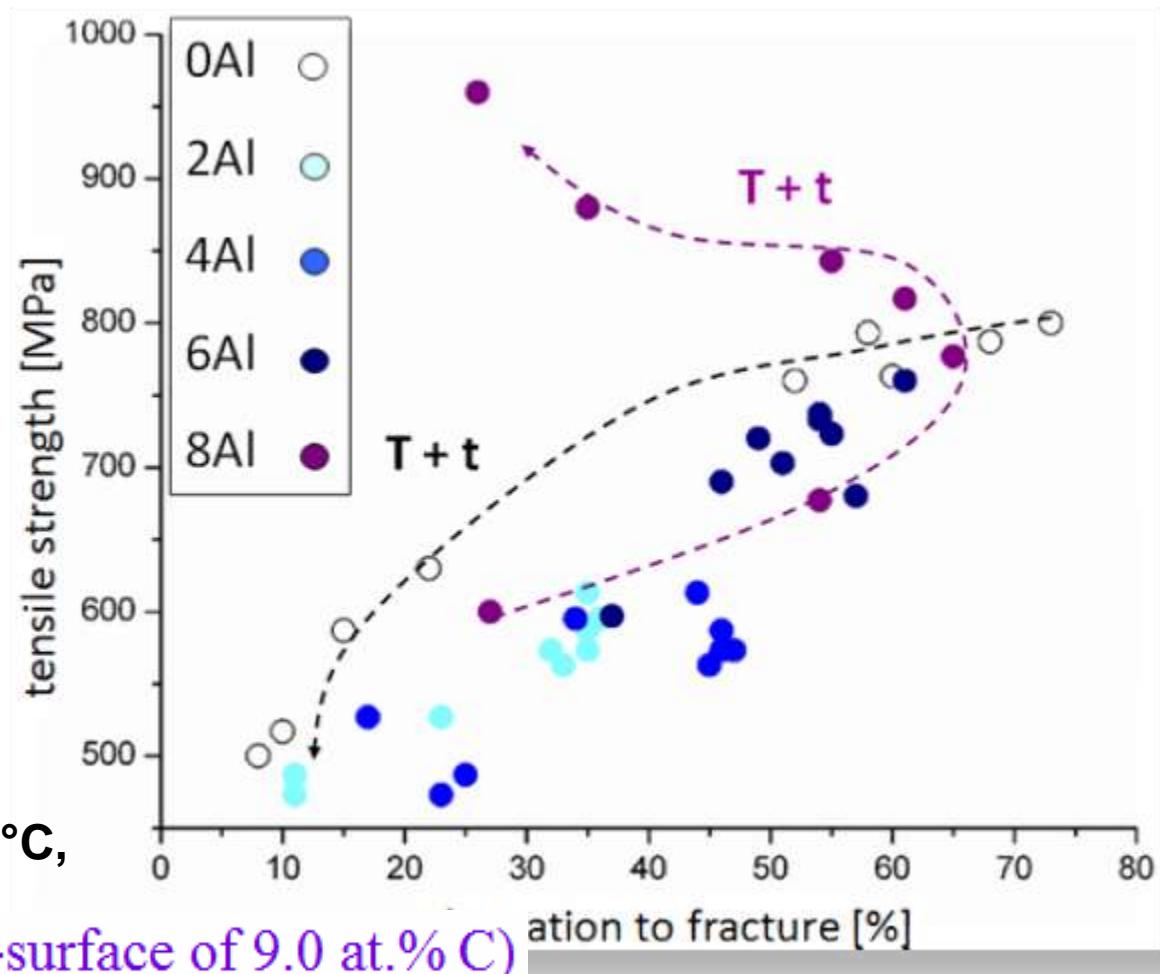
Fe – 30Mn – 1.2C

Fe – 30Mn – 1.2C – 2Al

Fe – 30Mn – 1.2C – 4Al

Fe – 30Mn – 1.2C – 6Al

Fe – 30Mn – 1.2C – 8Al



TMT (matrix) → 45 states

Hot rolling 1100°C, WQ

Homogenise 1100°C, WQ

Tempering 450, 500, 550, 600°C,

T: 1h T κ -carbide (iso-surface of 9.0 at.% C)

Alloys [wt.%] "TRIP+

Fe – 30Mn – 1.2C

Fe – 30Mn – 1.2C – 2Mn

Fe – 30Mn – 1.2C – 2Mn

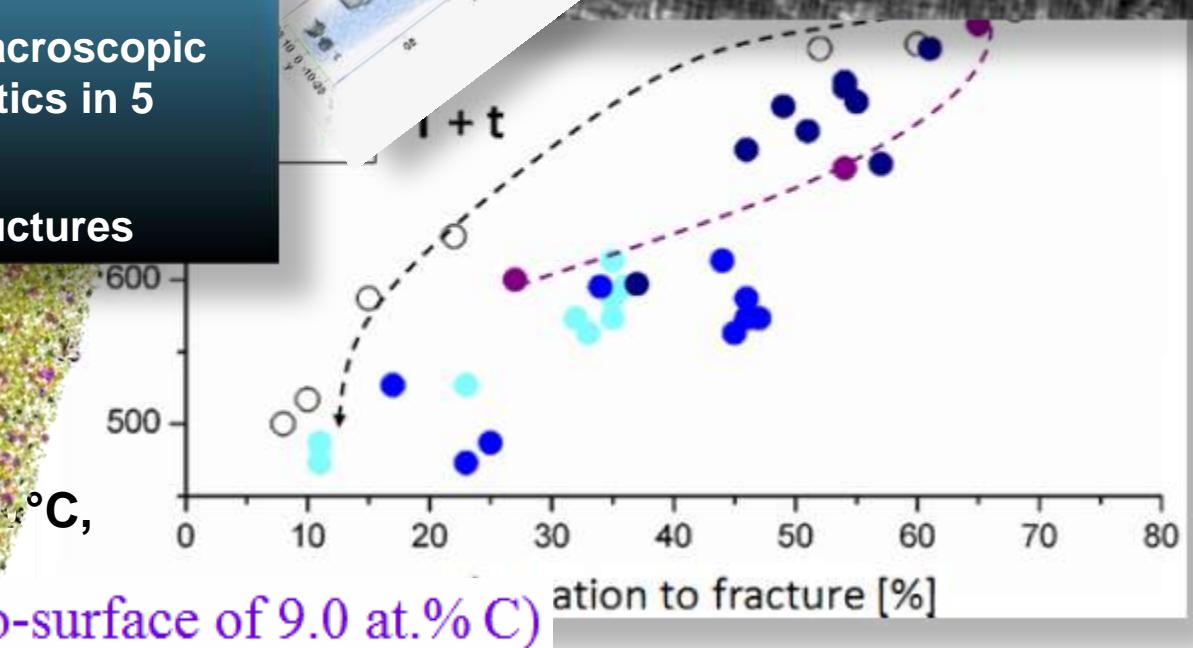
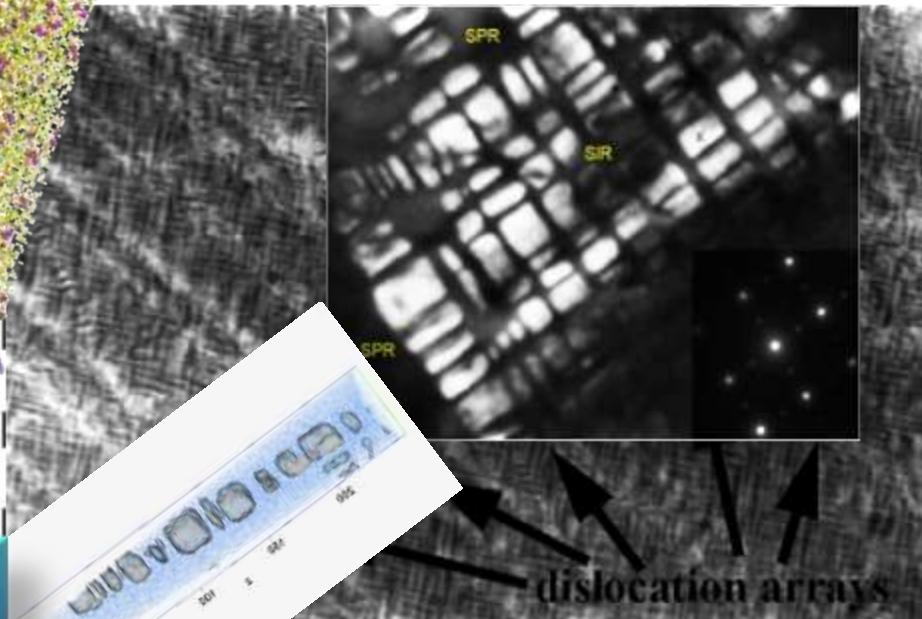
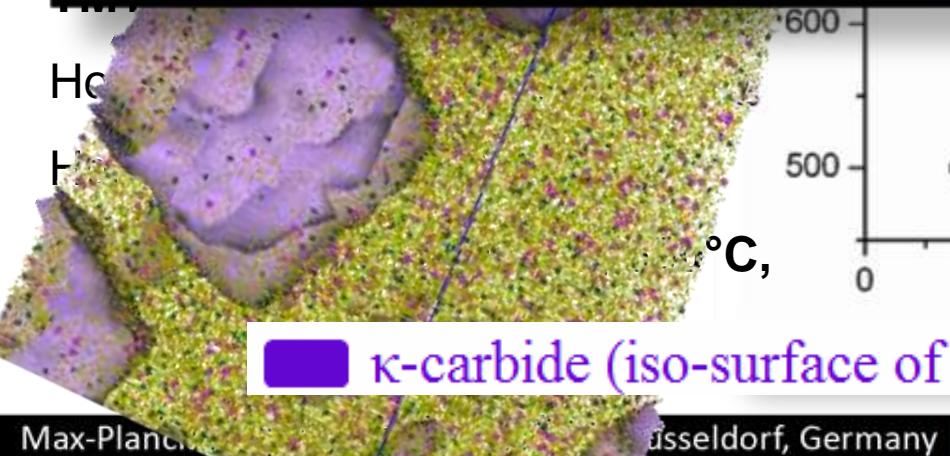
Fe – 30Mn – 1.2C

Fe – 30Mn – 1.2C

Message:

Probe 45 material states at macroscopic scale and with good statistics in 5 days (instead 6 weeks)

Watch out for unexpected structures



■ κ -carbide (iso-surface of 9.0 at.% C)



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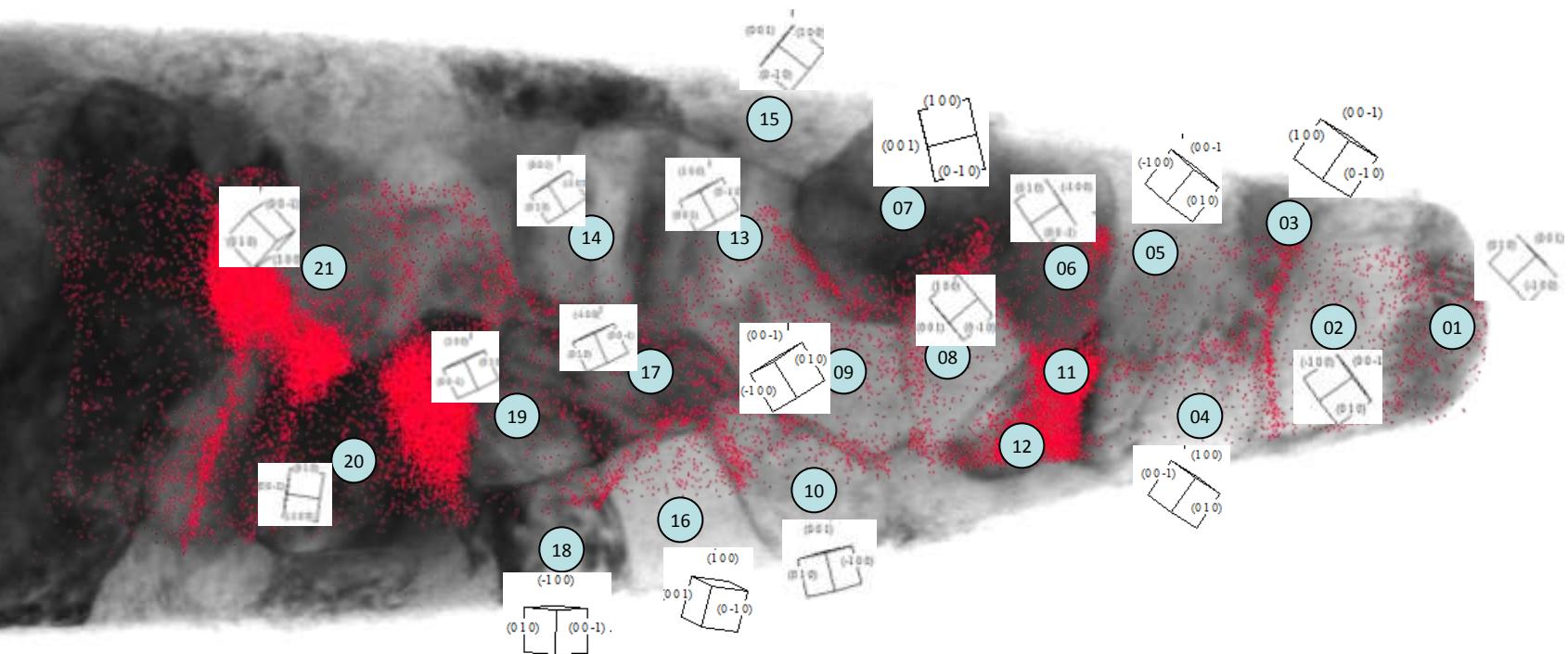
Dislocation Dynamics

