



Micromechanics of Metallic Crystals and Fresh Lobster

Professor Dierk Raabe

Roters: crystal mechanics

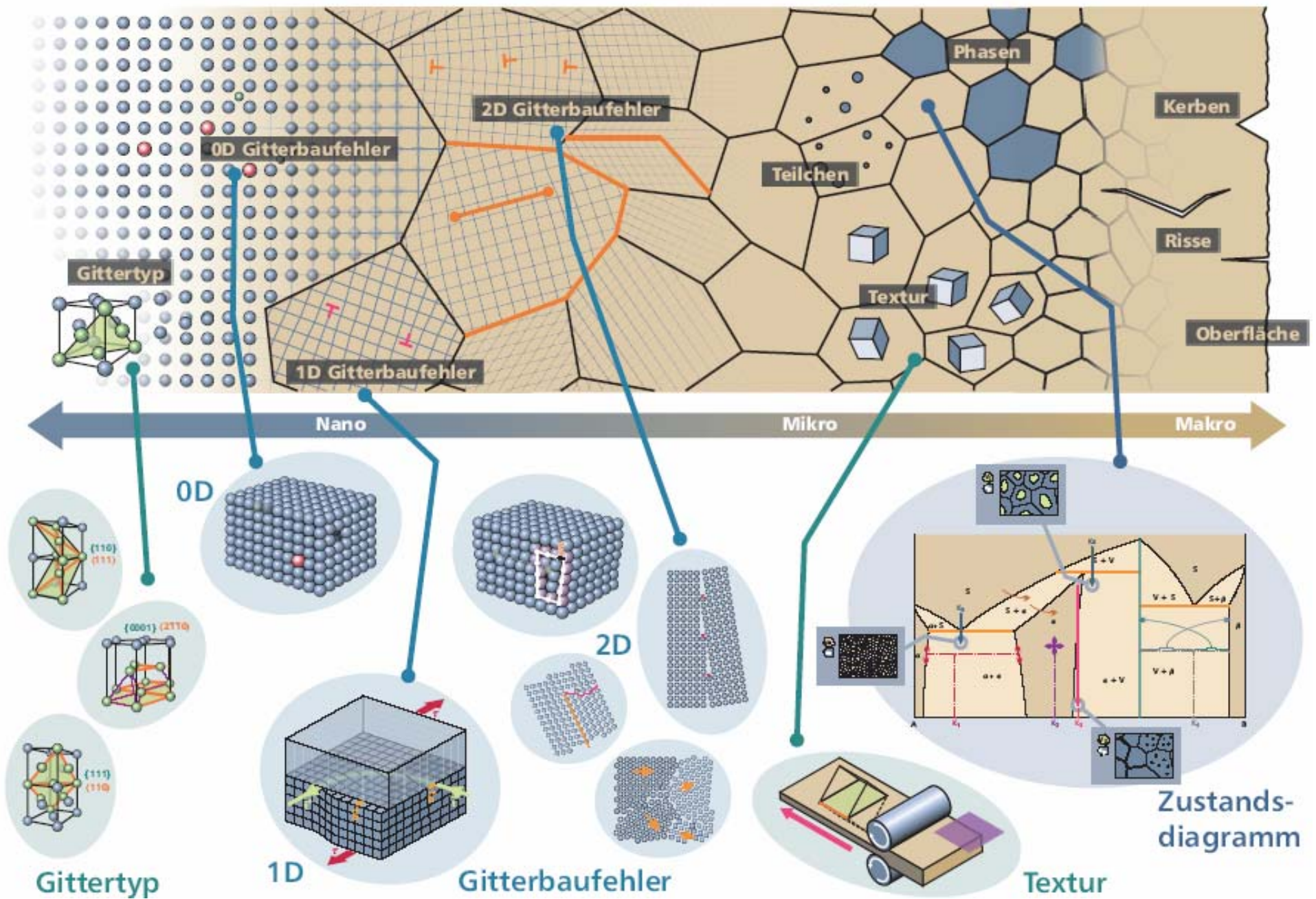
Sachs, Romano, Al-Sawalmih, Fabritius: chitin-composites

Zaefferer, Bastos: 3D Microscopy

Neugebauer, Petrov, Limperakis: ab initio and MD



- **Mechanics of few crystals**
- **Mechanics of many crystals**
- **3D electron microscopy**
- **Chitin-composites**



Dislocations



Burgers-Vektor

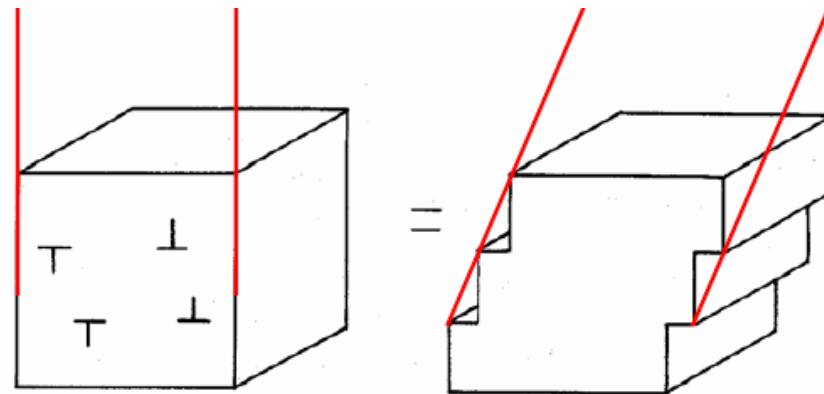
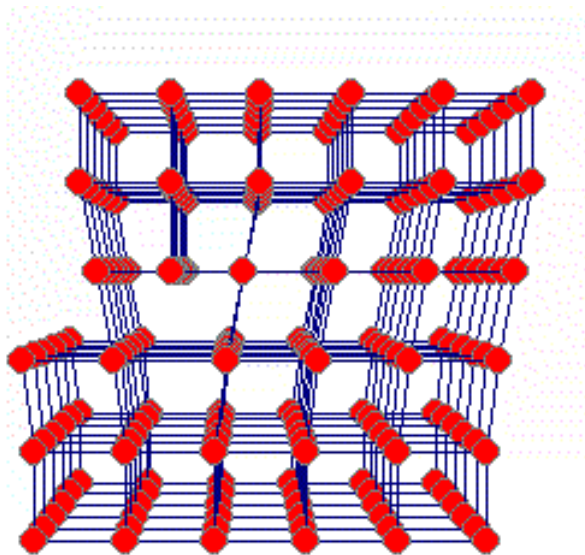
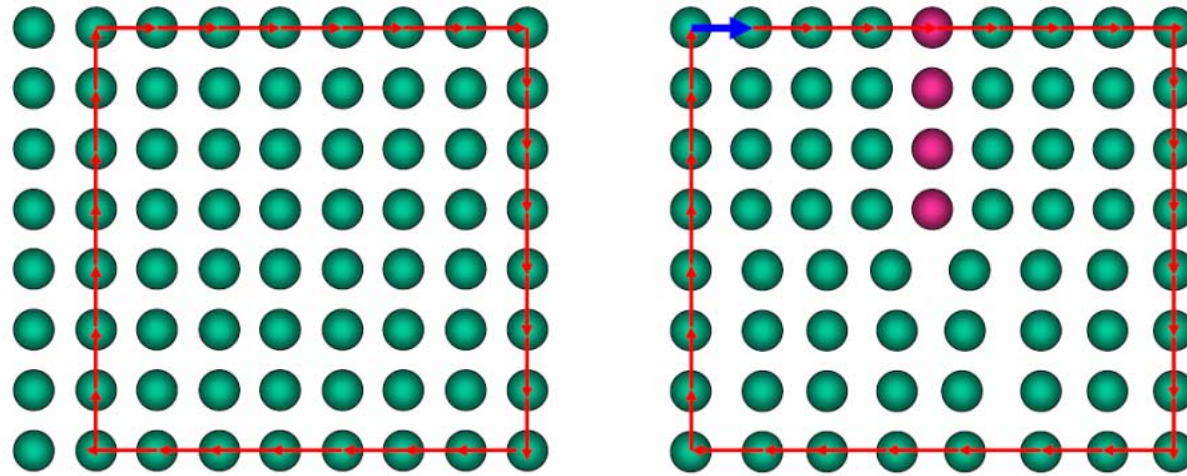
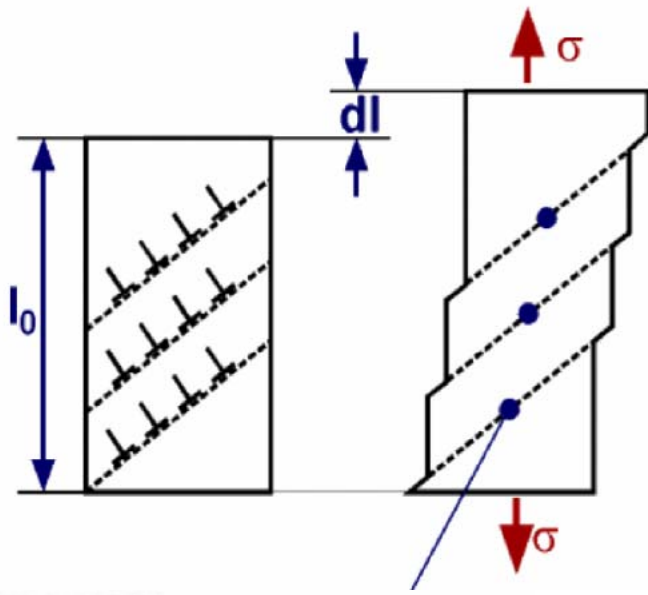
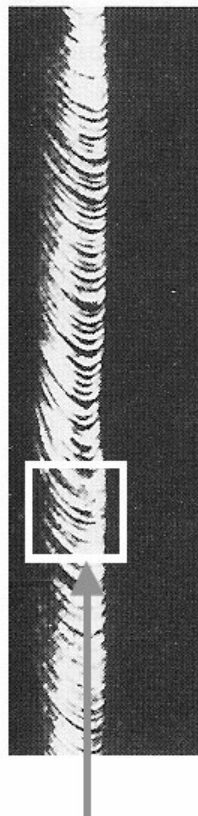
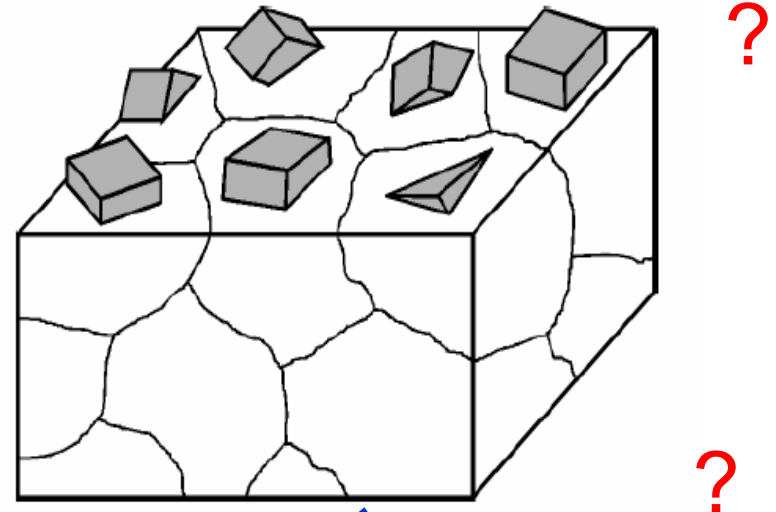


FIGURE 1-11. Slip produced by motion of many edge dislocations.

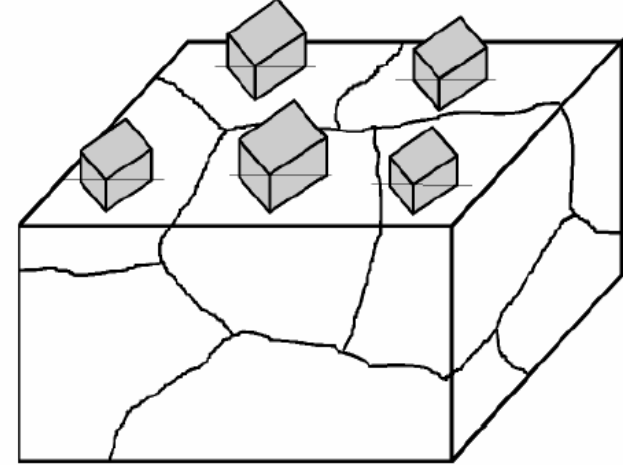
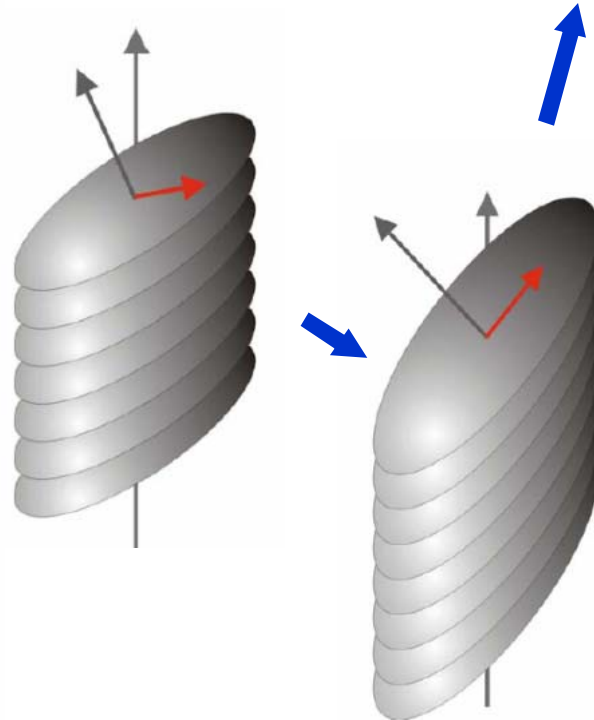


strain is the symmetric part of plasticity



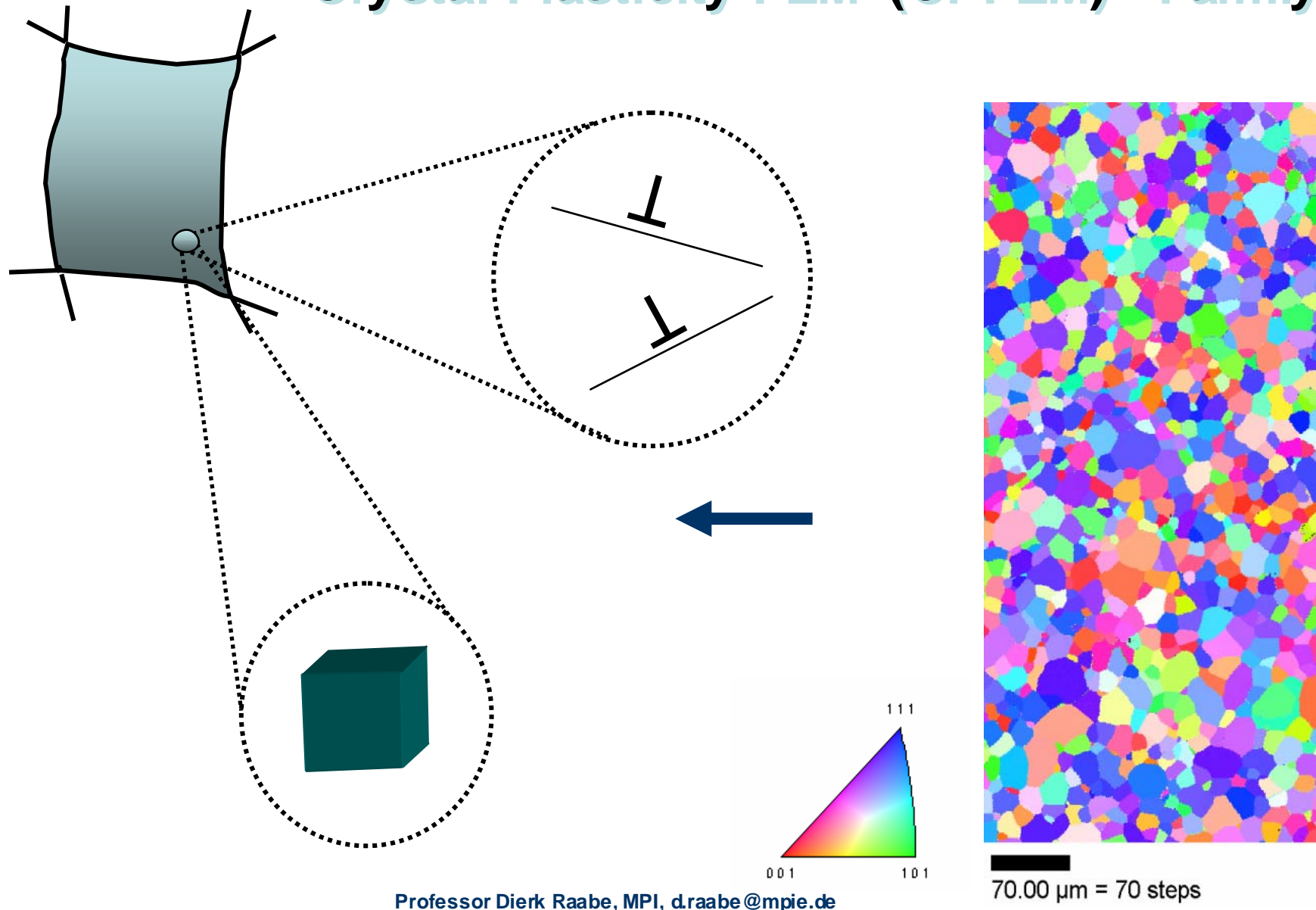
Plastically stretched zinc single crystal.

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.)

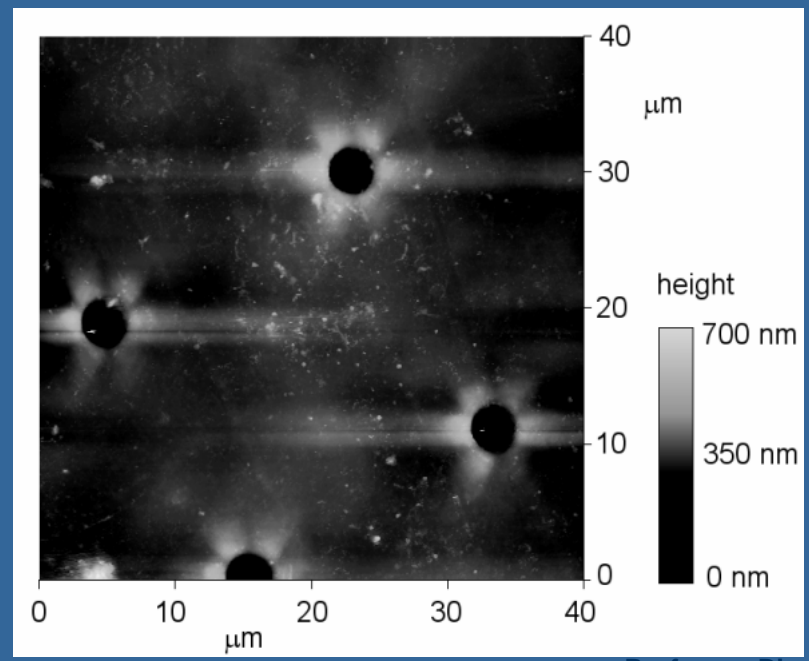
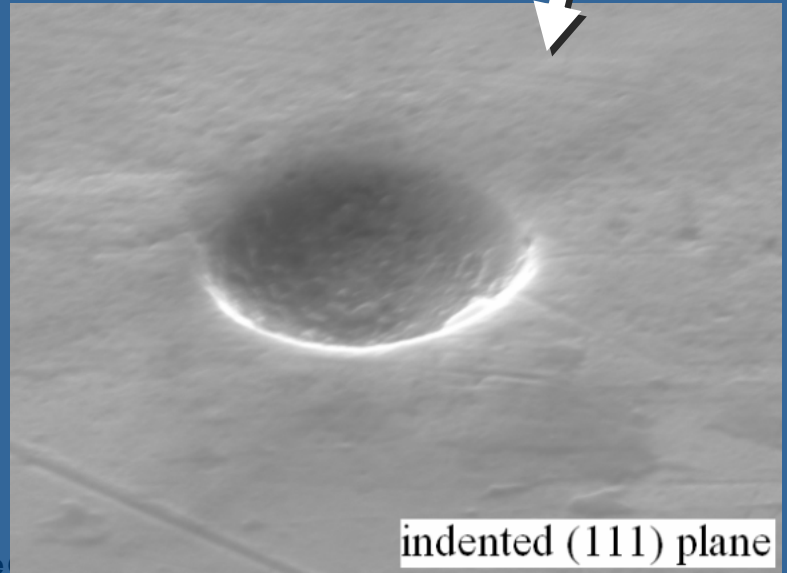
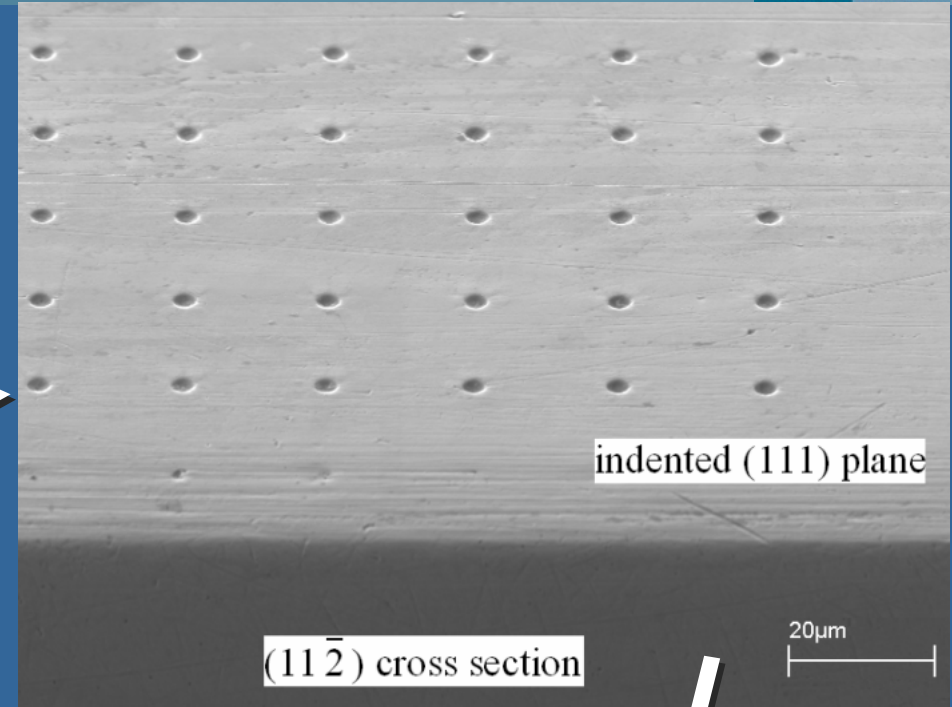
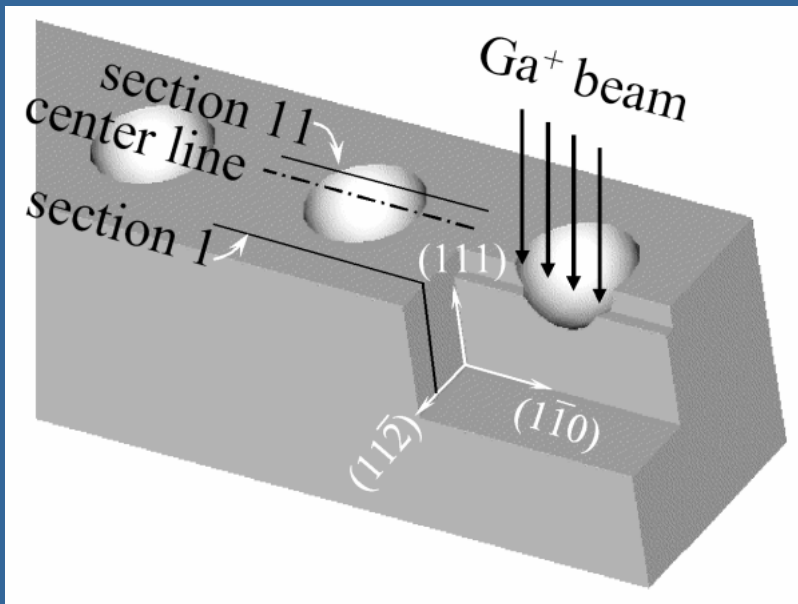


rotation (texture) is the antisymmetric part of plasticity

Crystal Plasticity FEM (CPFEM) - Family



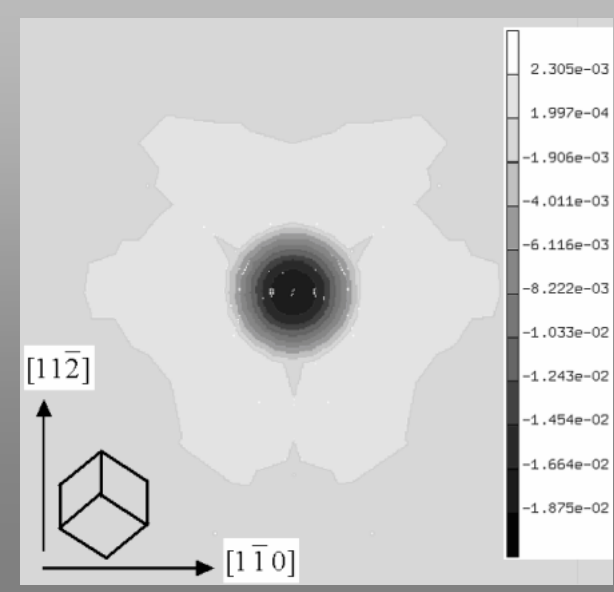
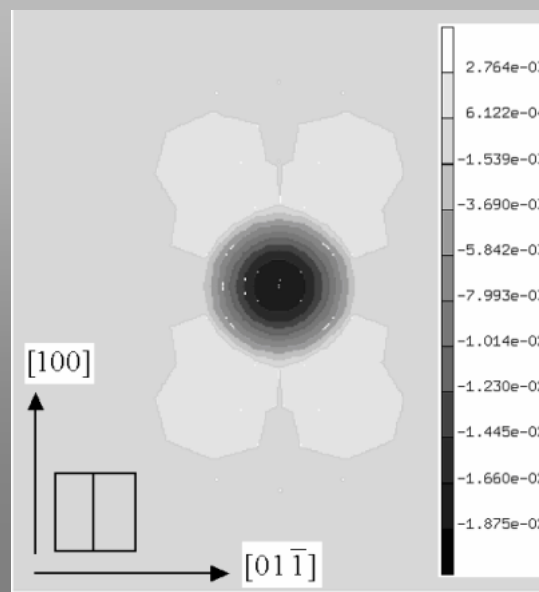
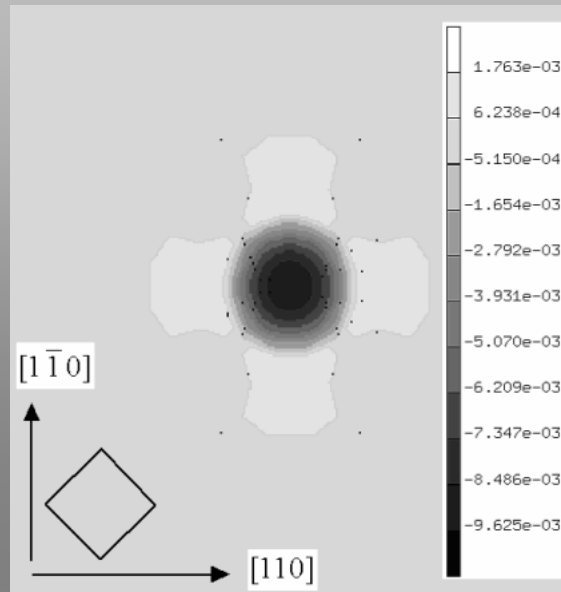
Nanoindentation - 3D