Cluster Homogenization

Crystal Plasticity FEM / Spectral Solver

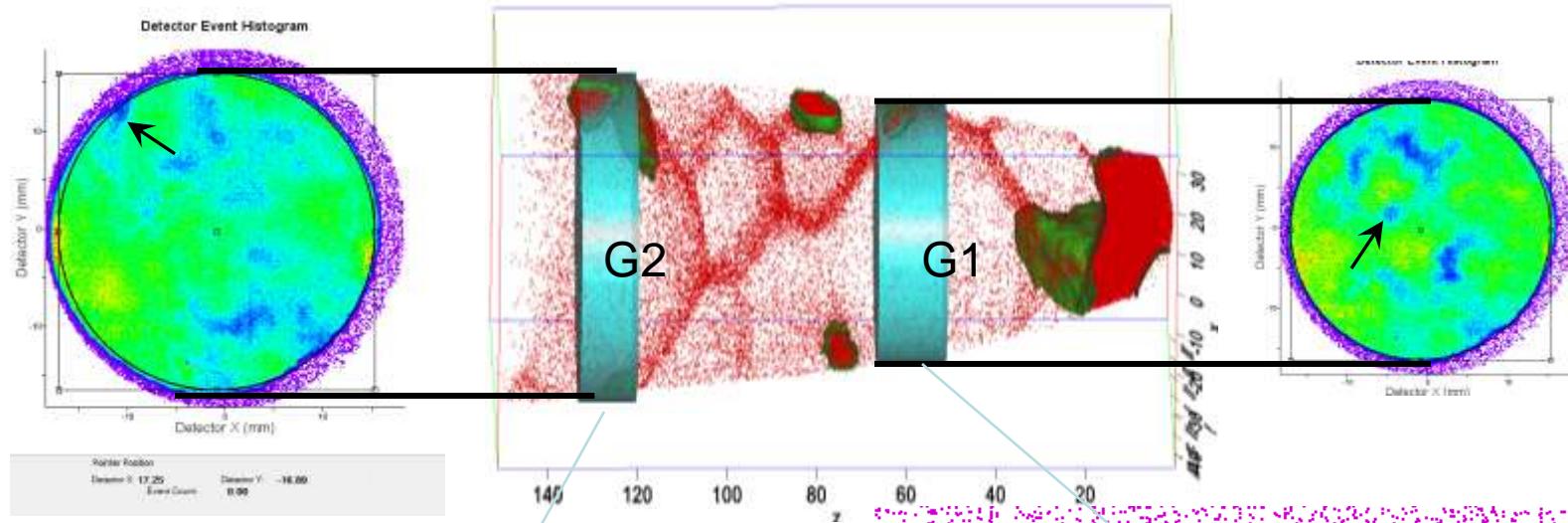
Virtual Forming Lab

Structure and composition at grain boundaries: Fe-C



•C

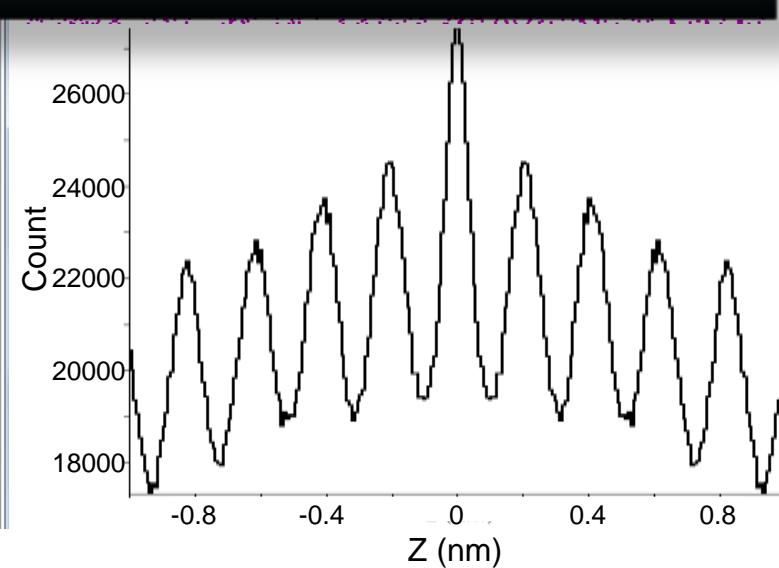
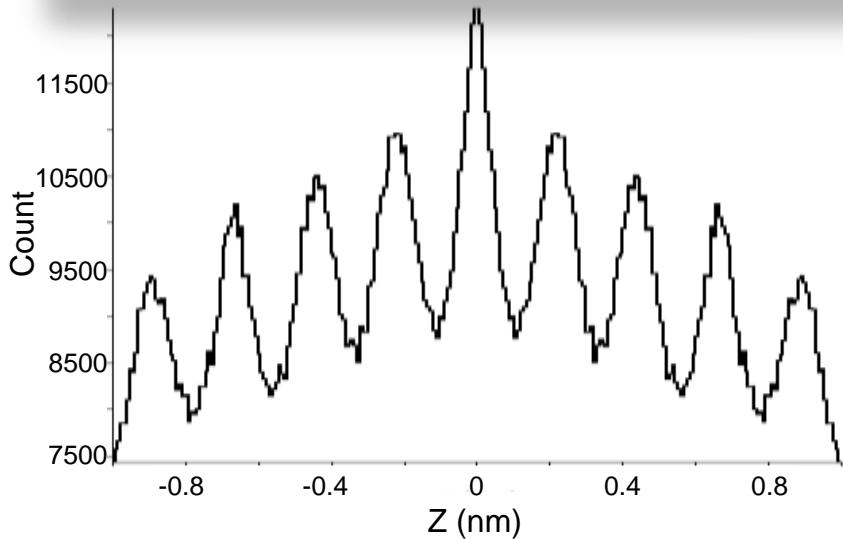
10 nm



Grain2 Grain1

Message:

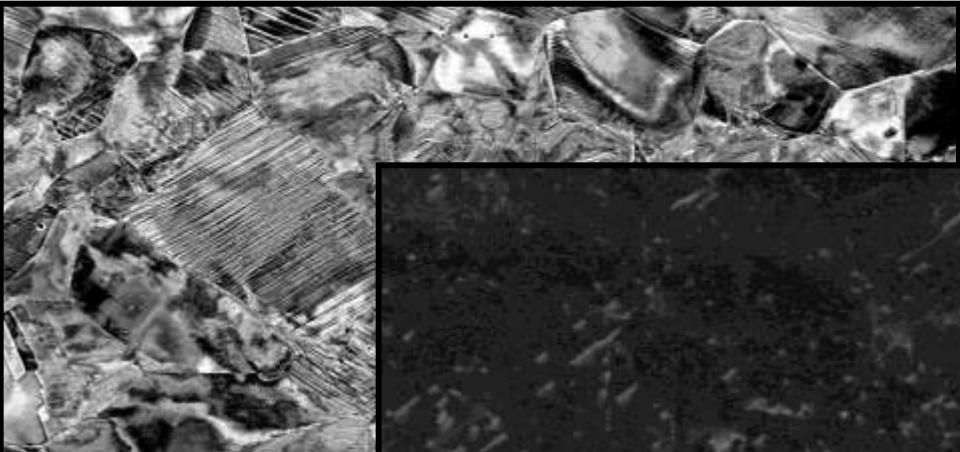
Understand structure and chemistry of interfaces at near-atomic scale: mean free path, damage, toughness, segregation, decohesion, corrosion



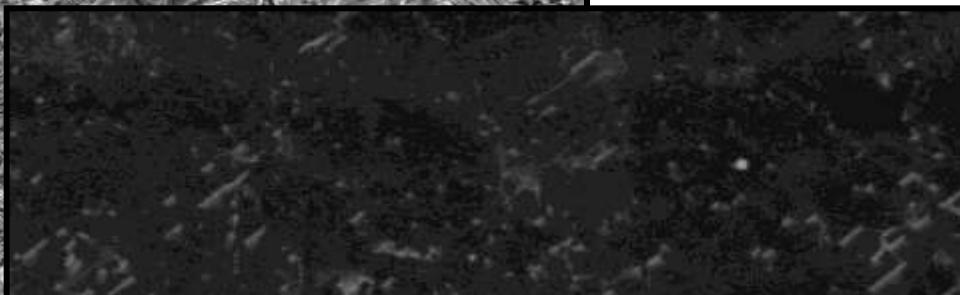


200 nm

Mag = 100.00 KX WD = 6 mm EHT = 10.00 kV Signal A = BSD Date :19 Jul 2023



large area defect observations



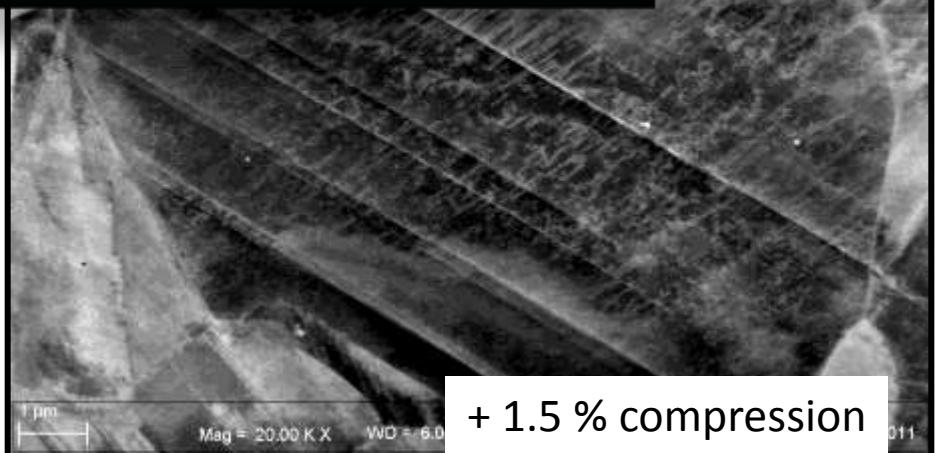
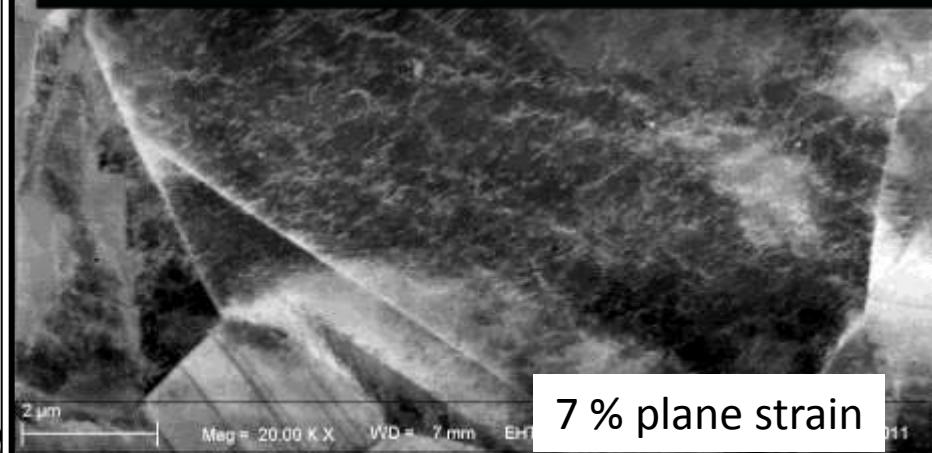
dislocation density
determination
 $\rho : 1.4 \dots 2 \times 10^{13} \text{ m}^{-2}$

Message:

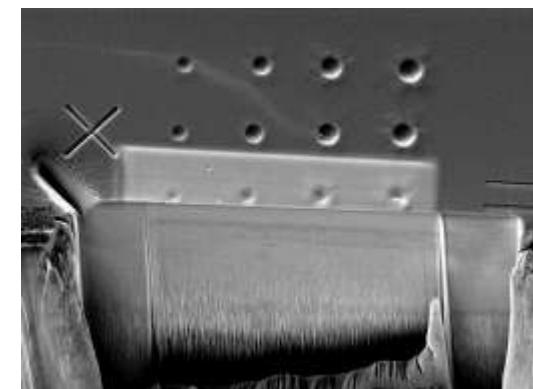
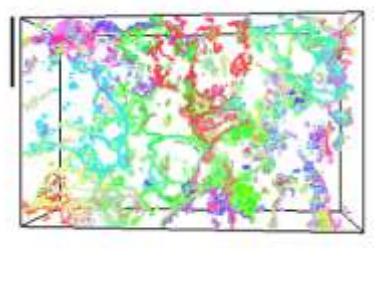
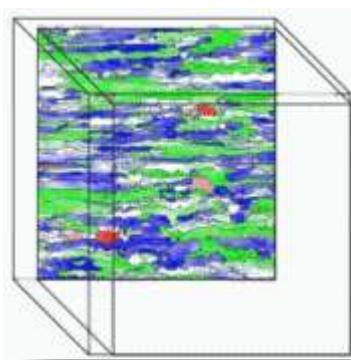
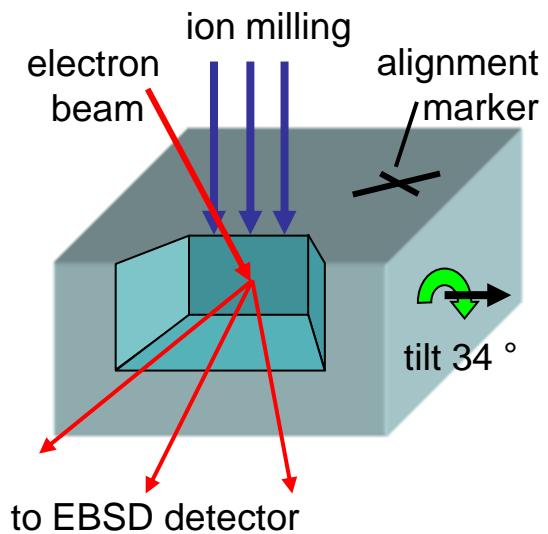
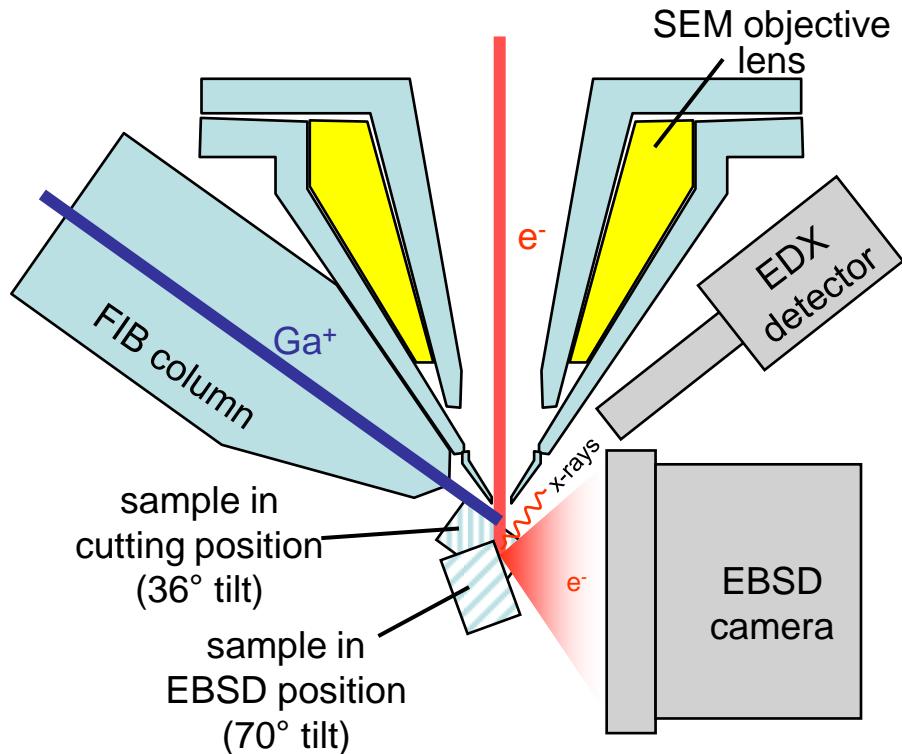
Get constitutive parameters (dislocation density, twin spacing, gradients)
directly from SEM at wide field of view