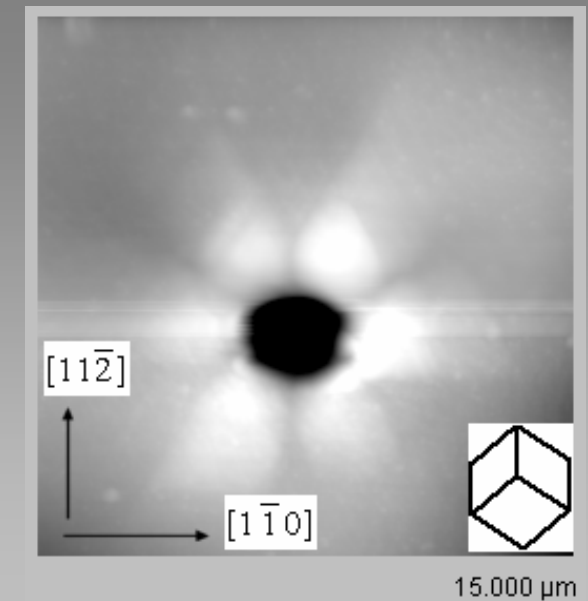
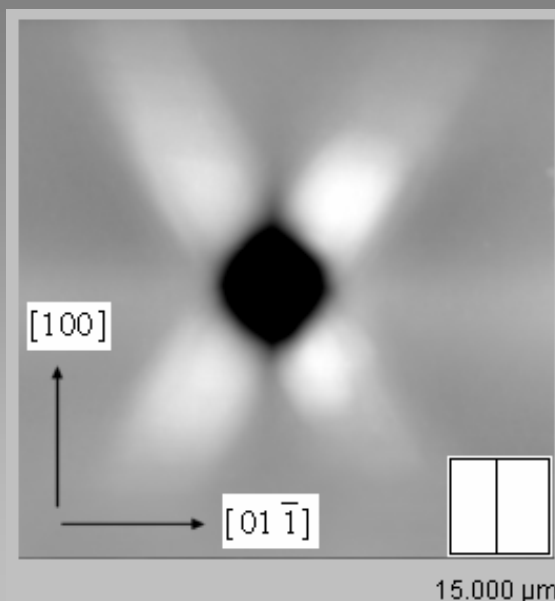
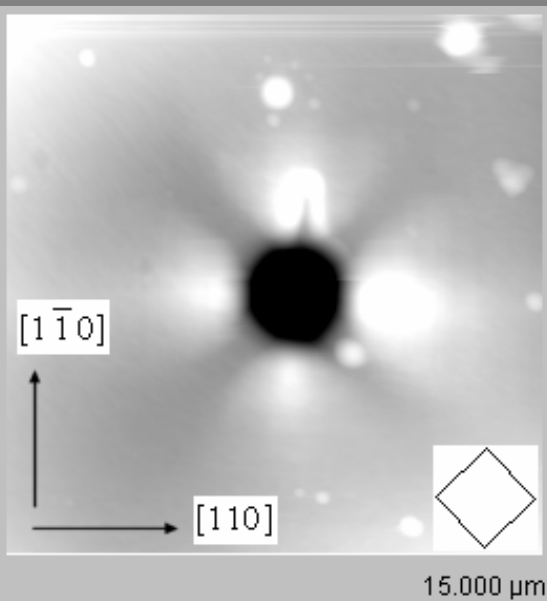
Nanoindentation - 2D



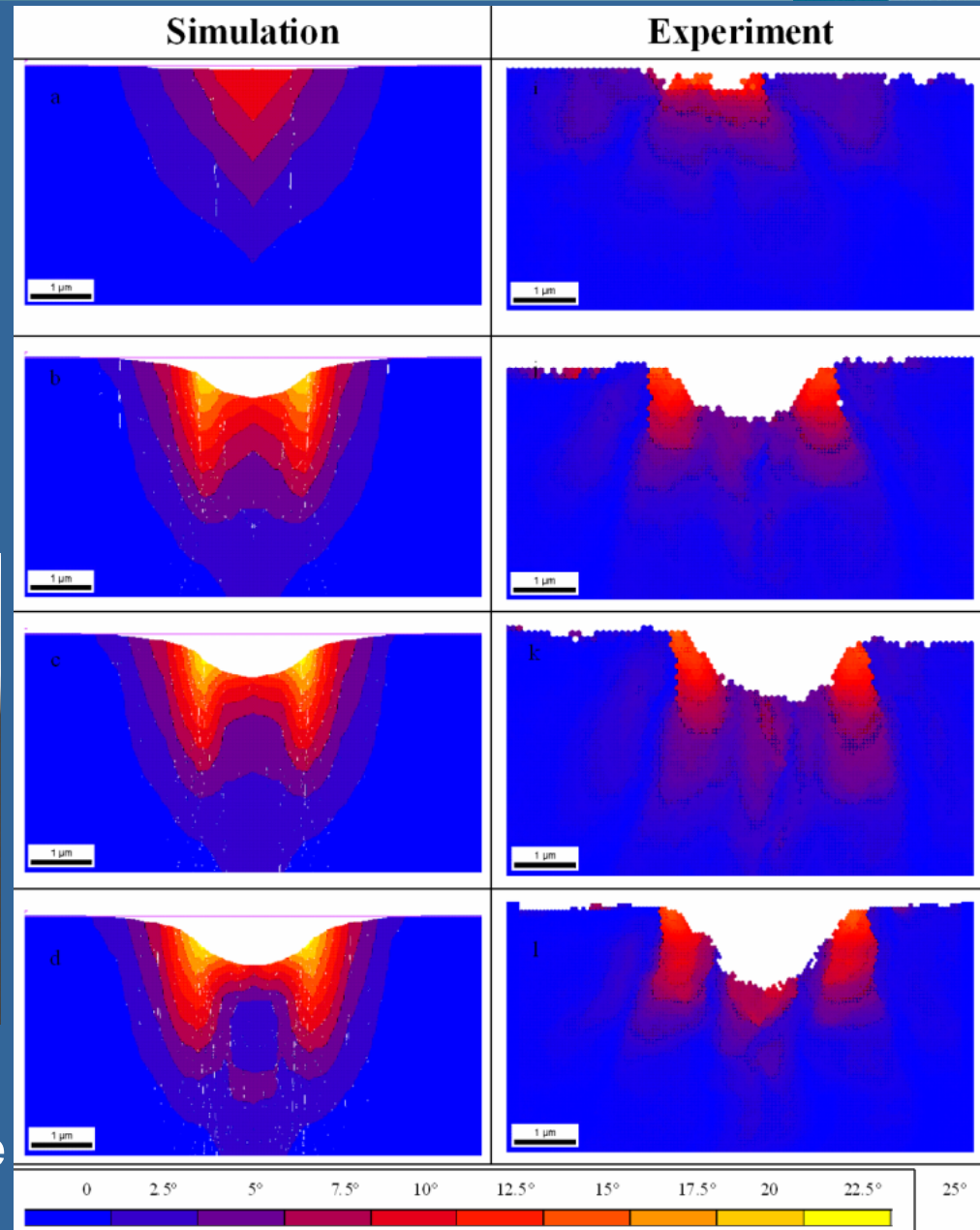
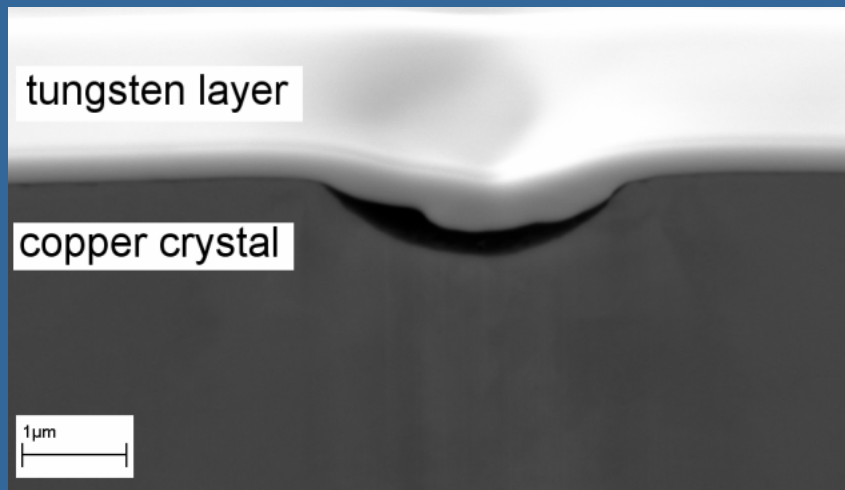
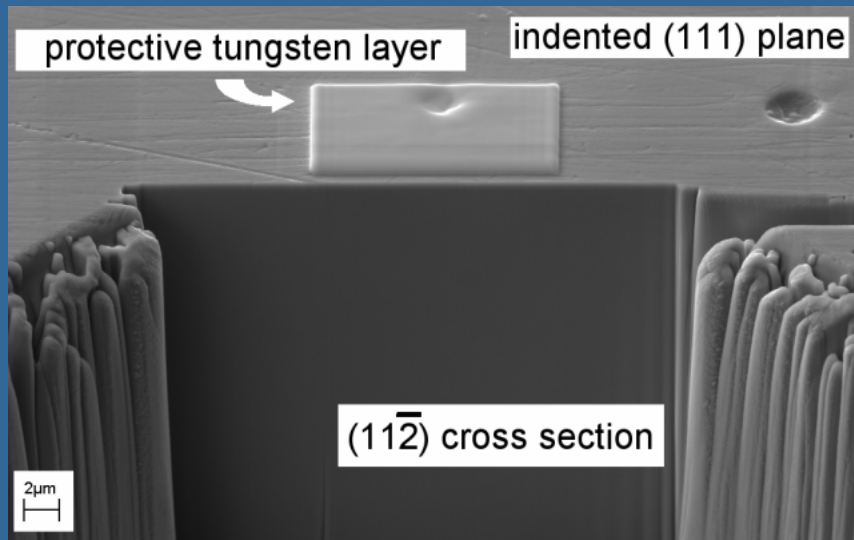
simulation



experiment

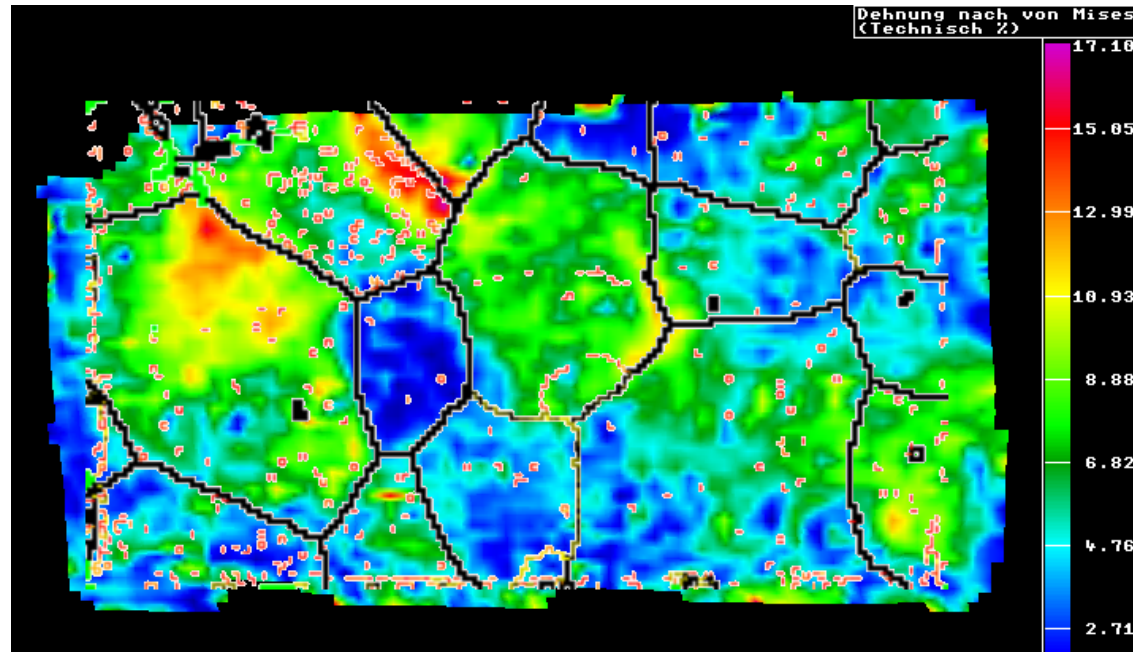
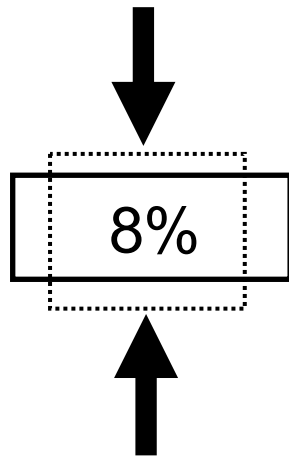


Nanoindentation - 3D



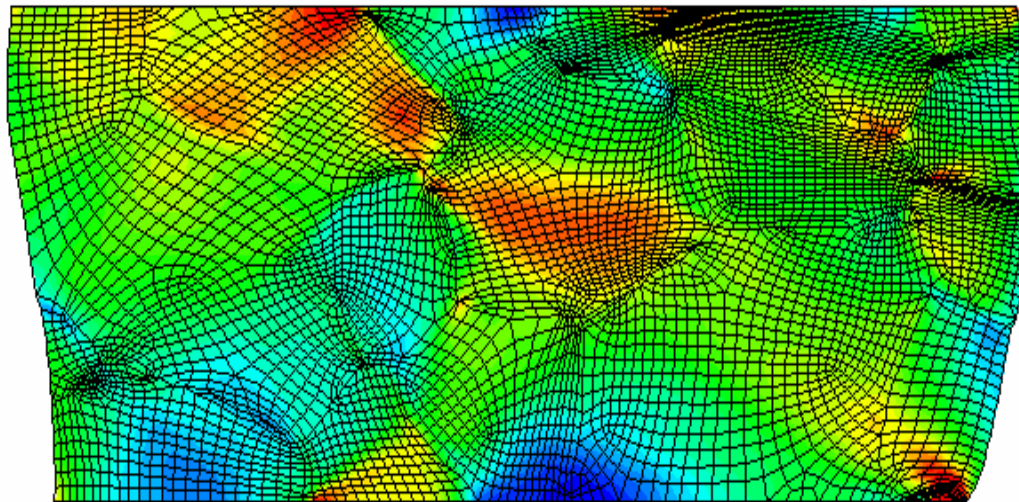
absolute values of orientation change 

2D Oligocrystals (few grains), Al, plane strain

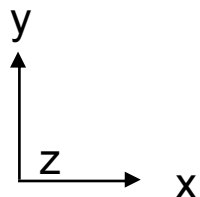


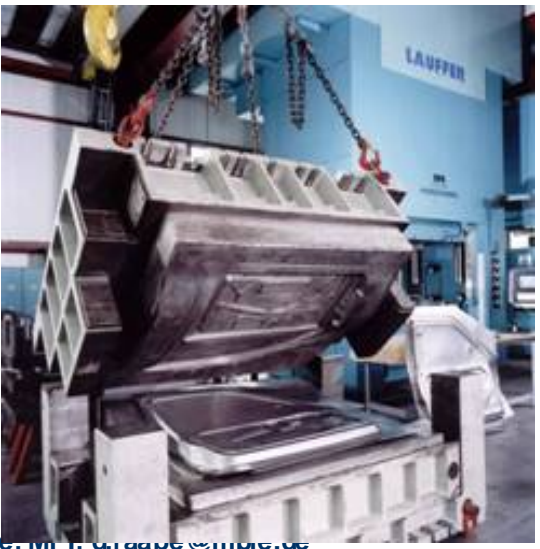
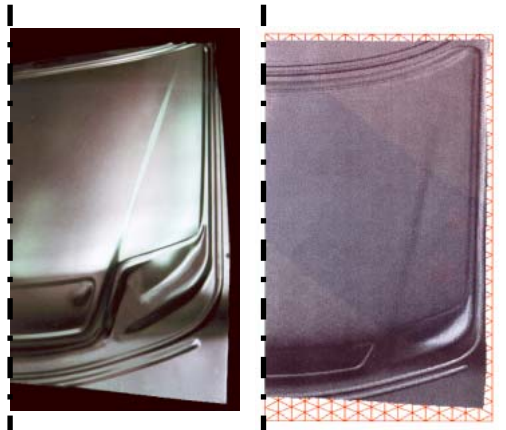
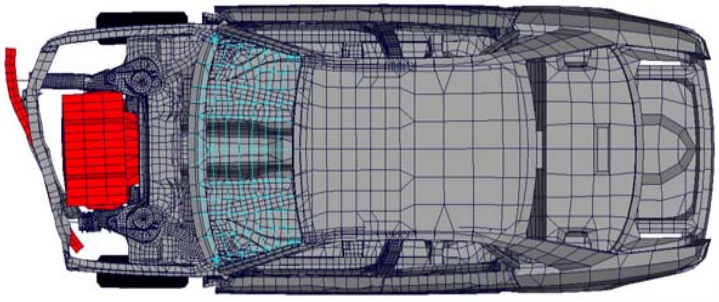
Experiment
(DIC, EBSD)
v Mises strain

von-Mises strain



Simulation
(CP-FEM)
v Mises strain

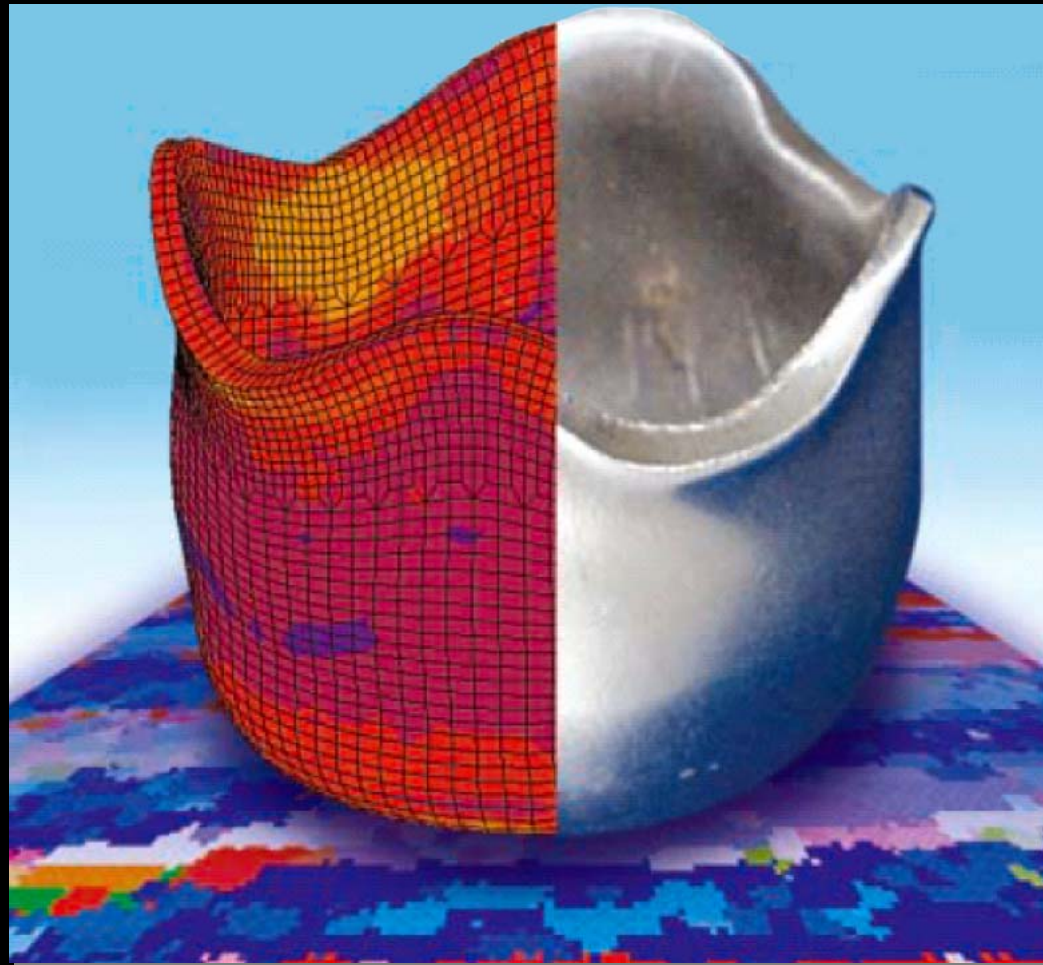




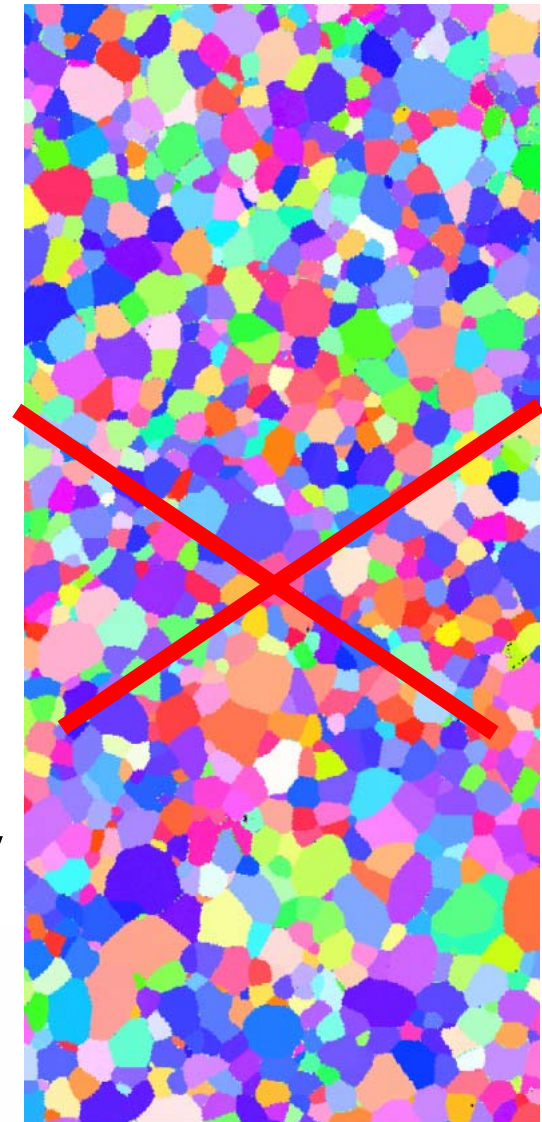
Crystal Mechanics FEM (large scale)



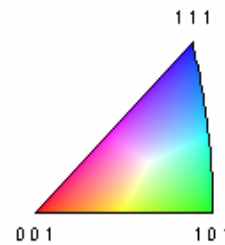
many crystals (10^{10})