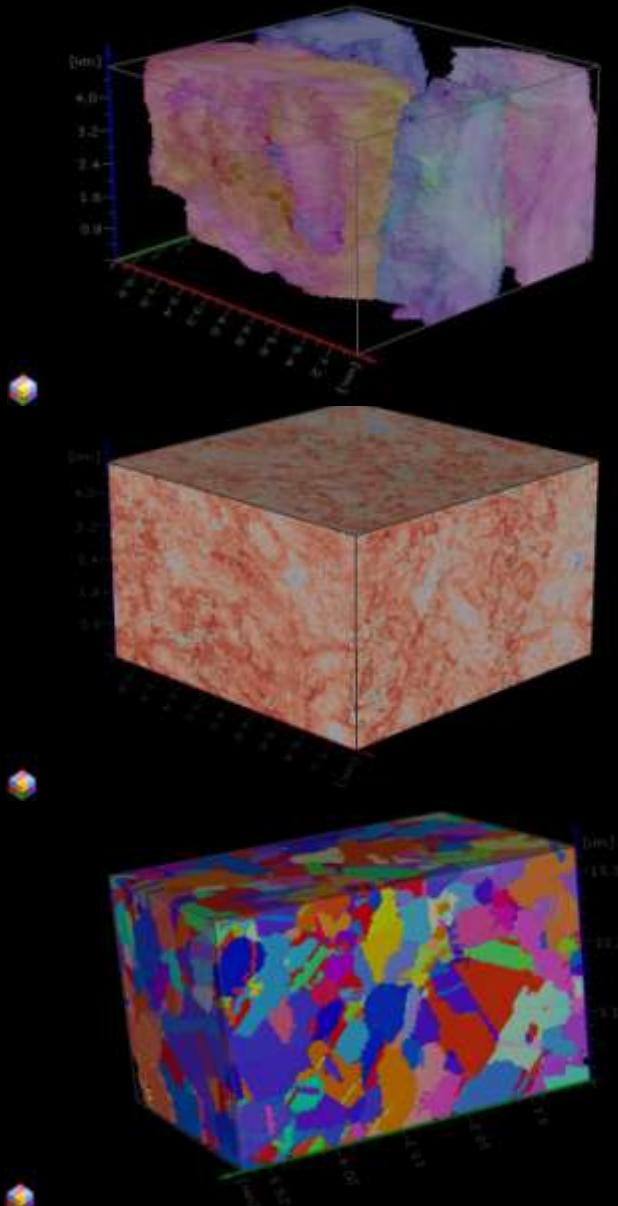
few days (instead of multiple months)

observations



Principle of serial sectioning & orientation microscopy: 3D EBSD





General features:

- Post processing only
- All Laue groups, quaternion based
- Generic structure wizard
- Filtering
- Geometry editor
- Slice re-alignment
- Data set import filters

Voxel based analysis:

- GND analysis with slip system resolution
- General orientation based analysis

Interface mesh based analysis

- 5-Parameter GBCD
- Local boundary analysis

Simulation tools / links

- Parallel Monte Carlo Potts model
- Full field elastic FFT model (R. Lebensohn)

Misorientation: $60^\circ<111> \pm 5^\circ<\dots>$

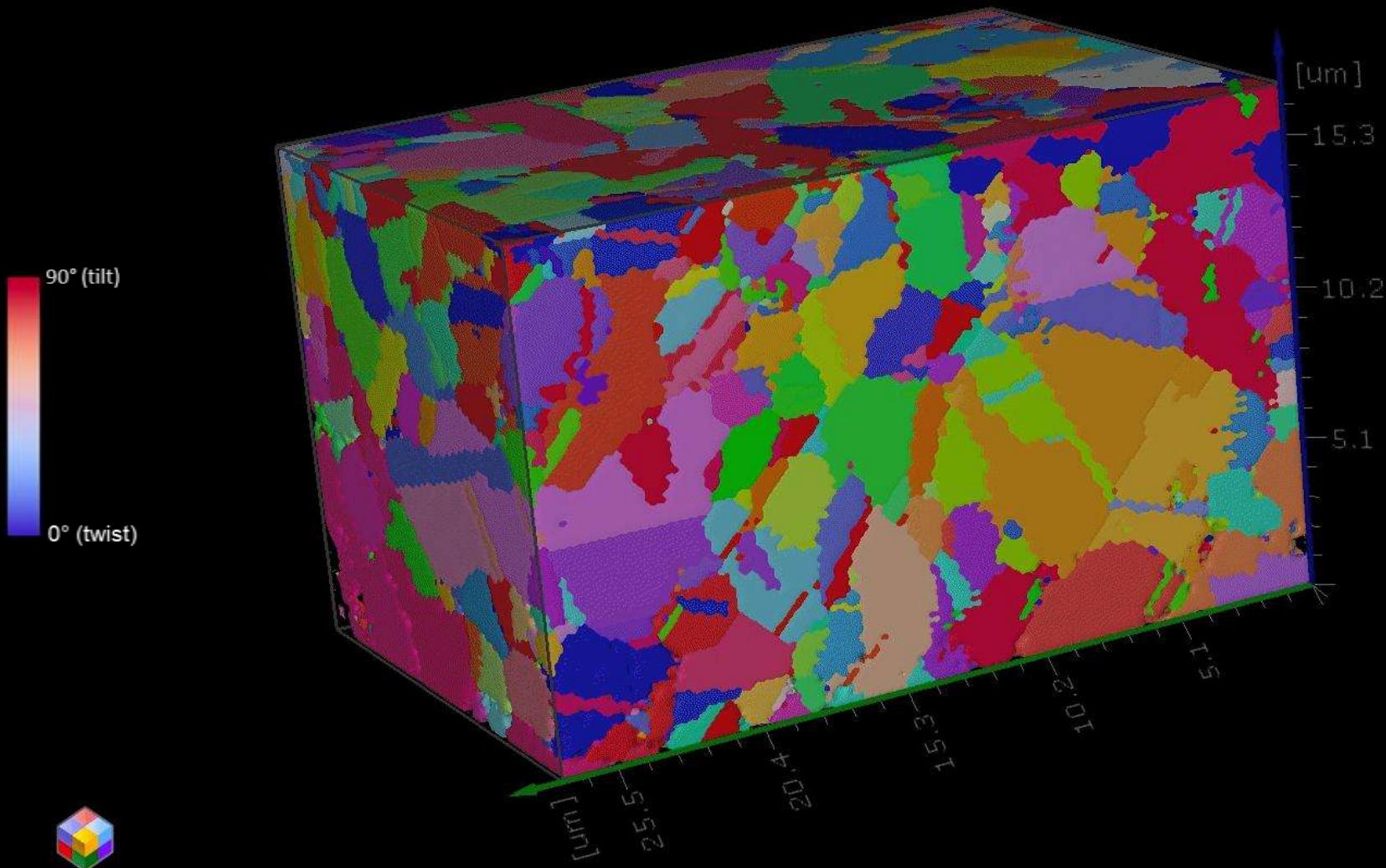
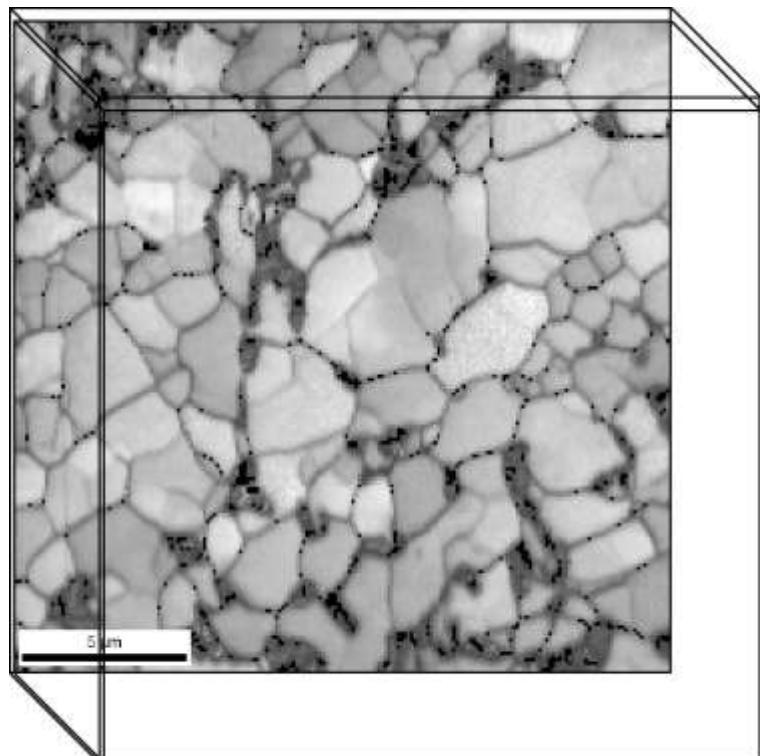
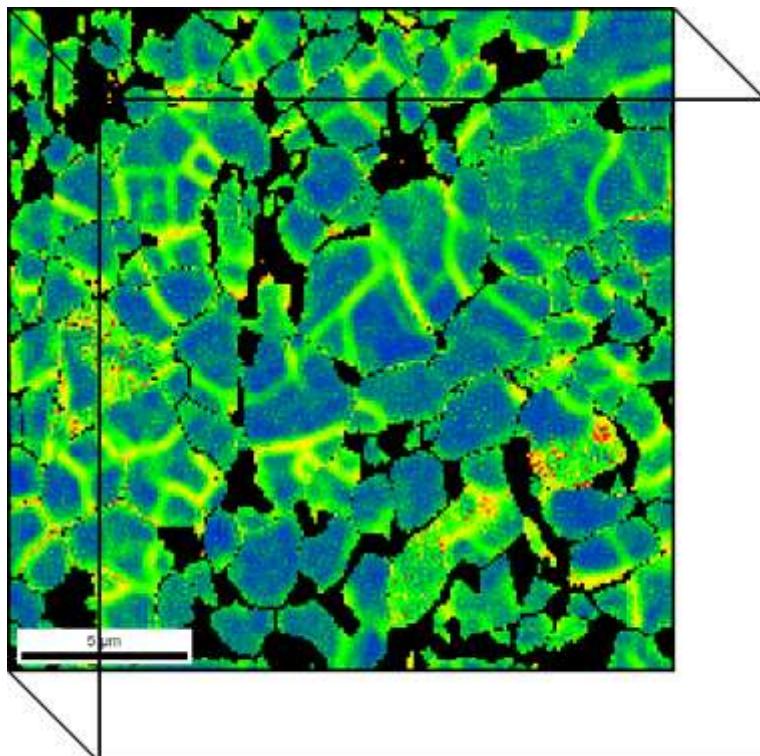
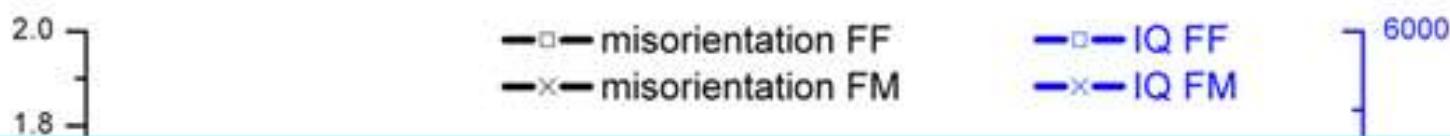


Image Quality



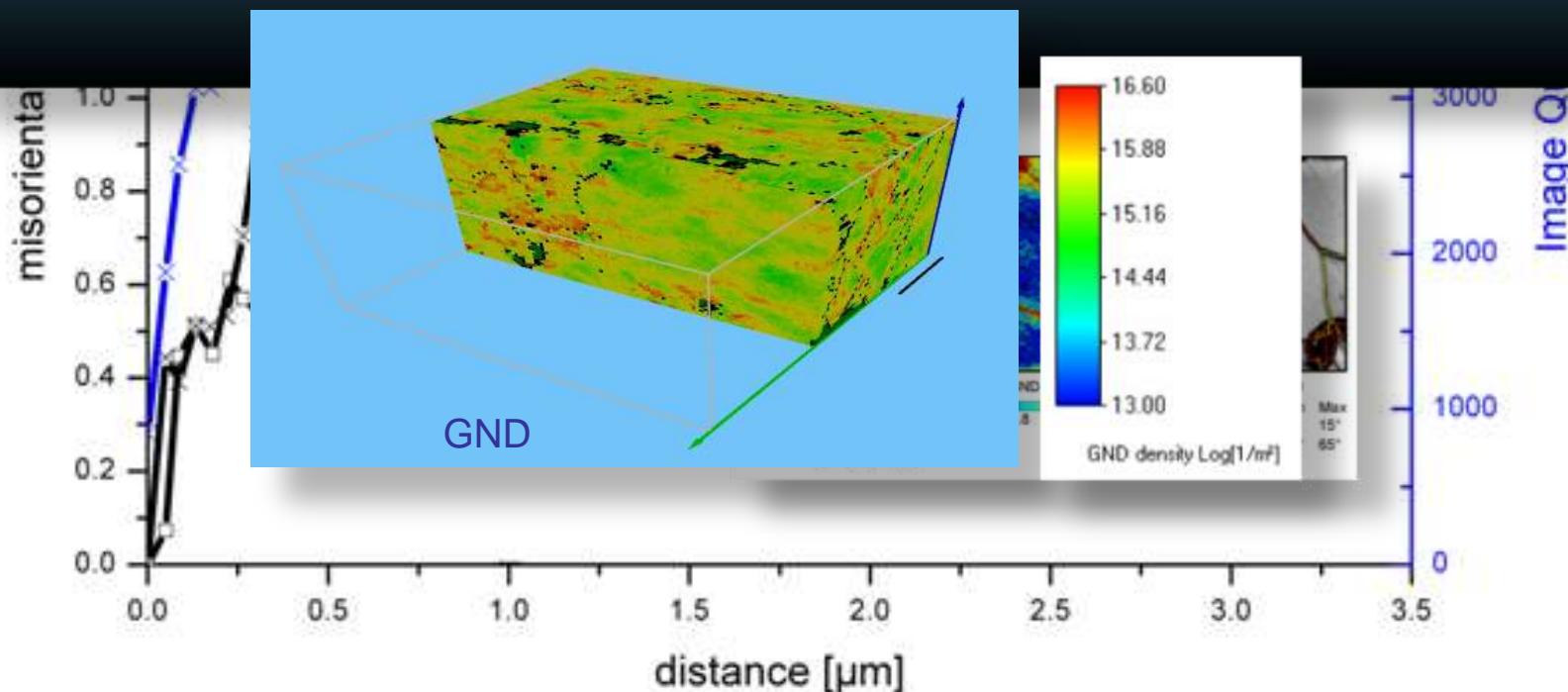
Kernel Average Misorientation
(martensite highlighted in black)



**Message:**

3D EBSD: phases, GND, gradients, texture, internal stresses in 3D for interface mechanics

integrate directly (meshless) into crystal plasticity FFT RVE solvers





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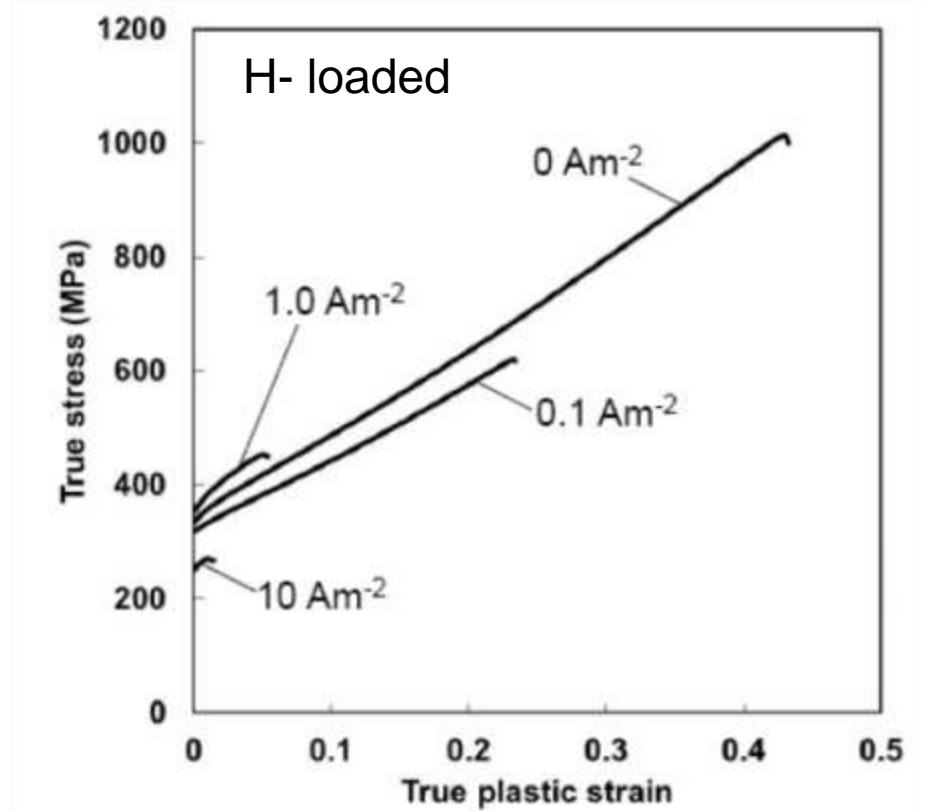
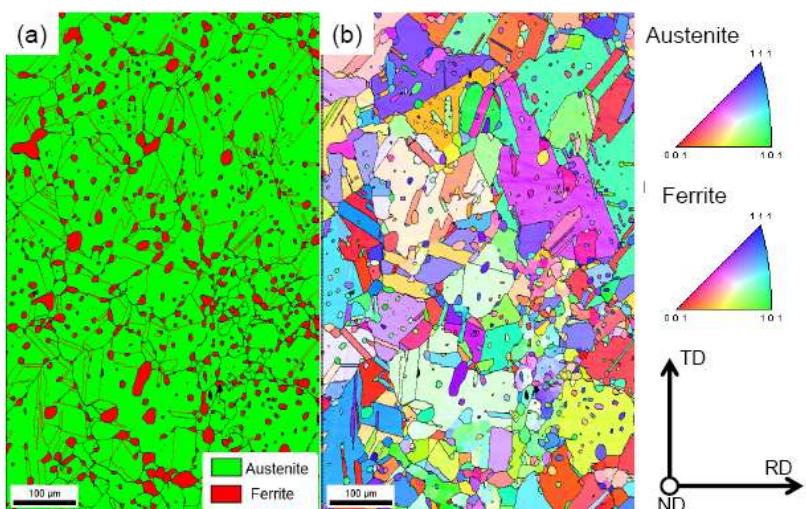
Dislocation Dynamics

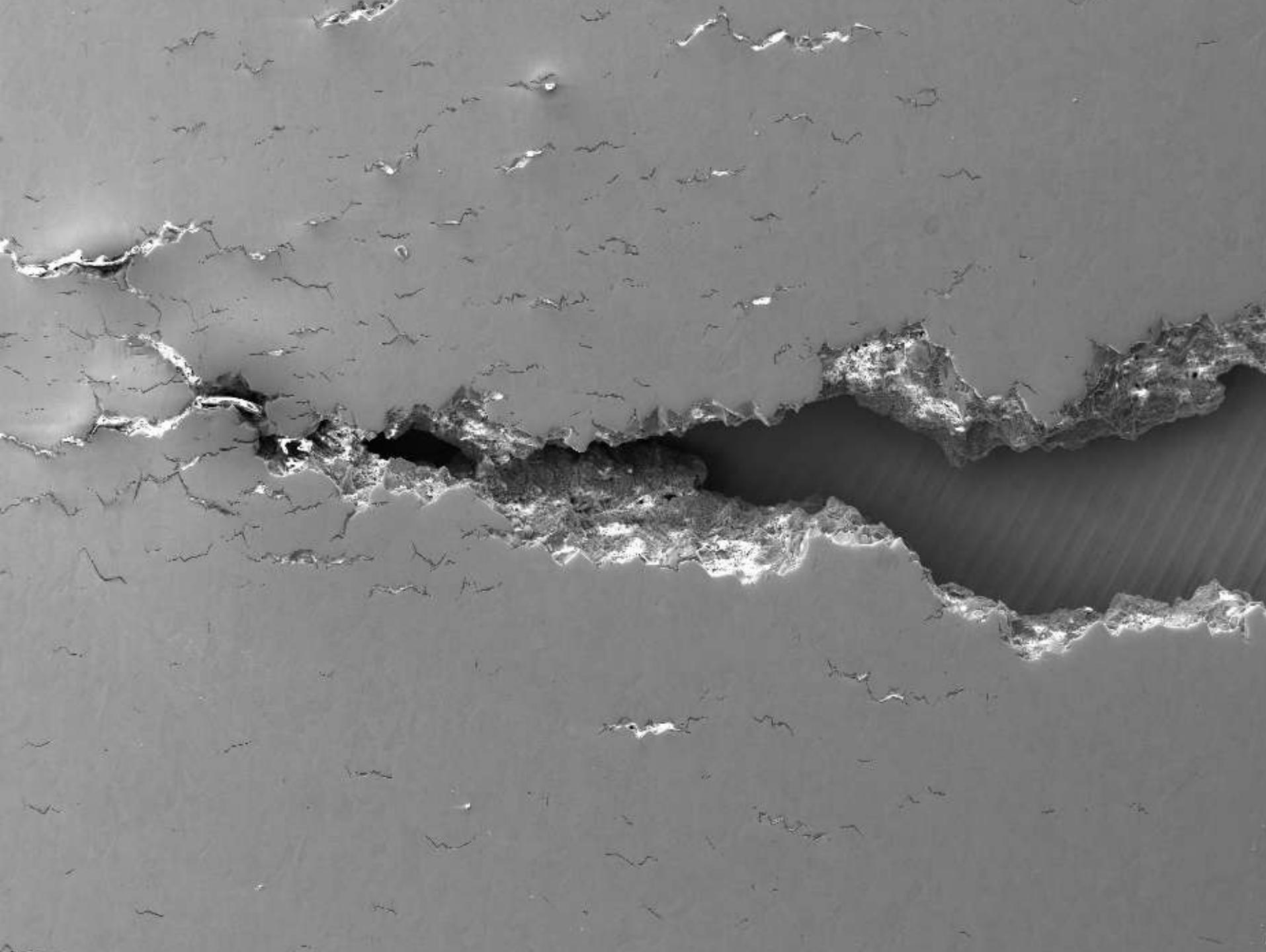
Cluster Homogenization

Crystal Plasticity FEM / Spectral Solver

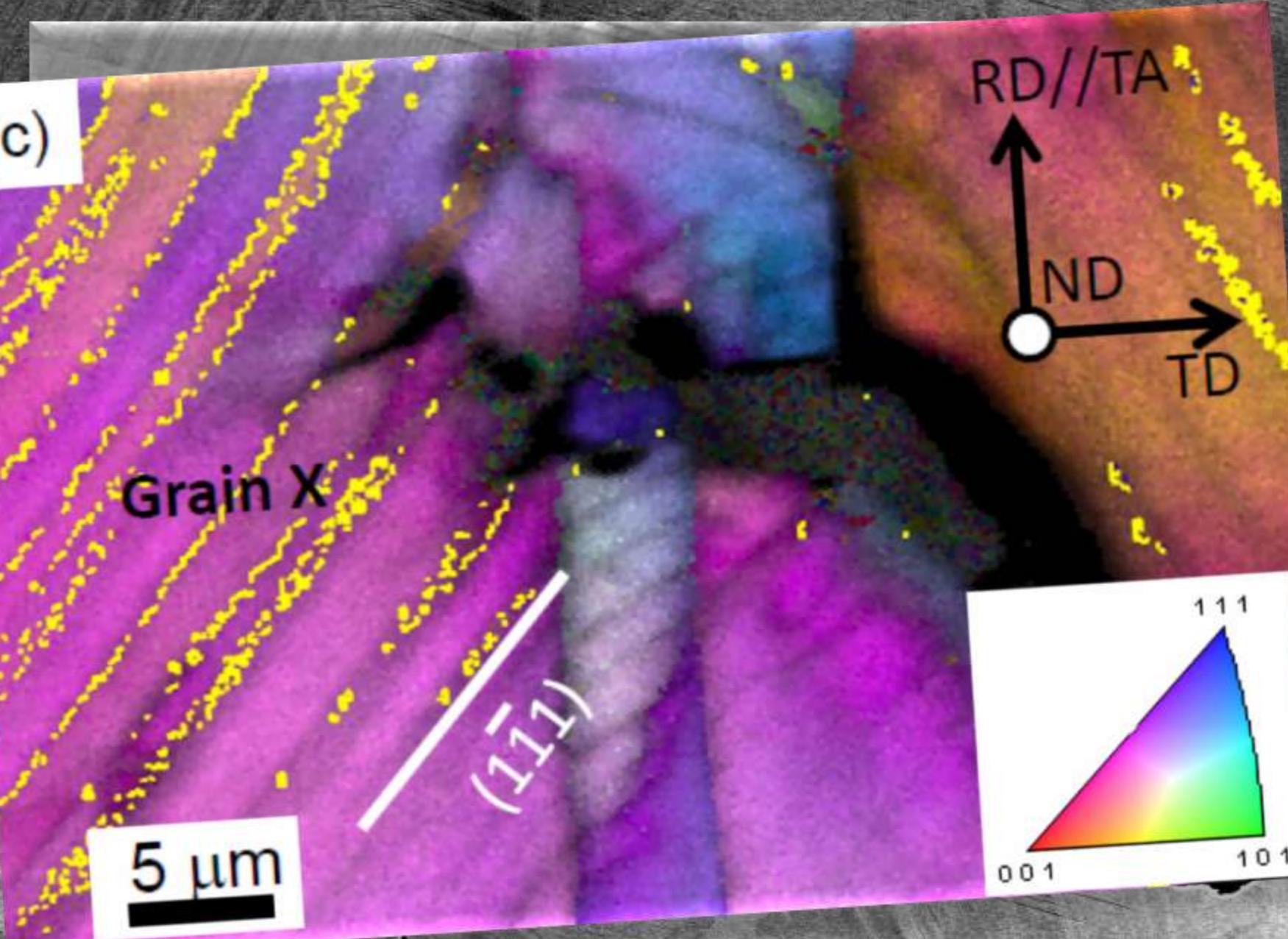
Virtual Forming Lab

Fe-24Mn-0.5C-8.6Al (wt%)





c)