10 billion grains

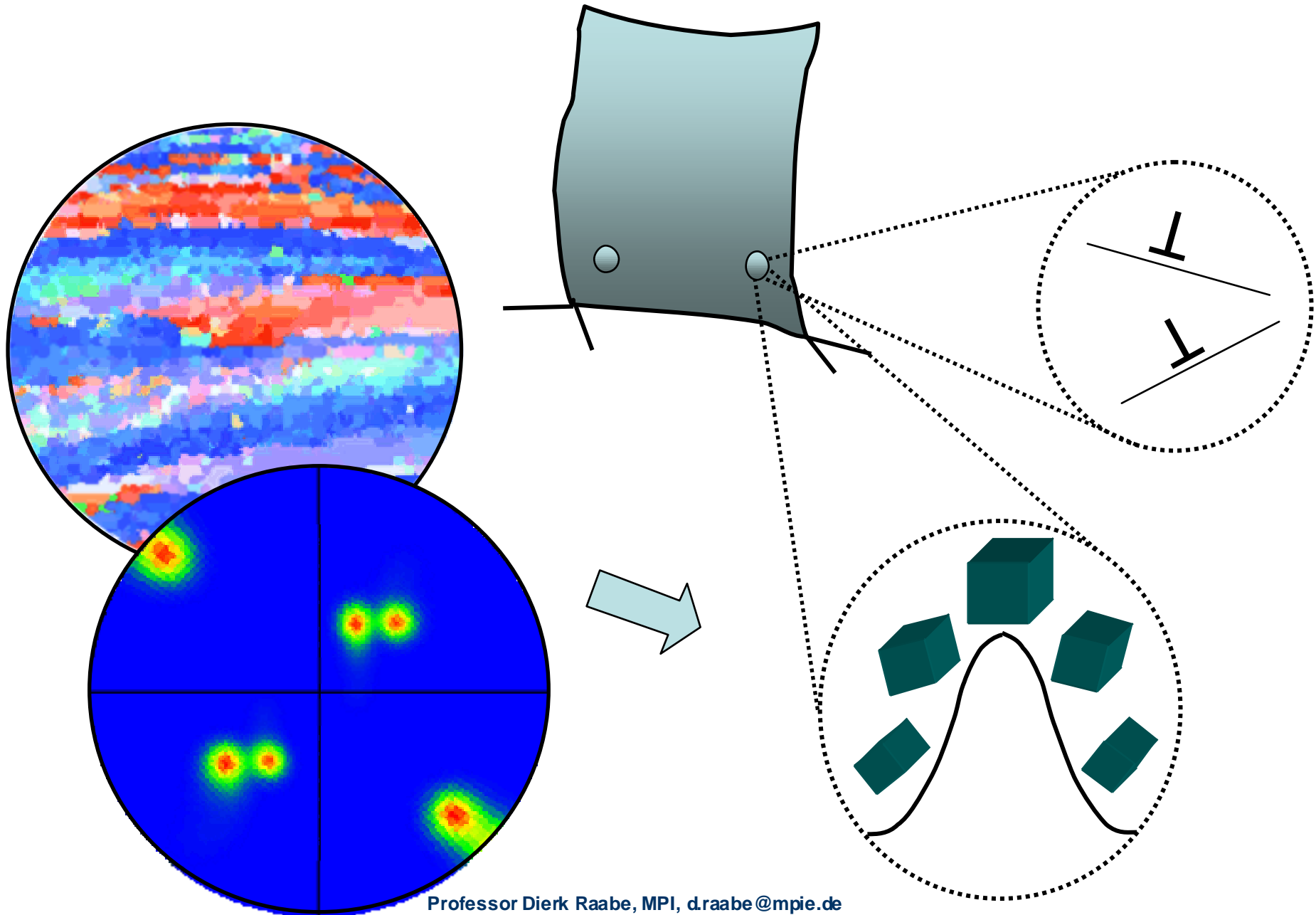


too many grains

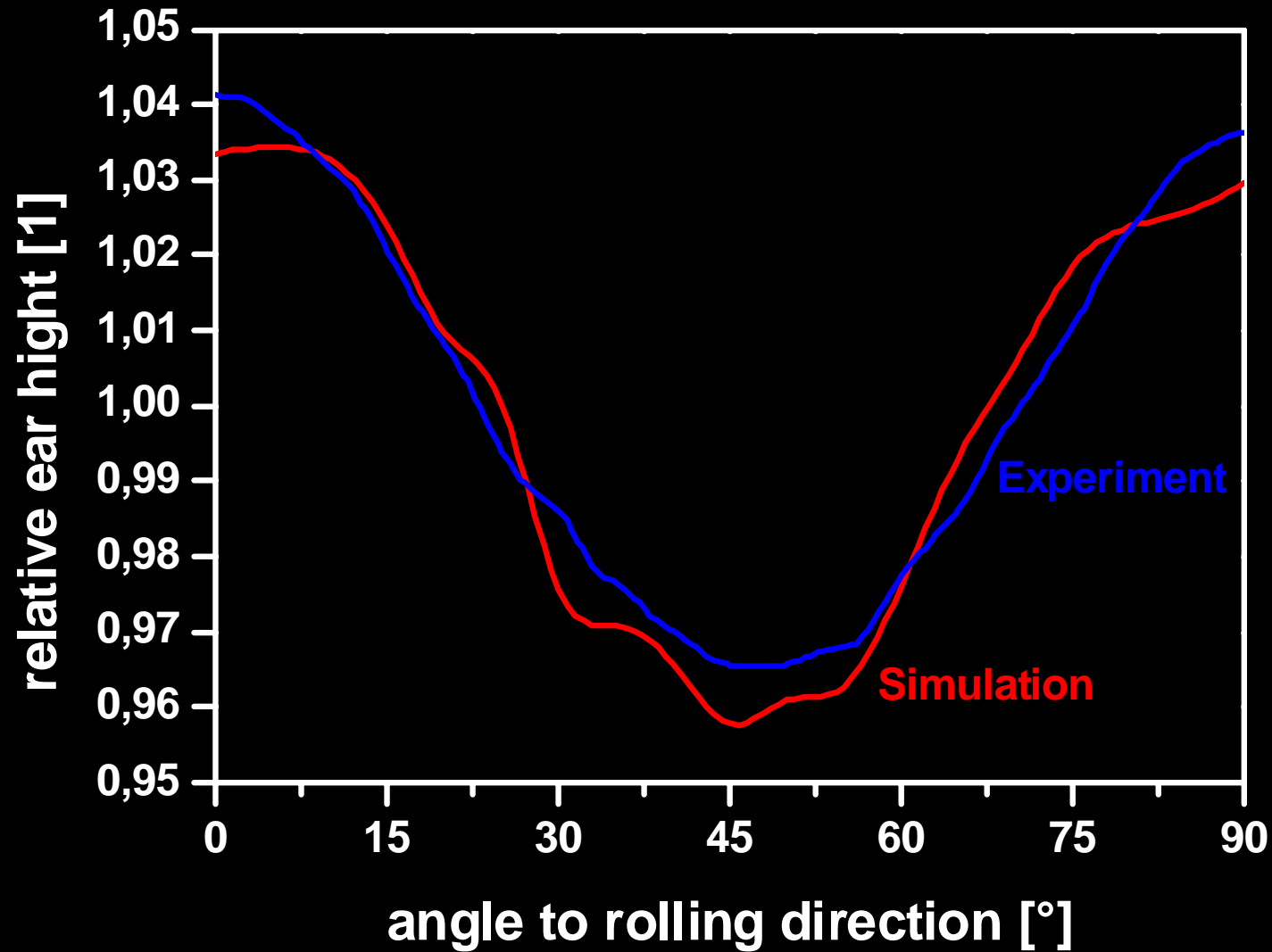


70.00 μm = 70 steps

Using spherical functions in FEM



Crystal Plasticity FEM



Applications



Biomedical parts, implant devices

Small mechanical and electronic parts

Automotive

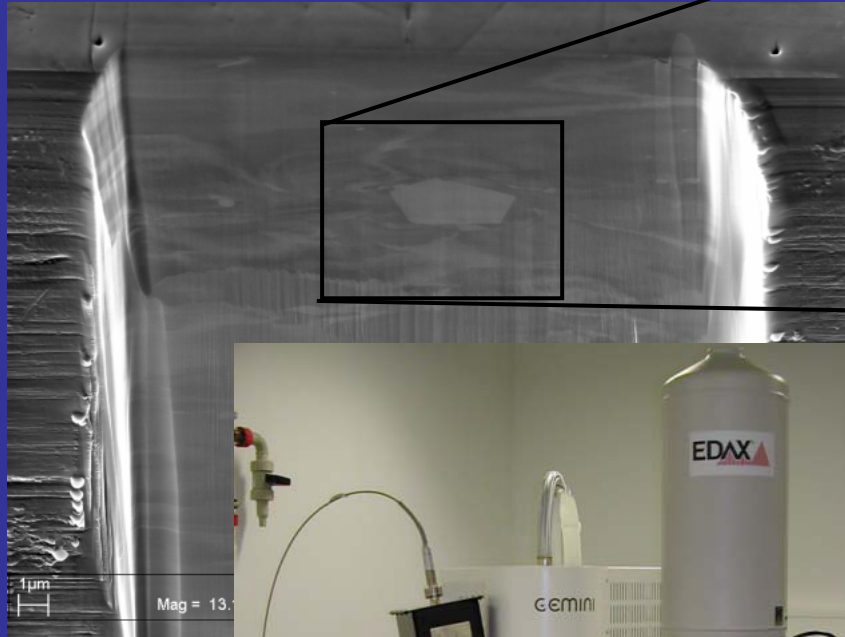
Structural aerospace and turbines

Numerical laboratories

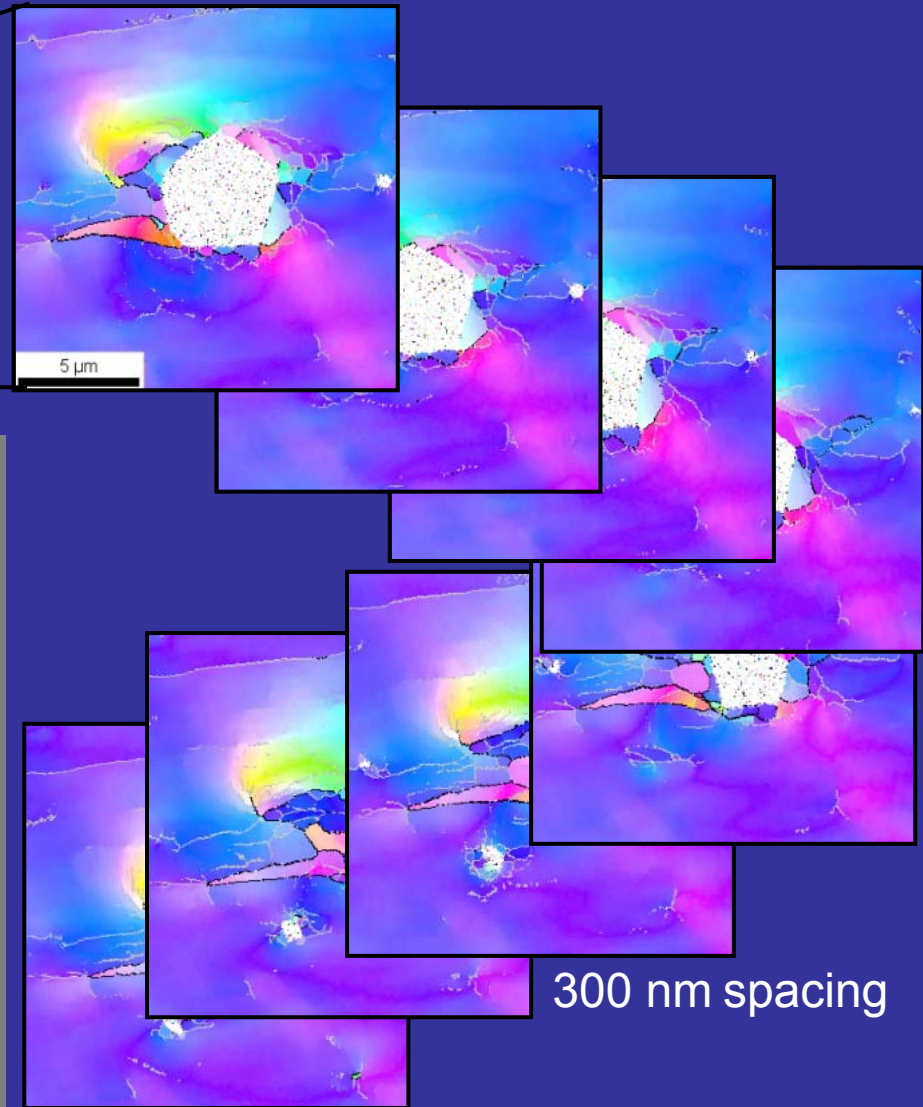
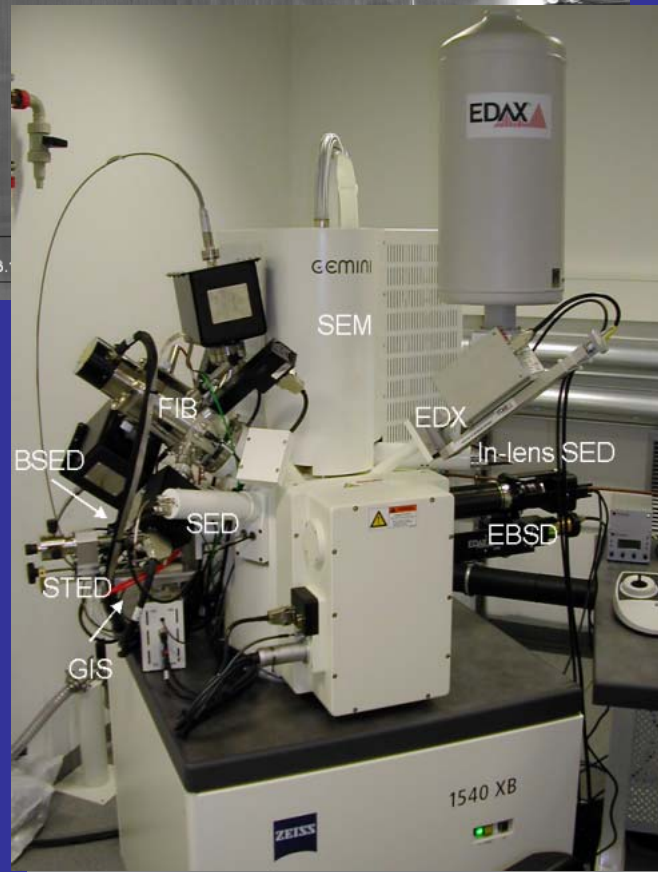
Homogenization Theory

Micromechanics and damage

3D electron orientation microscopy



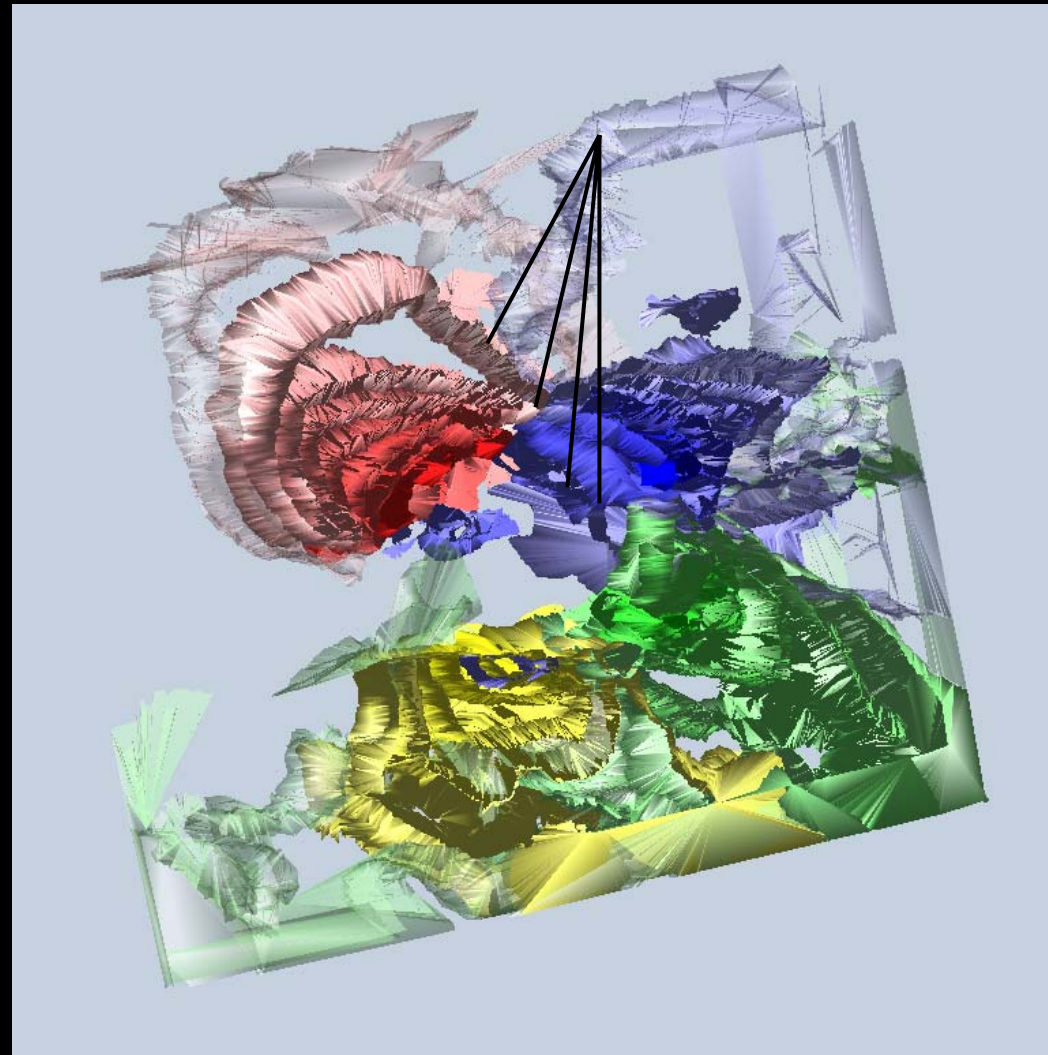
SE-image



3D electron orientation microscopy



5° misorientation steps from shell to shell



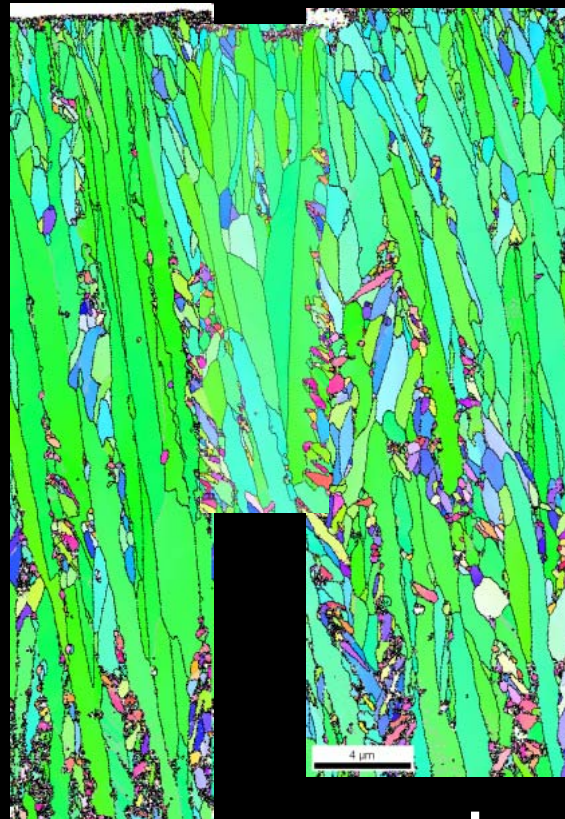
lattice rotations around Laves phase
in Fe_3Al