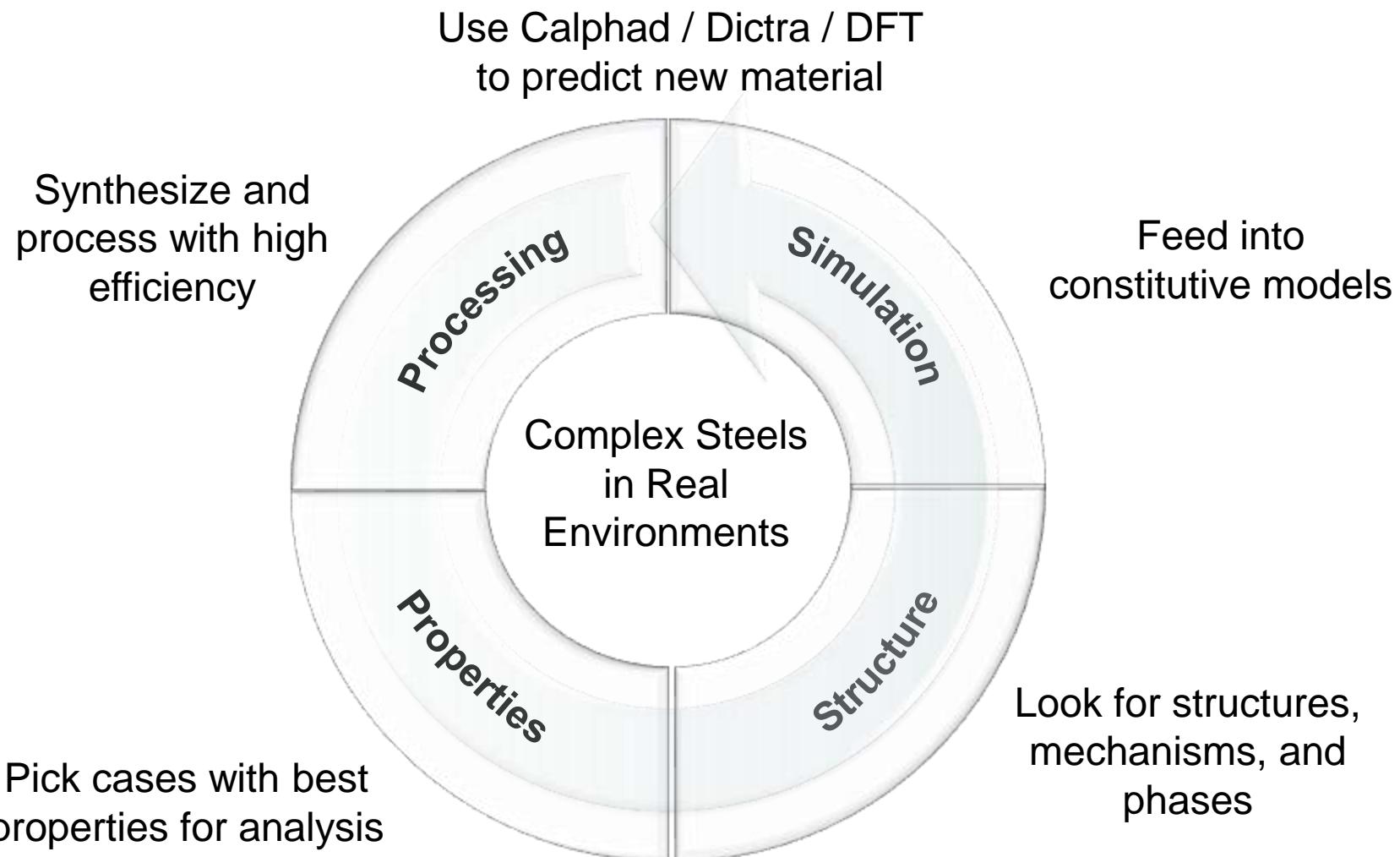
Message:

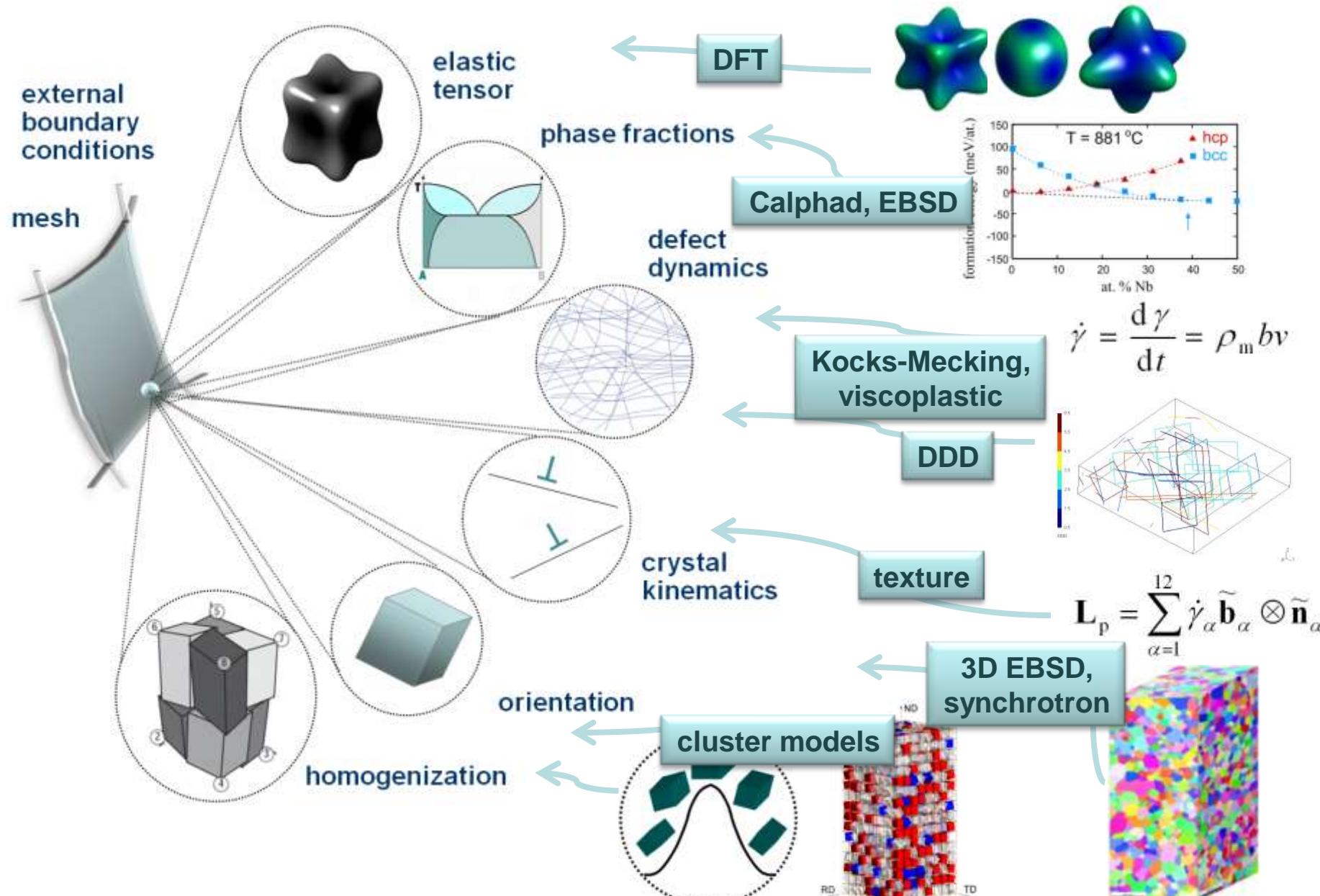
Consider complex microstructures AND real environments

Integrate damage into constitutive models: damage evolution curves

8 μm

Integration procedure

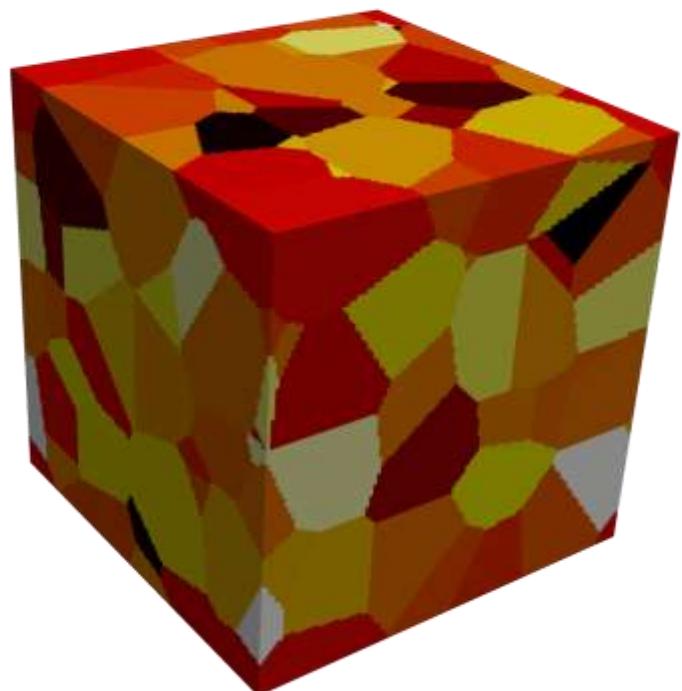




Comparison FEM vs. Spectral Method

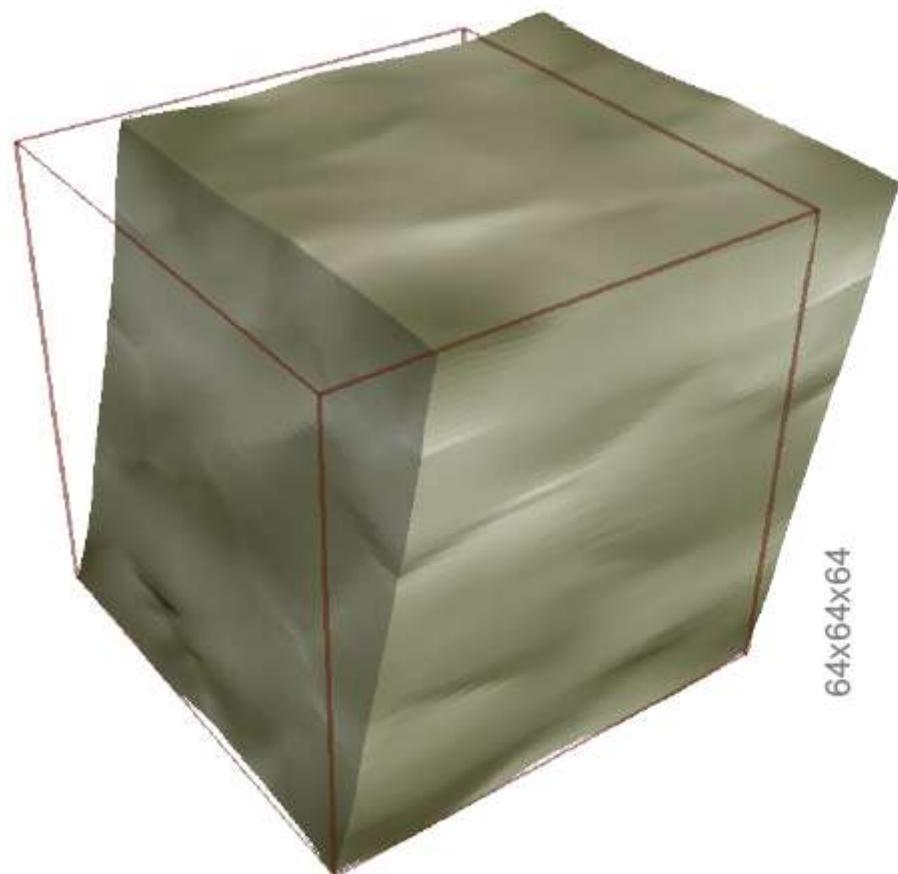
simple shear

50 randomly oriented crystals



Comparison FEM vs. Spectral Method

Finite Element Method

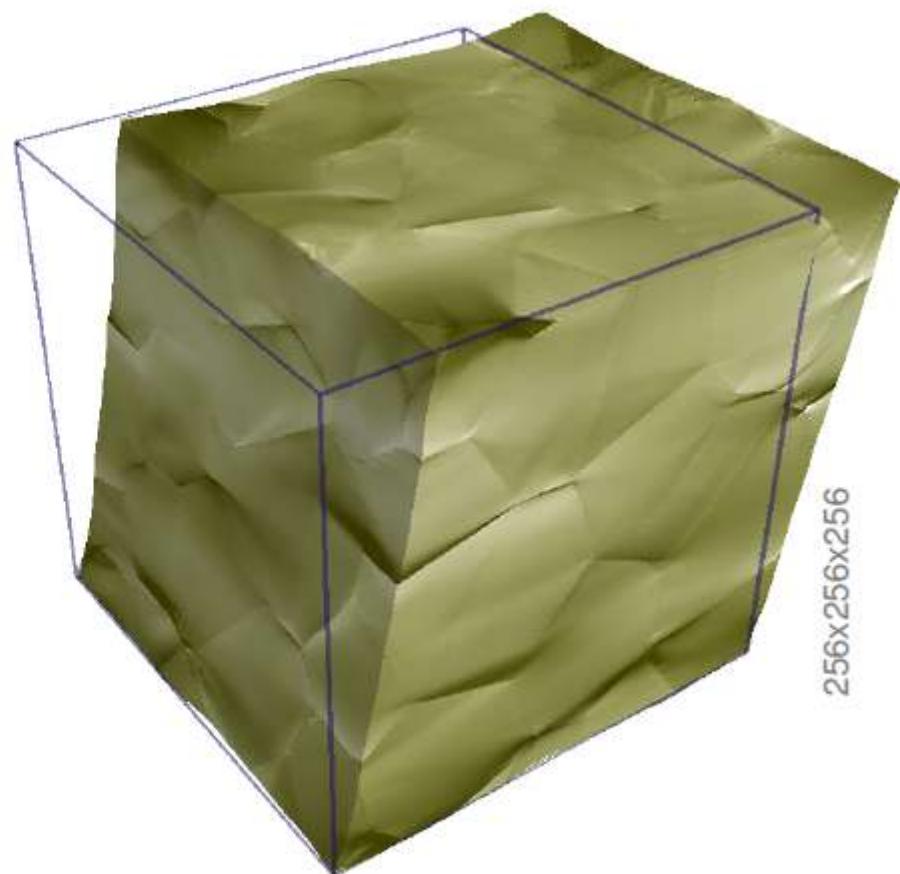


-0.1

F_{23}

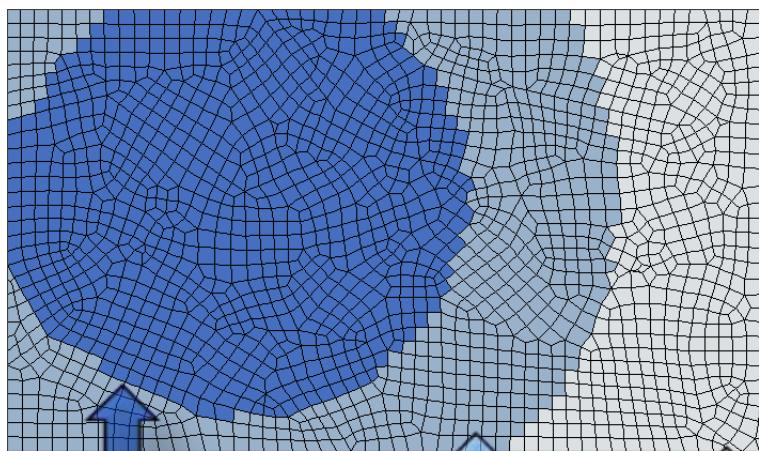
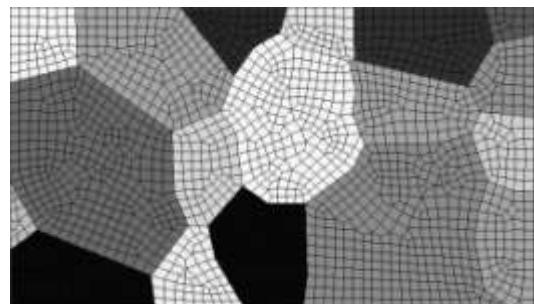
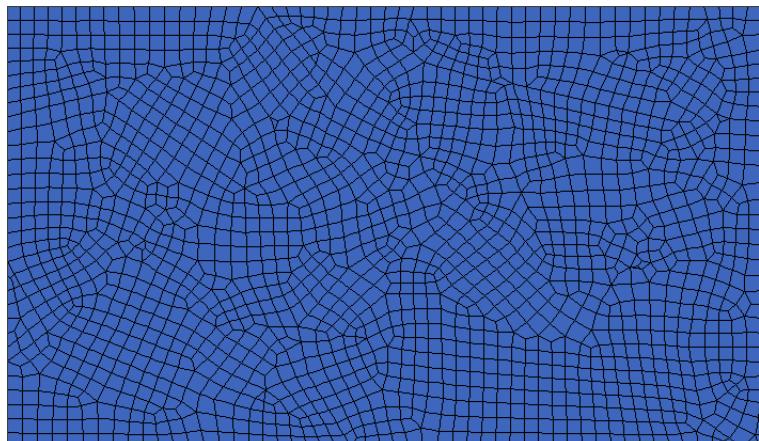
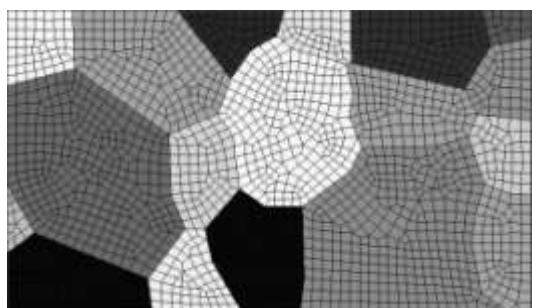
0.6

Spectral Method



Eisenlohr, et al. Journal of Plasticity (2012),

full-field dislocation density-based CPFEM



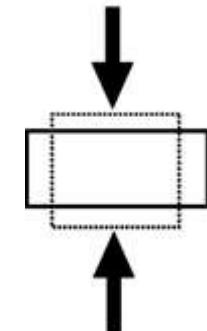
modular

dislocation density-based

phenomenological CP

J2 isotropic

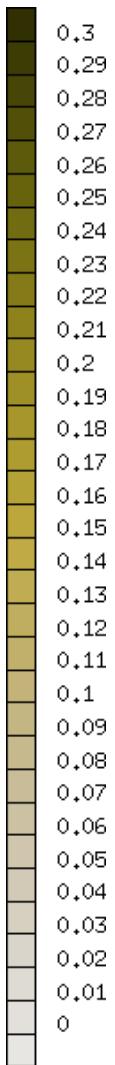
- Modular material point model can incorporate arbitrary constitutive laws within same mesh



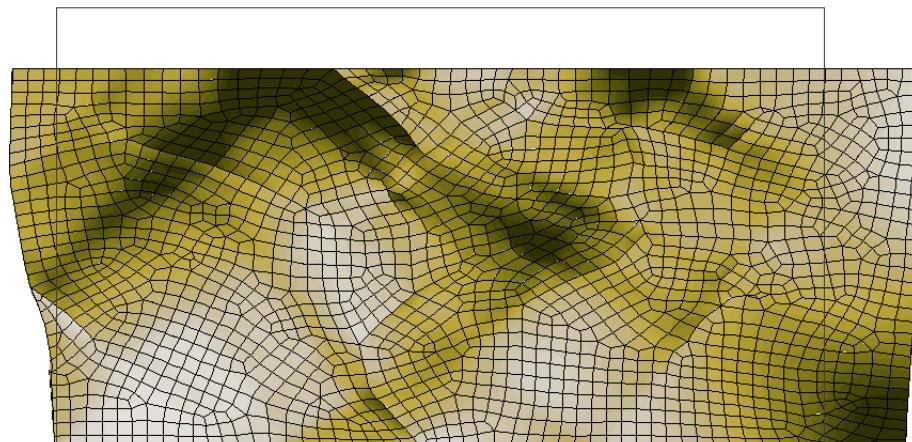
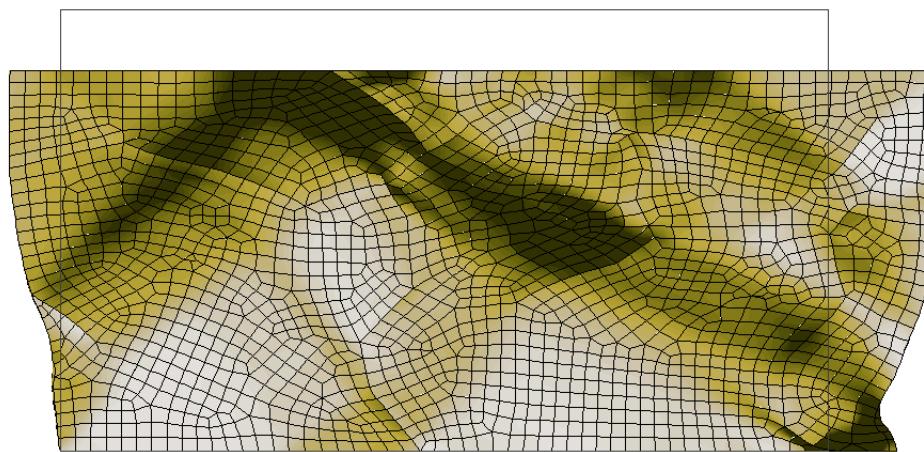
Using dislocation-based hardening laws in CPFEM simulations



logarithmic strain
(normal)



full-field dislocation density-based CPFEM



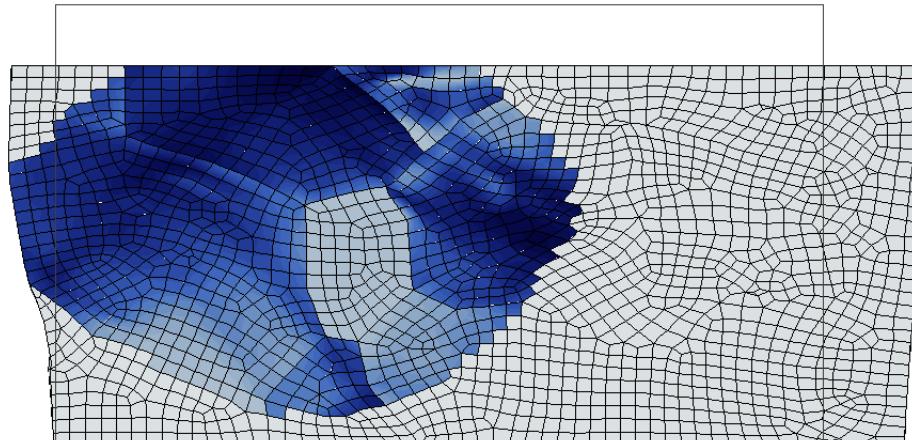
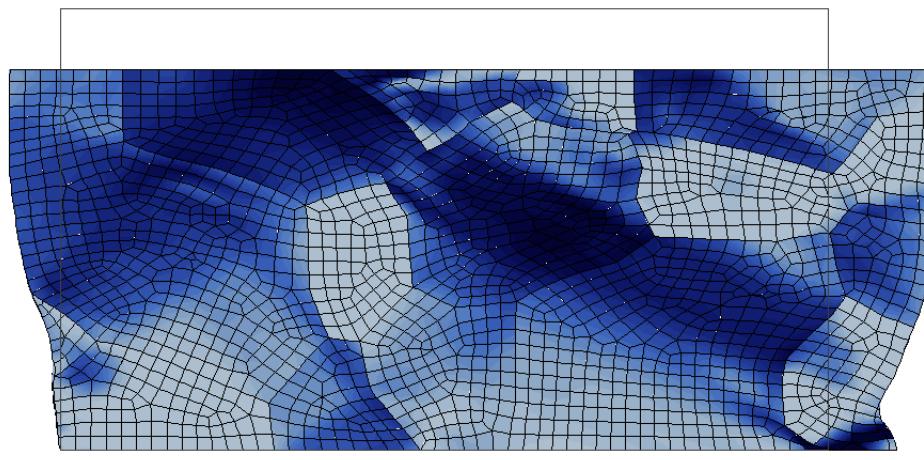
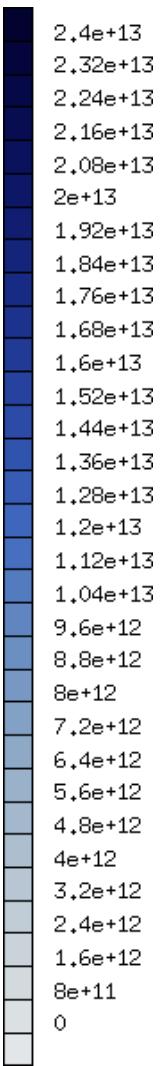
modular

Using dislocation-based hardening laws in CPFEM simulations



dislocation
density

full-field dislocation density-based CPFEM

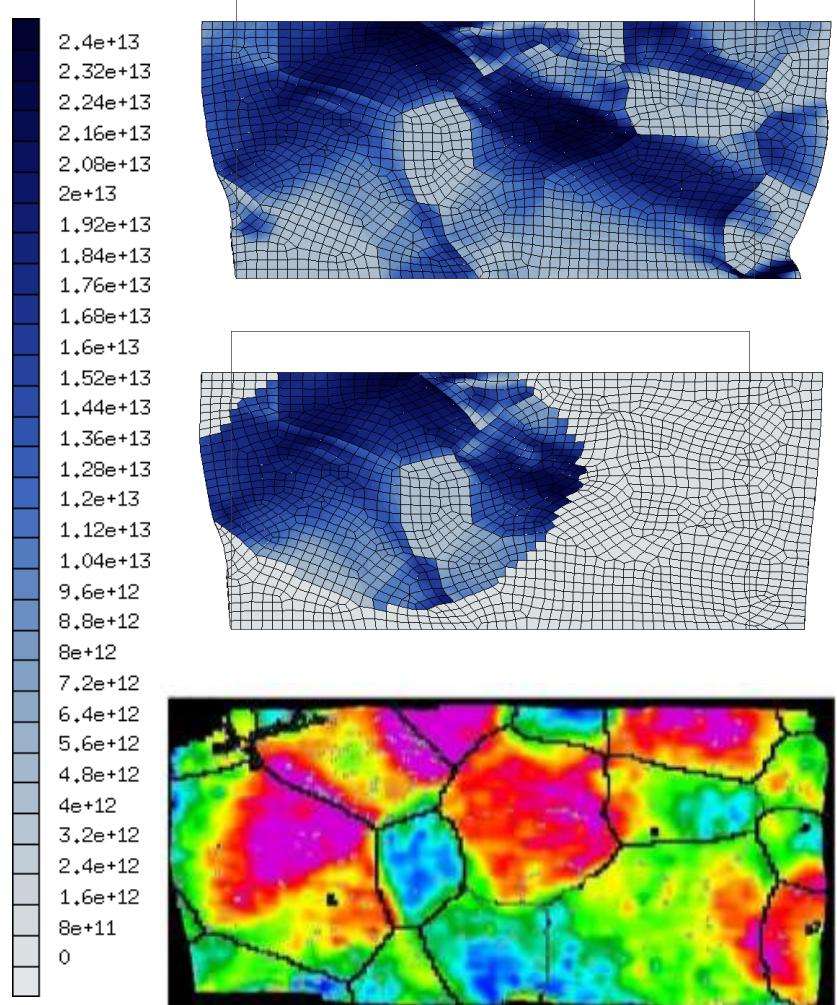


modular

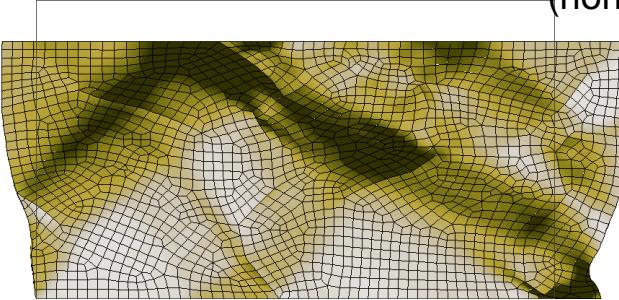
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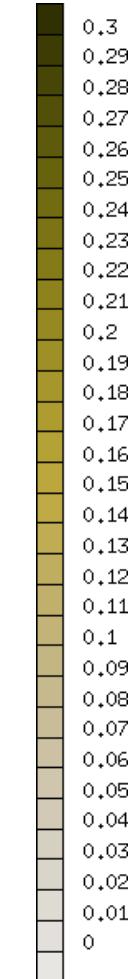
dislocation
density



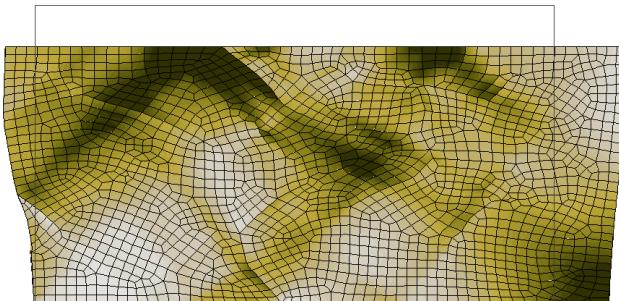
full-field



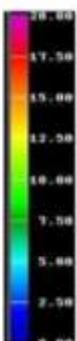
logarithmic strain
(normal)