3D : EBSD, EDX, SEM, FIB

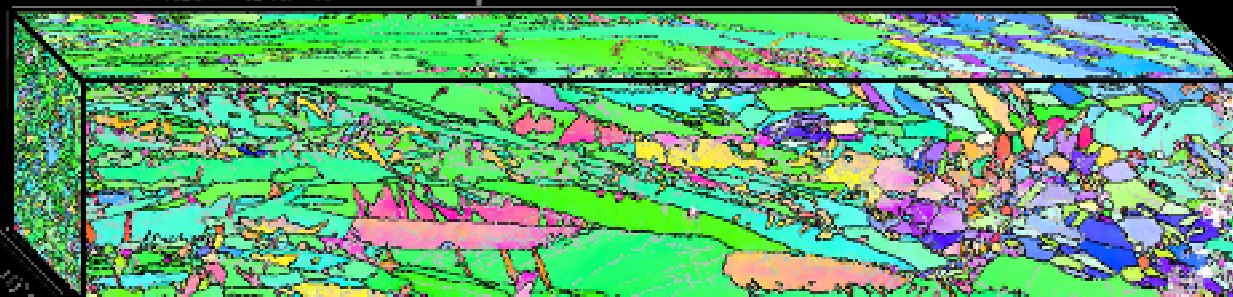
3D electron orientation microscopy

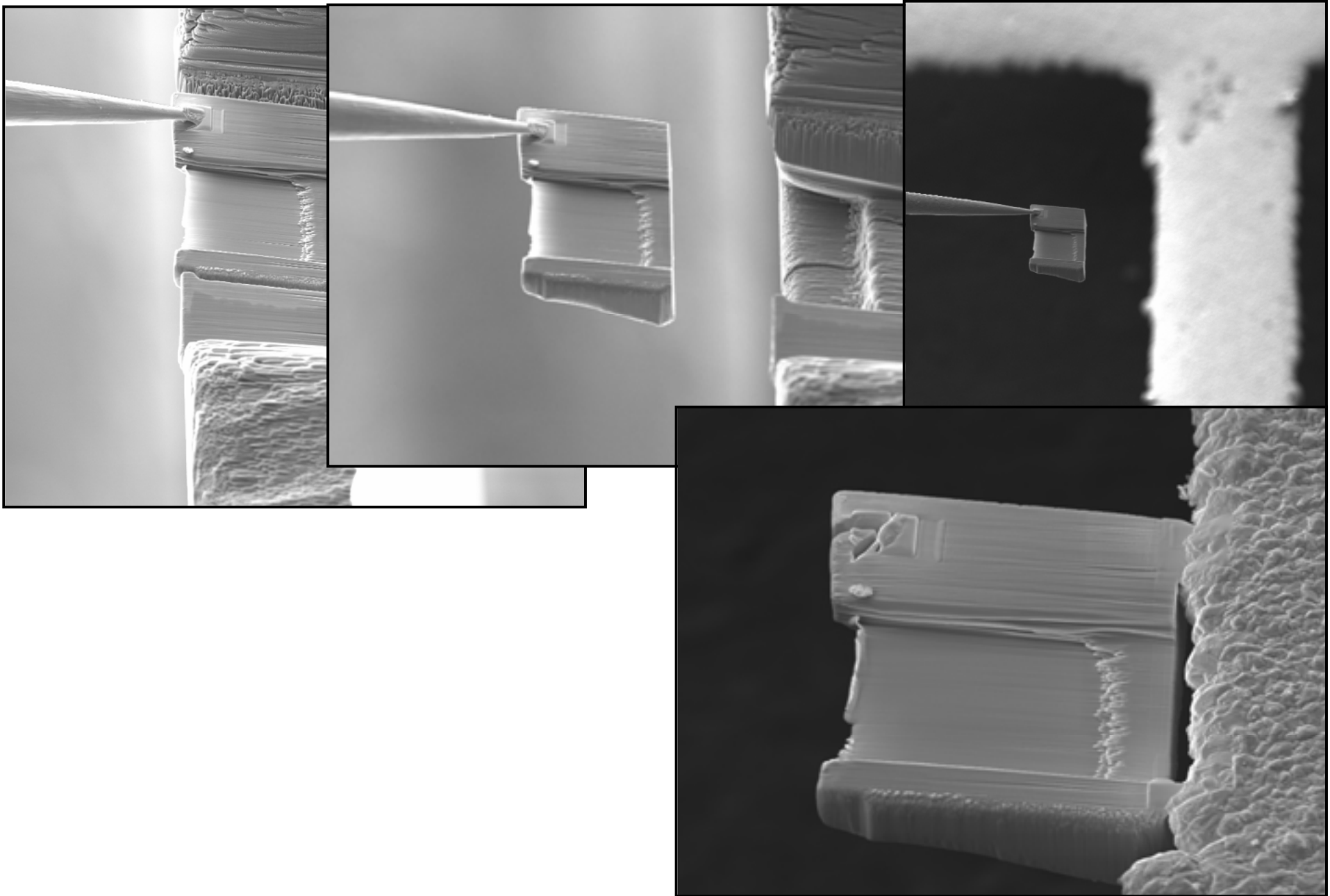


isolated pyramid



cross view





Multiphase Materials

Professor Dierk Raabe, MPI, d.raabe@mpie.de

Methods and systematics



1) structure, texture

TEM, SEM, EBSD, EDX, FIB, X-ray (lab-scale), Synchrotron

2) properties

indentation, compression tests, tensile tests, photogrammetry

3) specimens

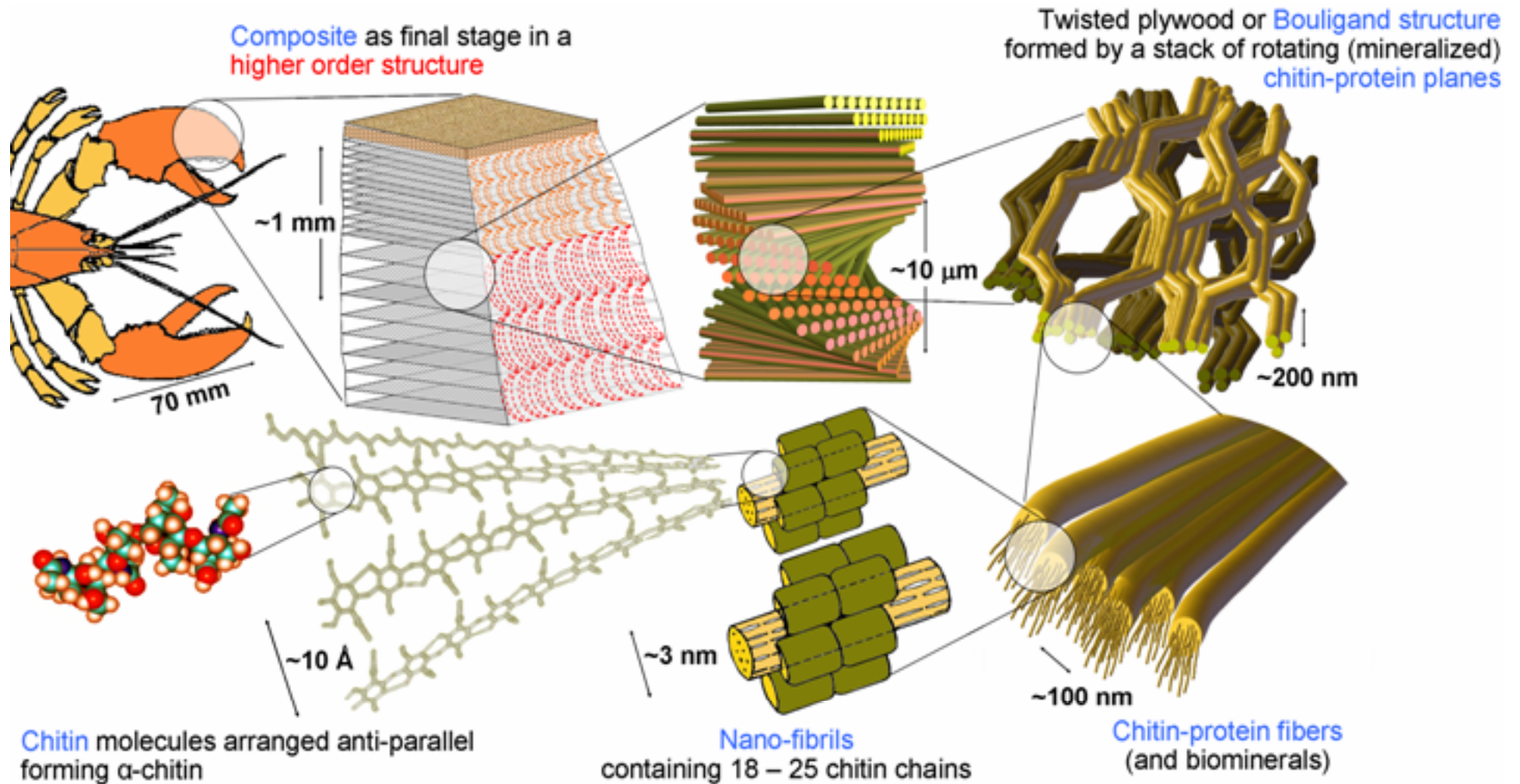
mineralized chitin-protein tissue

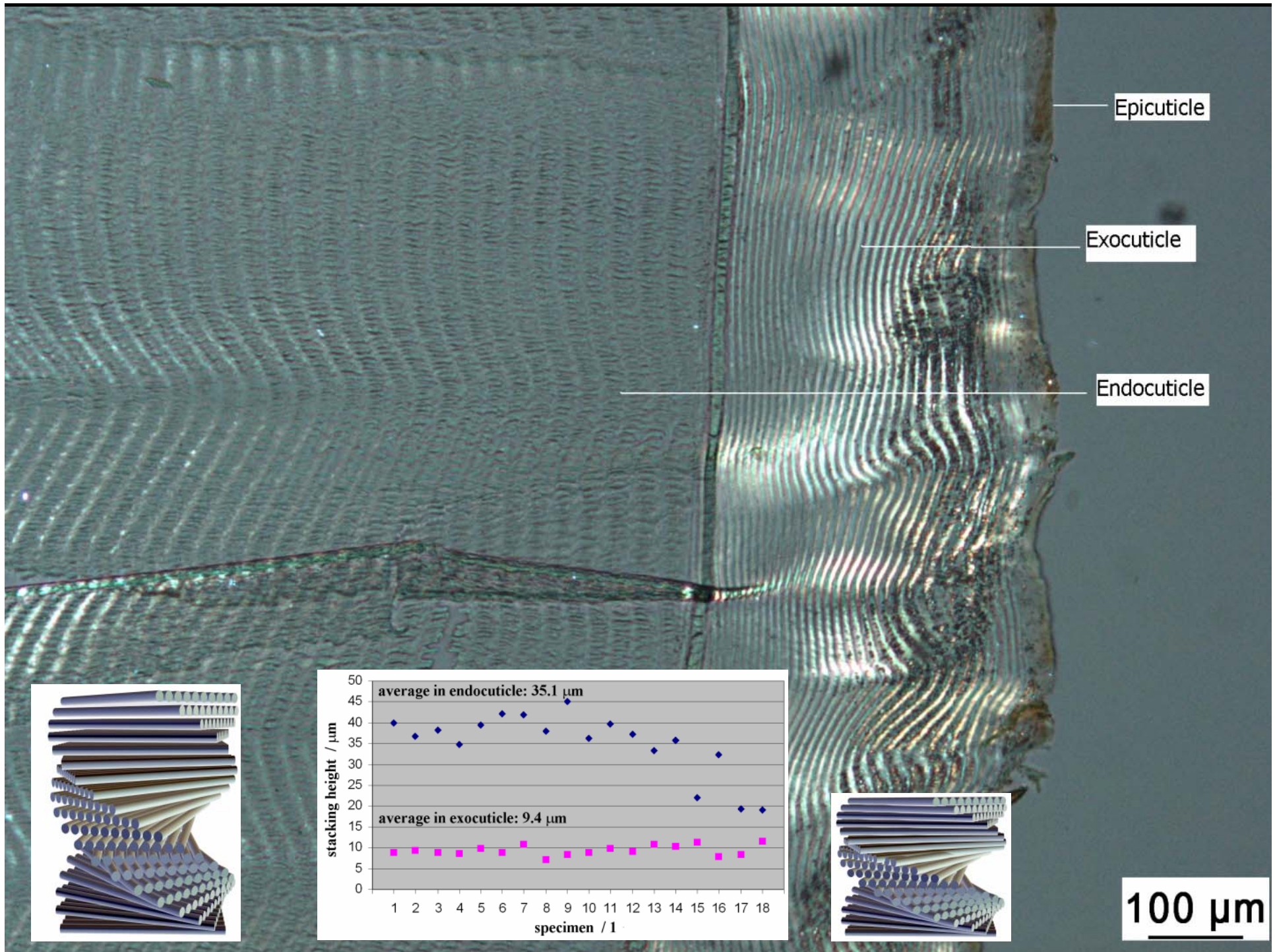


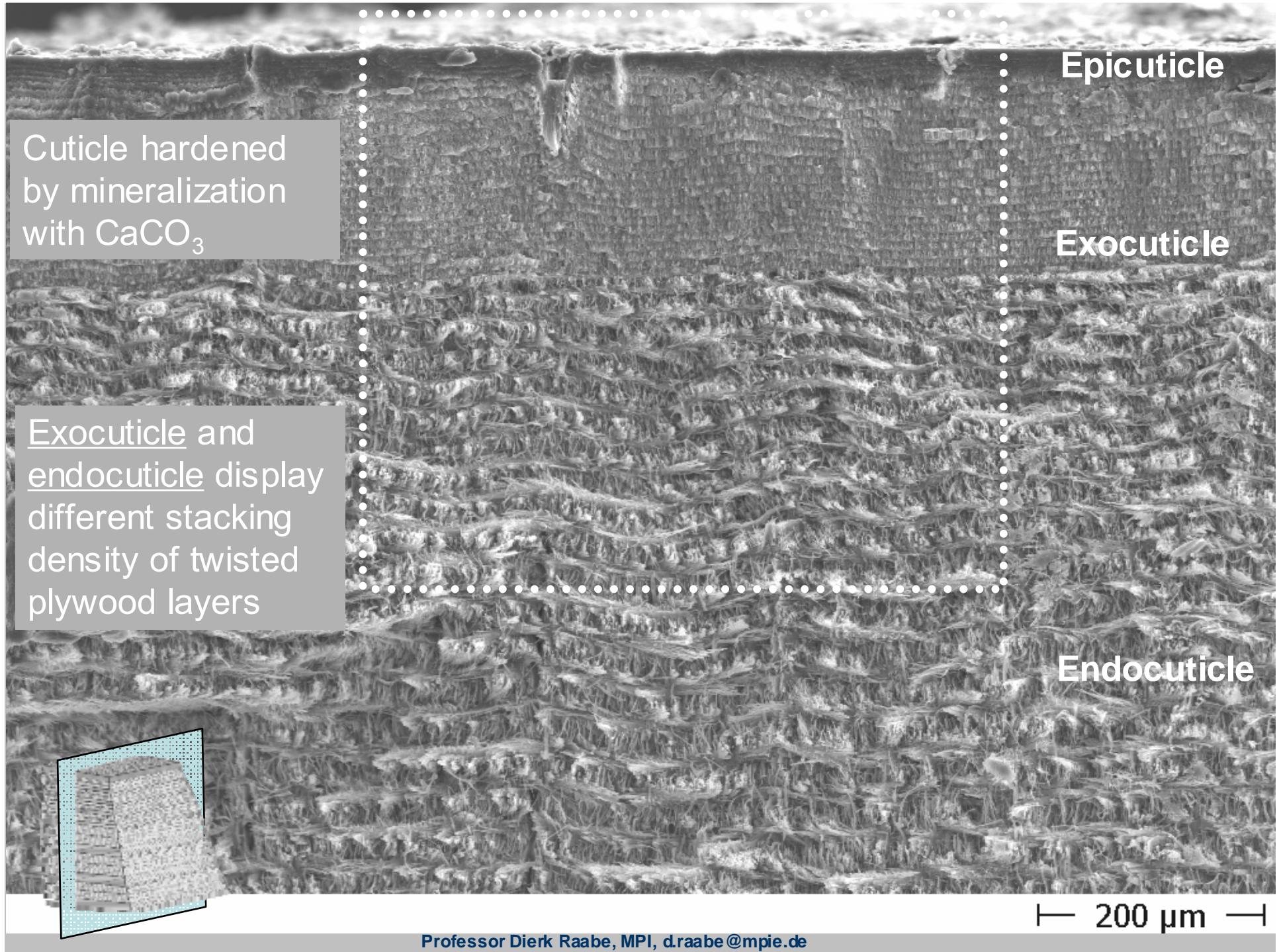
mineral content



Structure Hierarchy (*Homarus americanus*)







Cuticle hardened by mineralization with CaCO_3

Exocuticle and endocuticle display different stacking density of twisted plywood layers