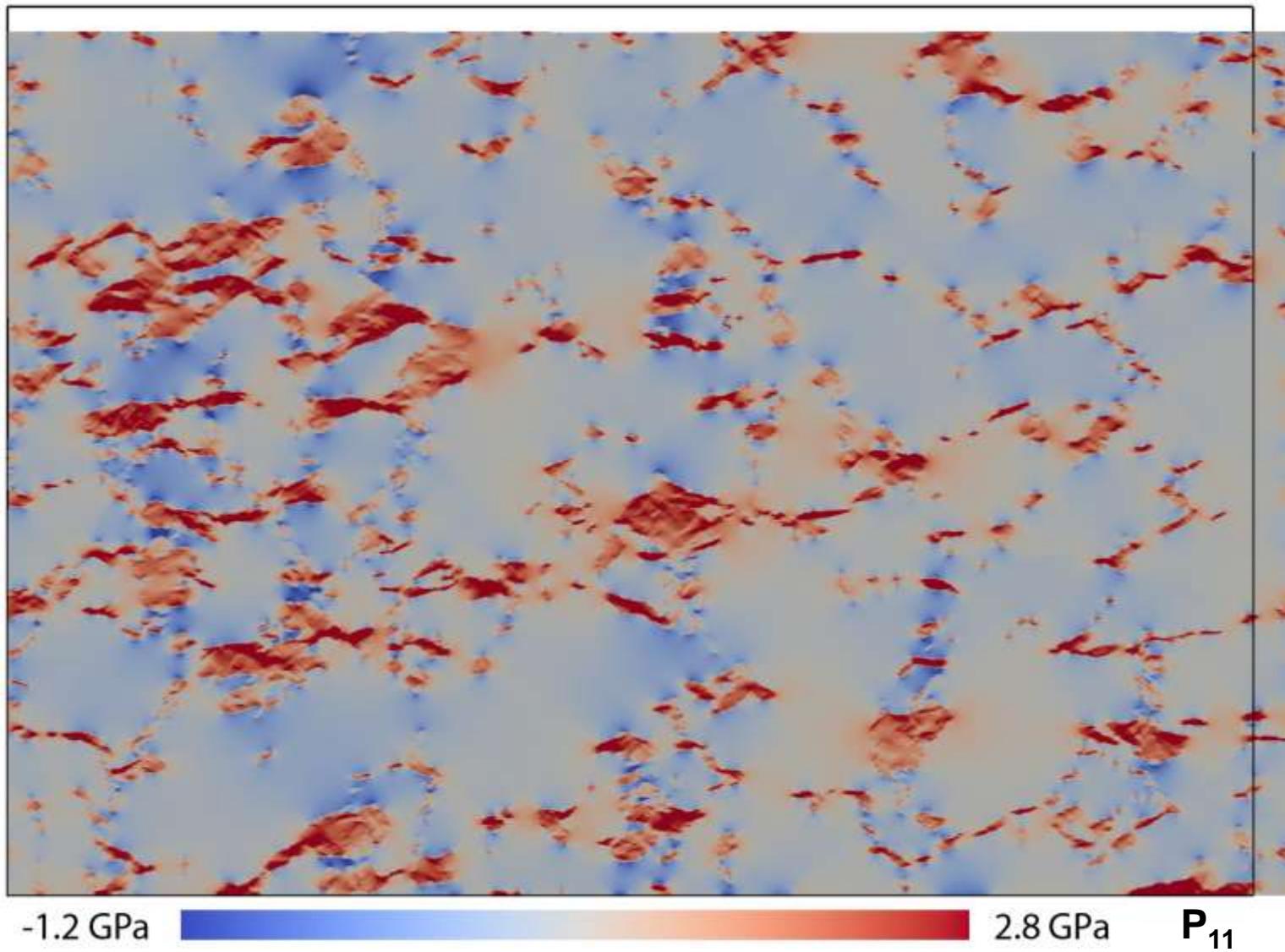
modular



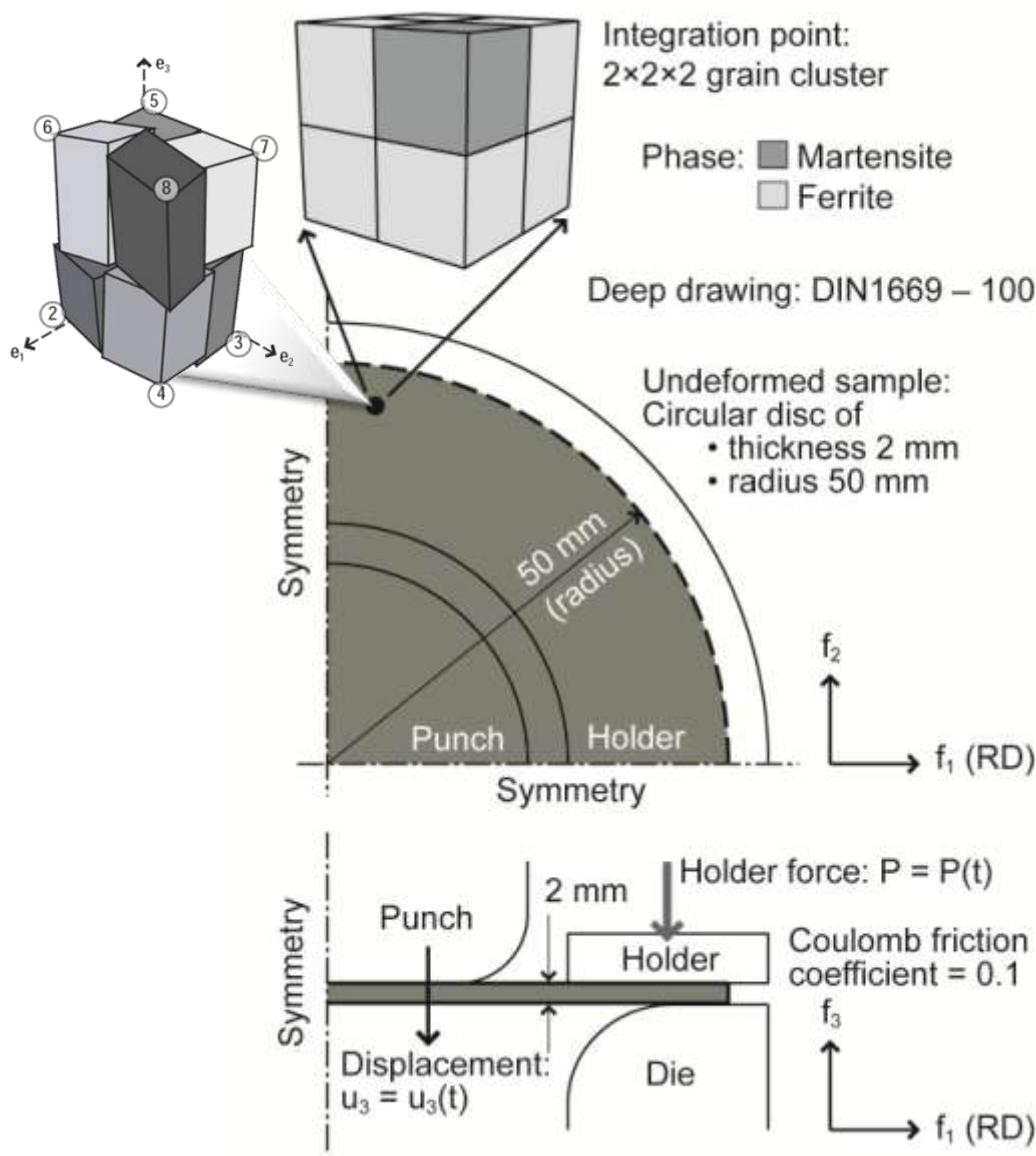
accumulated
von Mises
strain



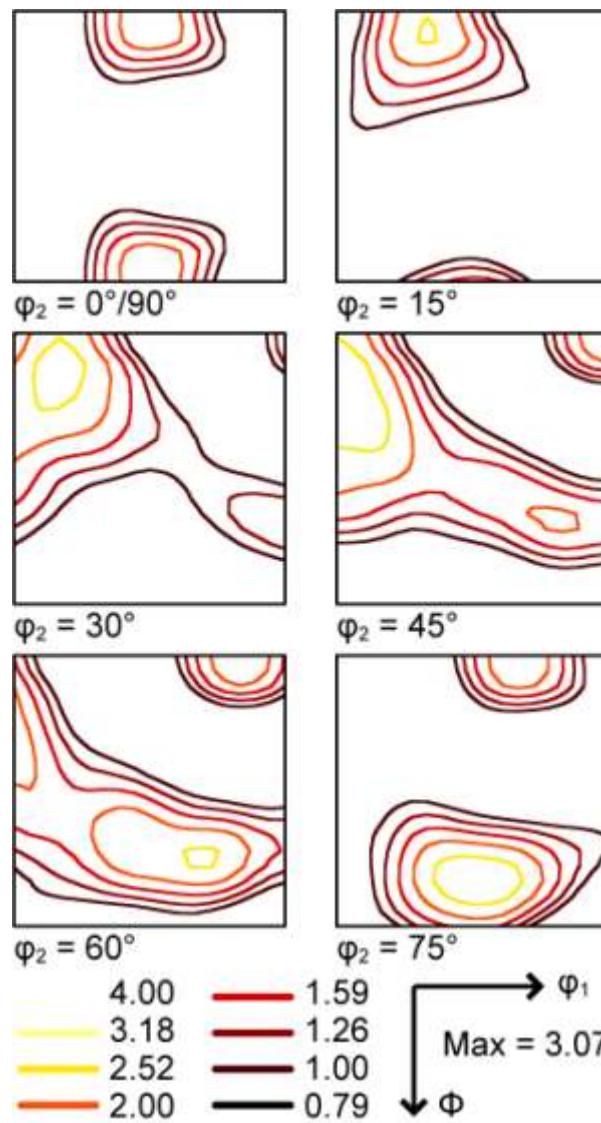
Full-field / large-scale RVE modeing for DP steels



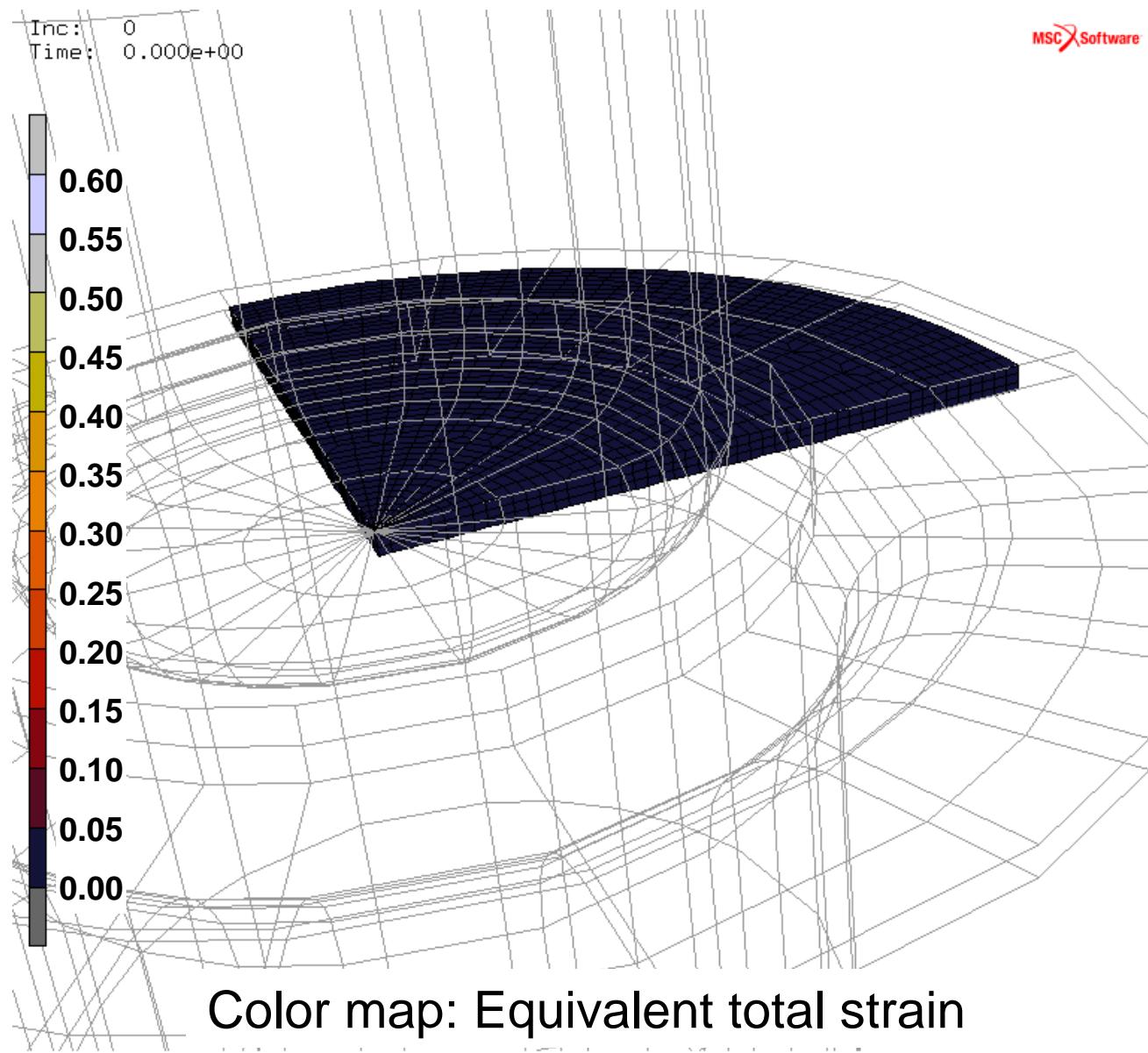
Simulation setup: grain cluster homogenization



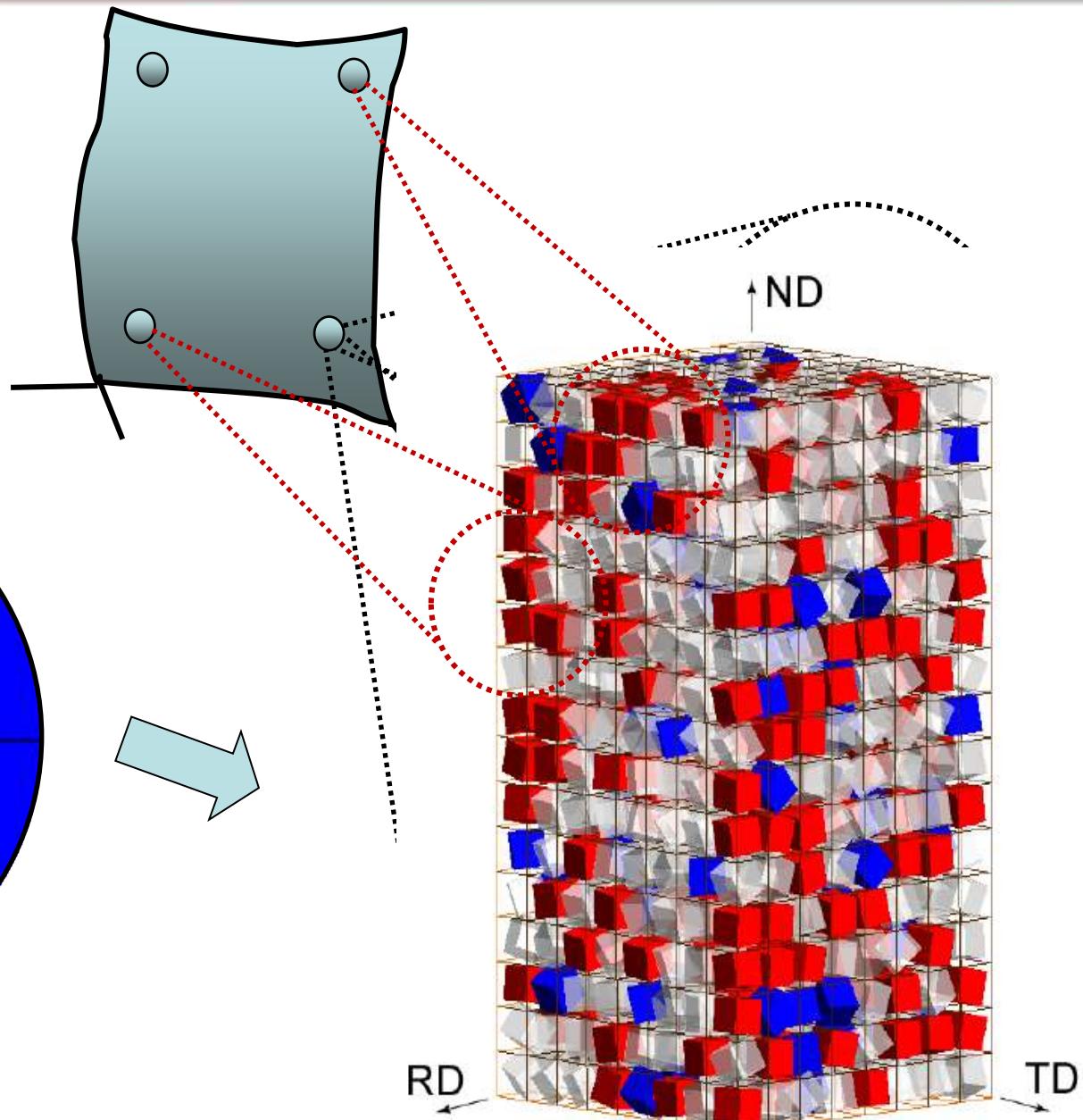
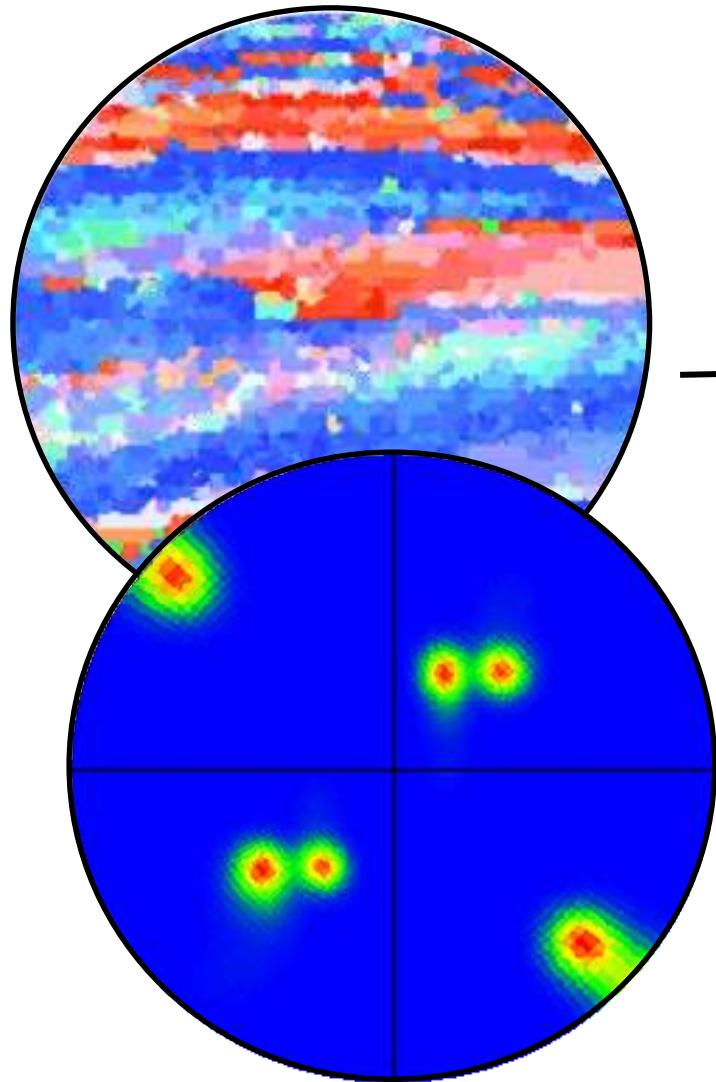
Initial texture of bcc ferrite:



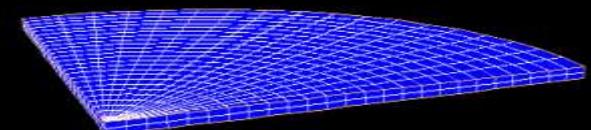
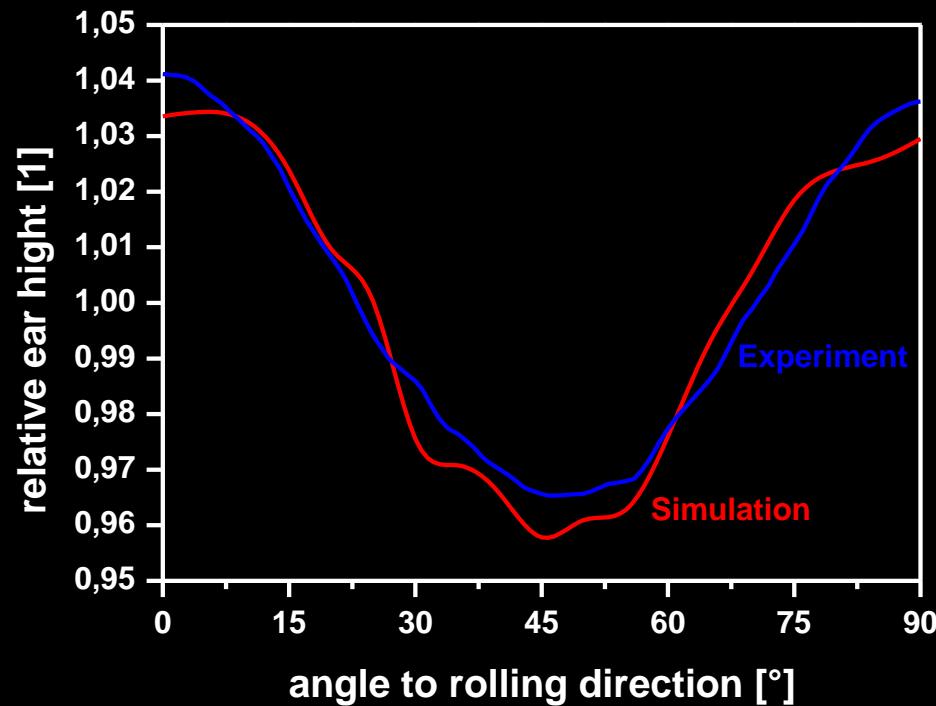
Simulation result



Texture component crystal plasticity FEM for large scale forming

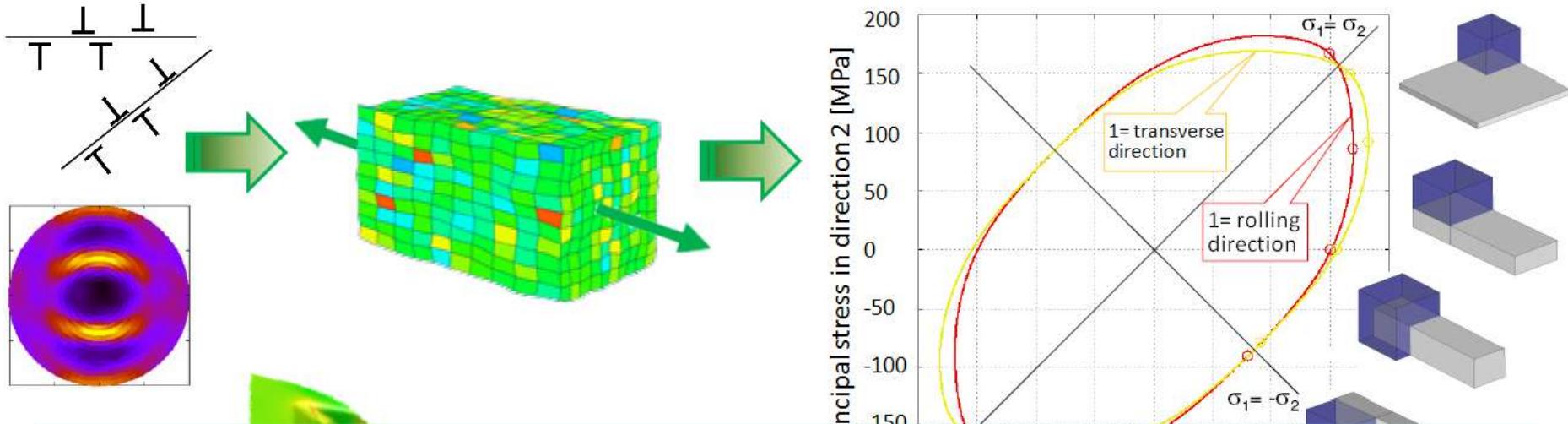


Texture component crystal plasticity FEM for large scale forming



vawisri

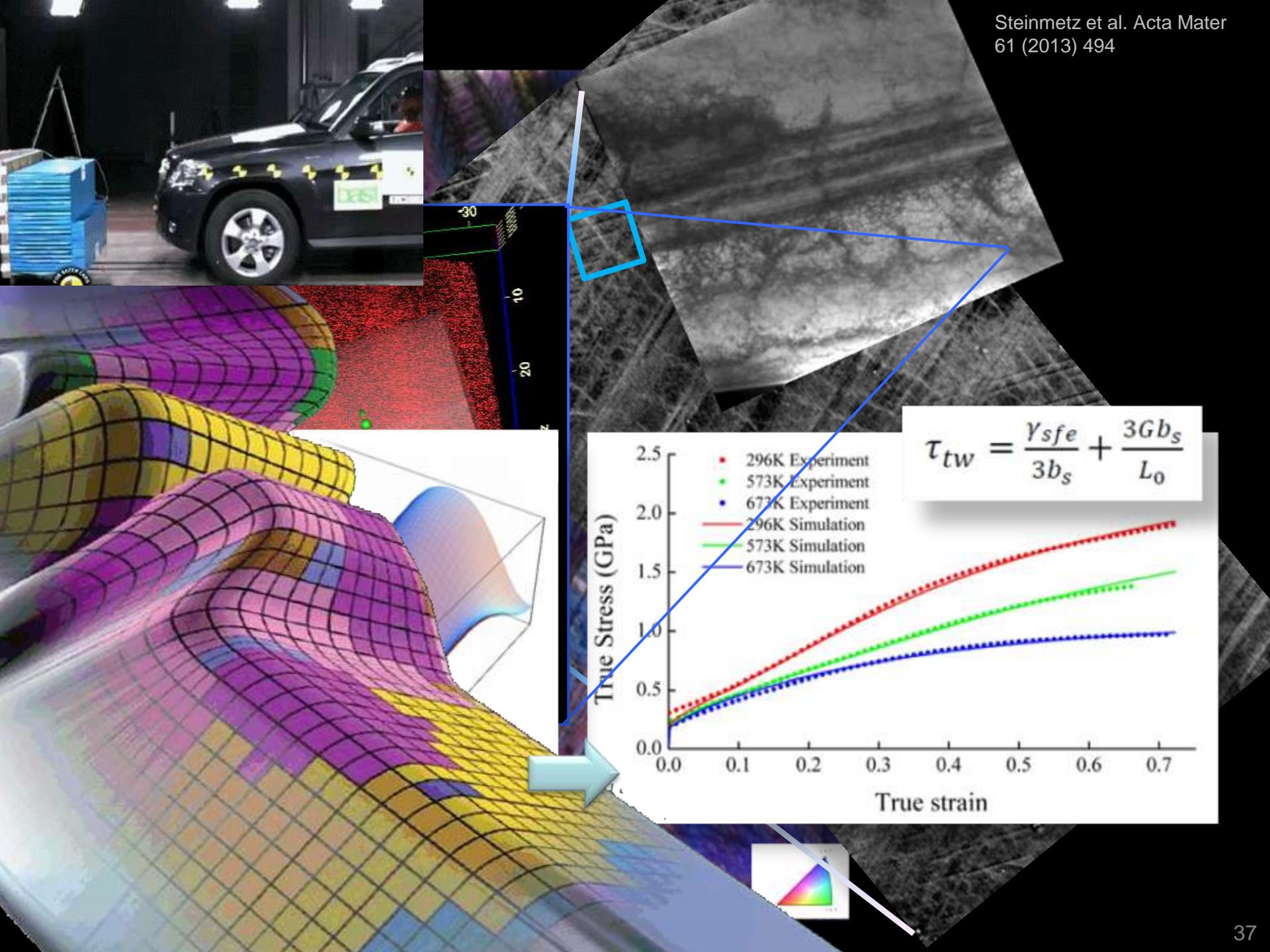
Numerical Laboratory: From CPFEM to yield surface (engineering)



Message:

RVE / virtual testing and high mechanical contrast: crystal plasticity FFT solvers

Complex global boundary condition treatment: FEM solvers in conjunction with yield surface / cluster homogenization / texture components



Düsseldorf Advanced MAterial Simulation Kit, DAMASK

- Available as freeware according to GPL 3
- Integrates into MSC.Marc and Abaqus (std. and expl.)
- Standalone spectral solver
- Web: <http://DAMASK.mpie.de>