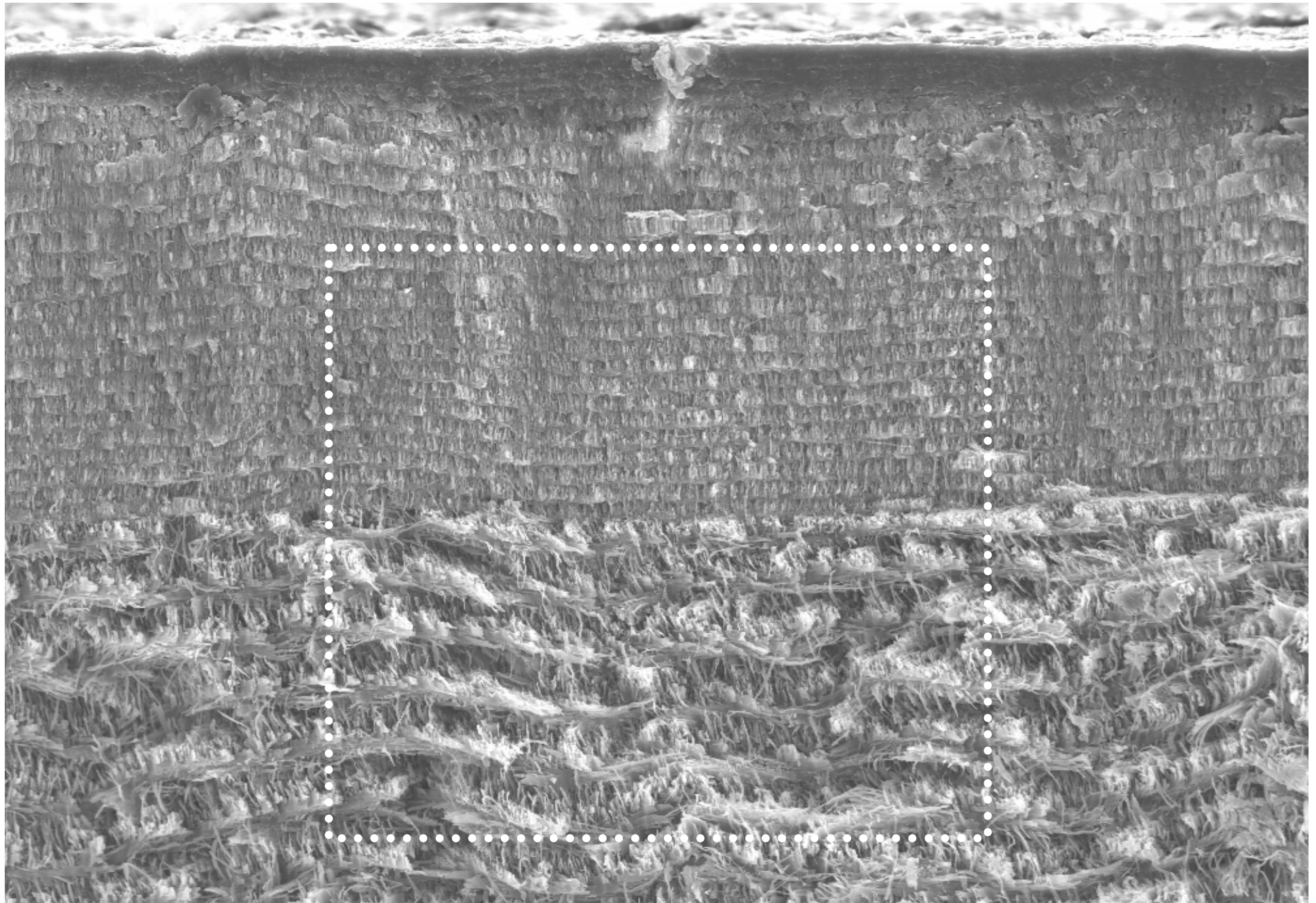
Epicuticle

Exocuticle

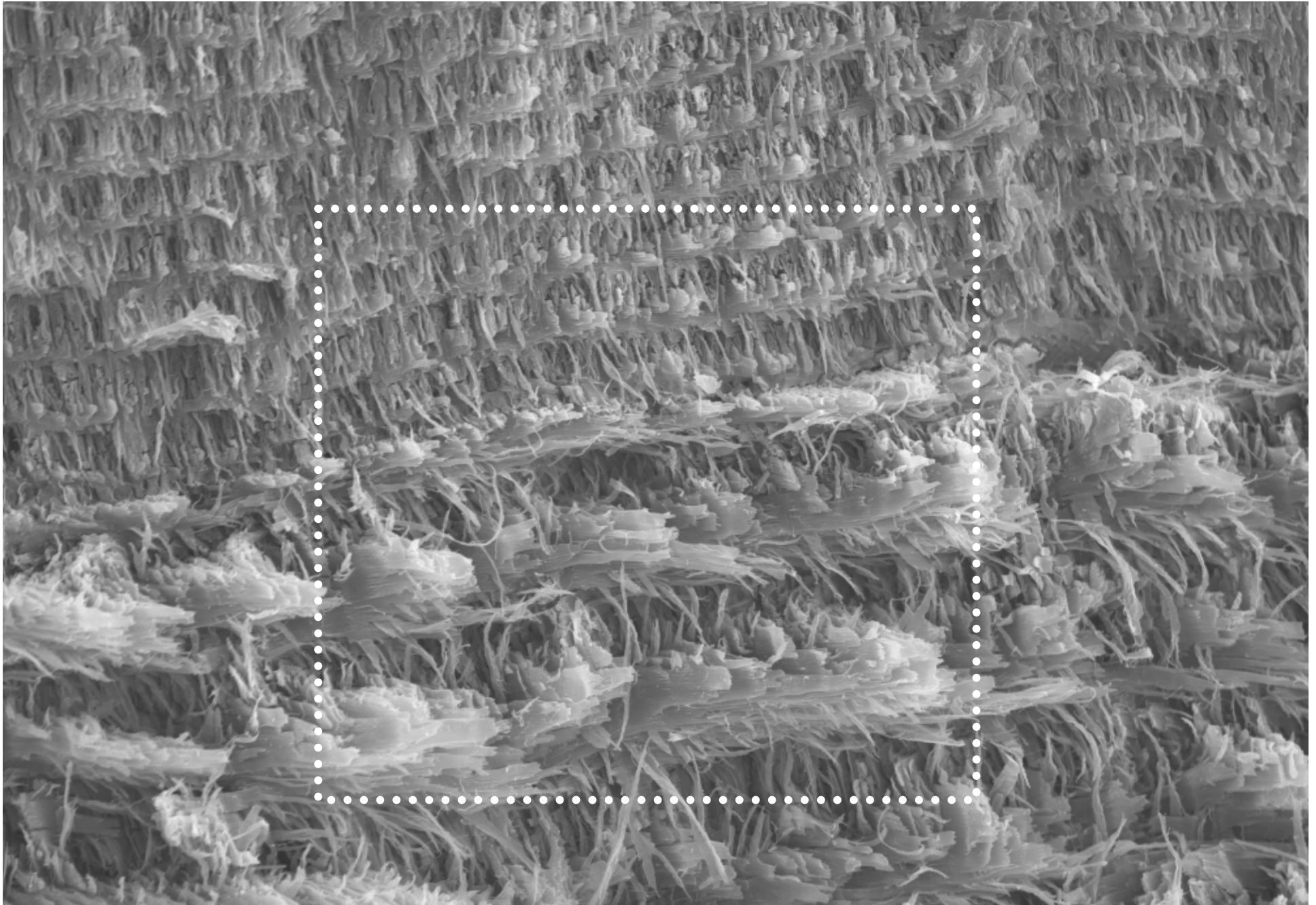
Endocuticle

— 200 μm —

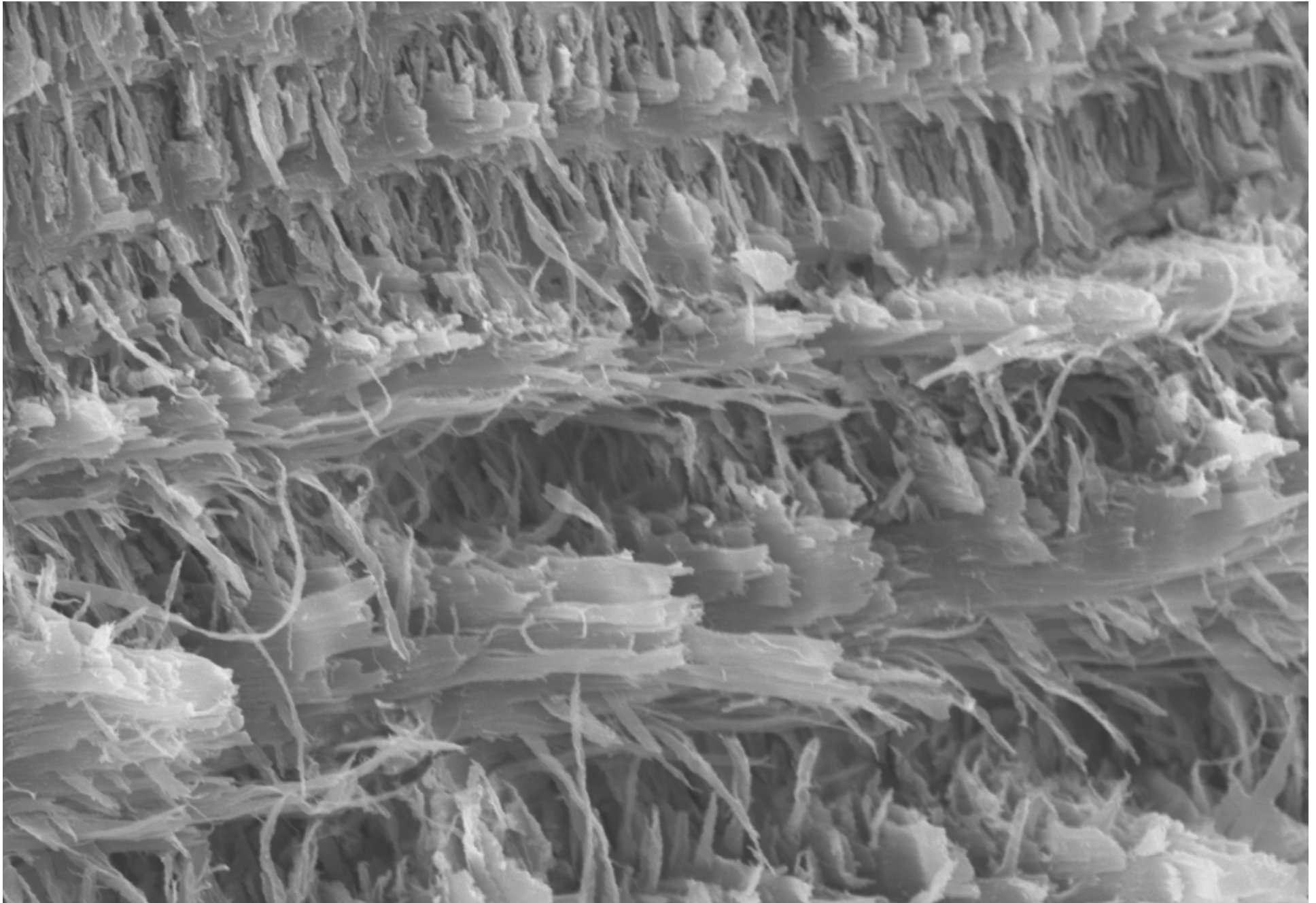




— 100 μm —

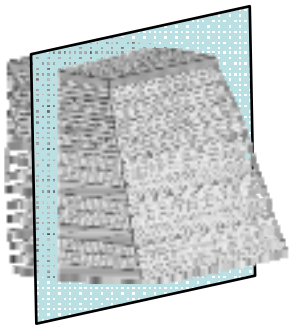
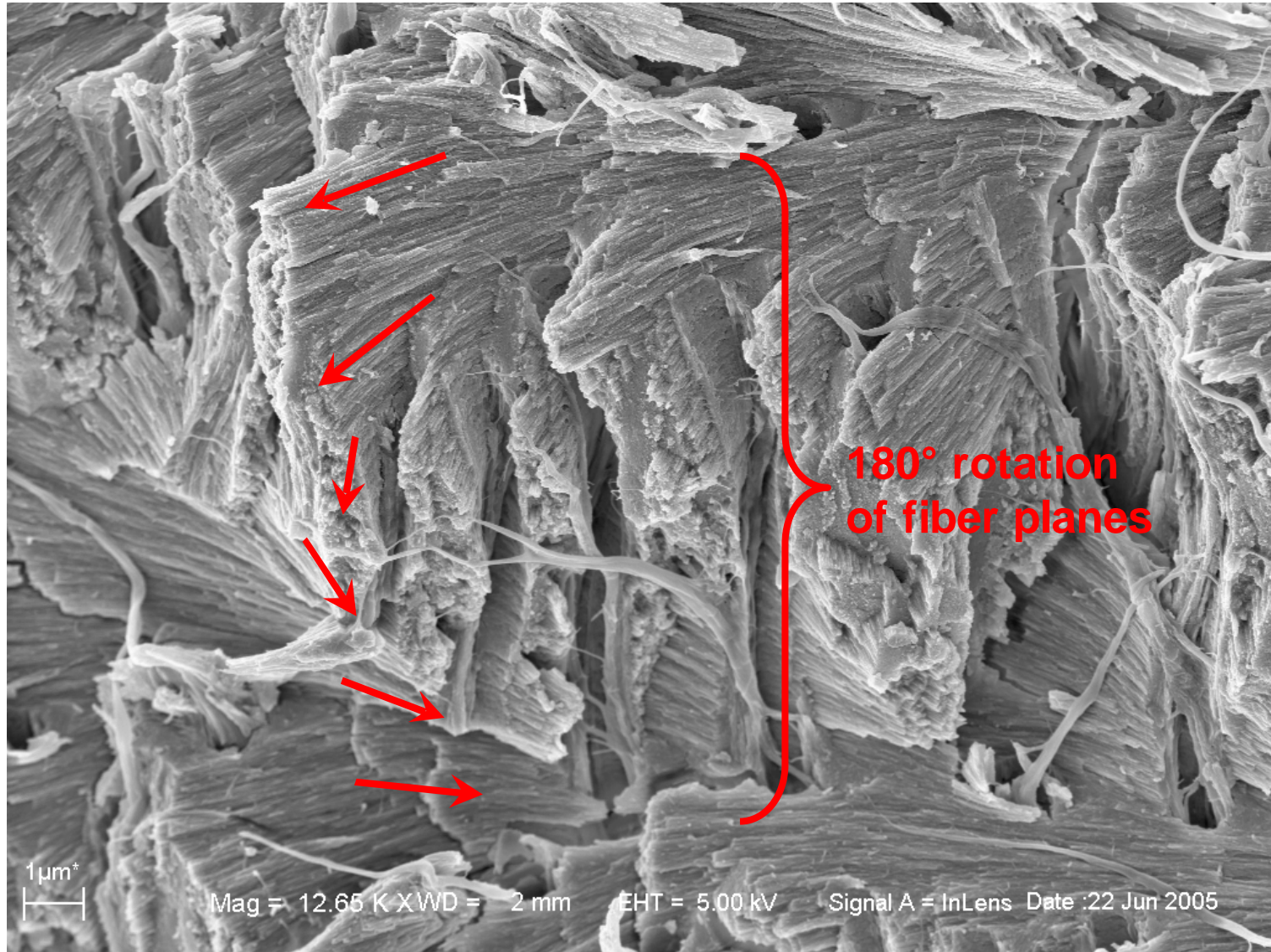


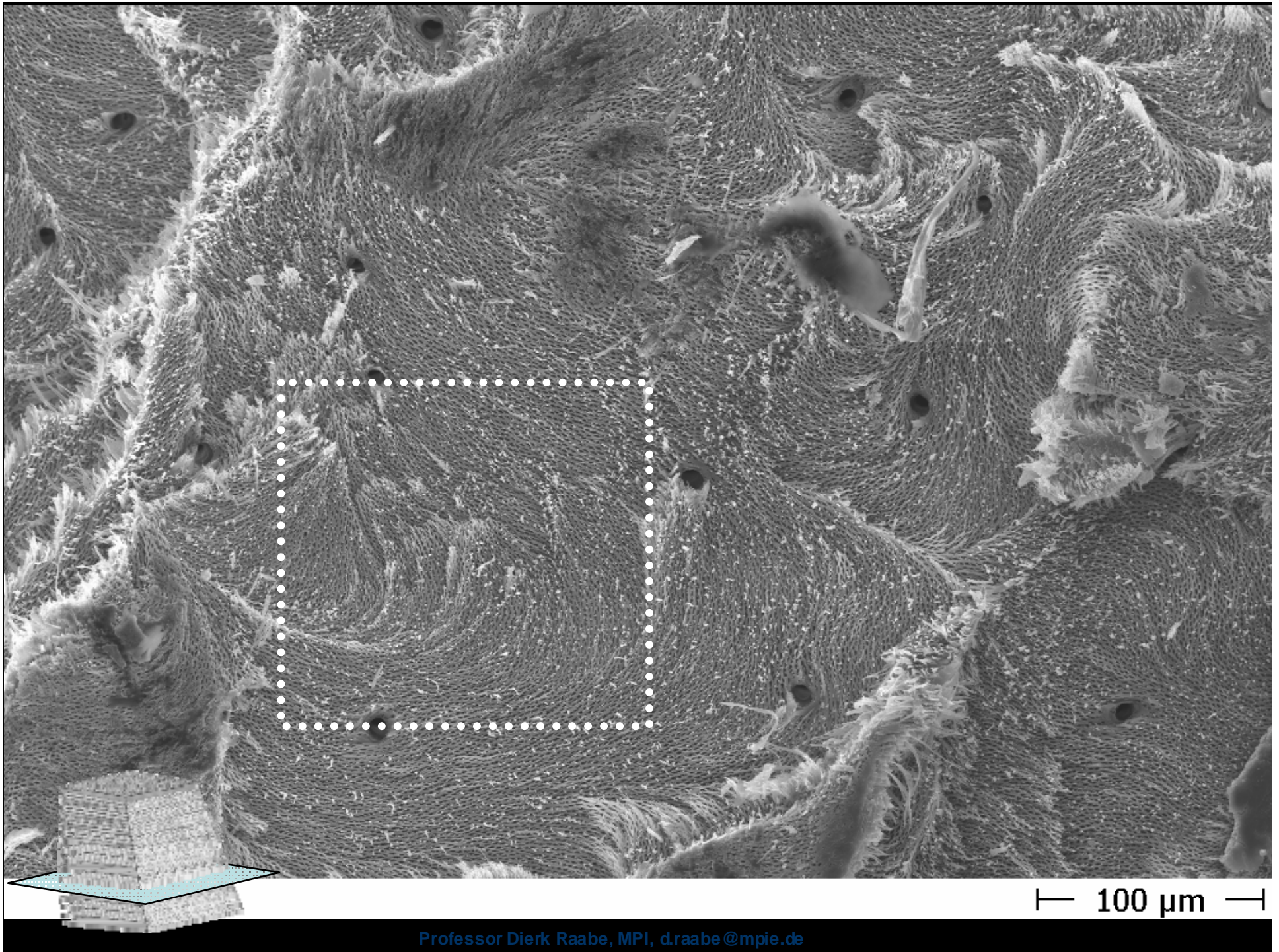
— 30 μm —

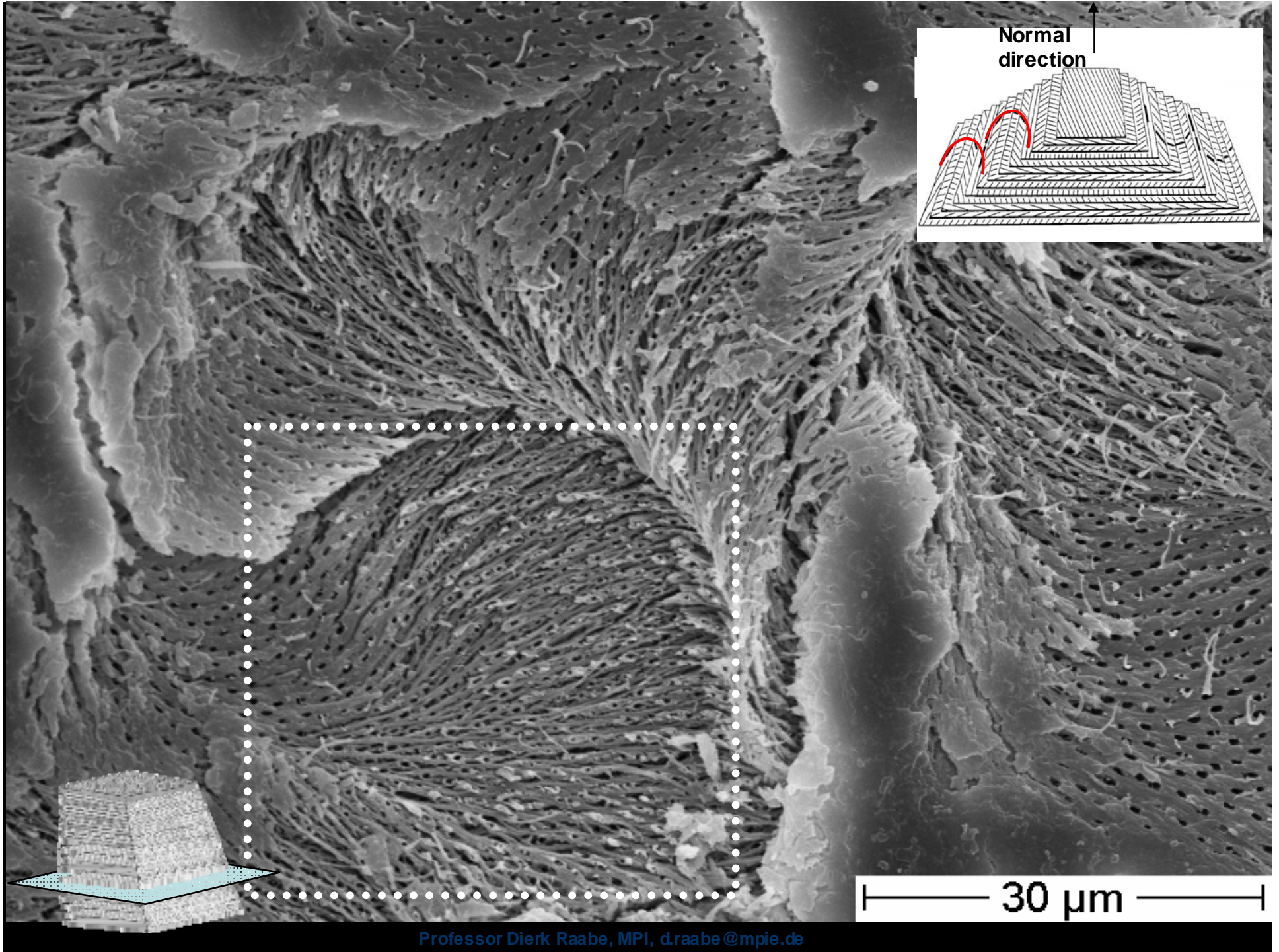


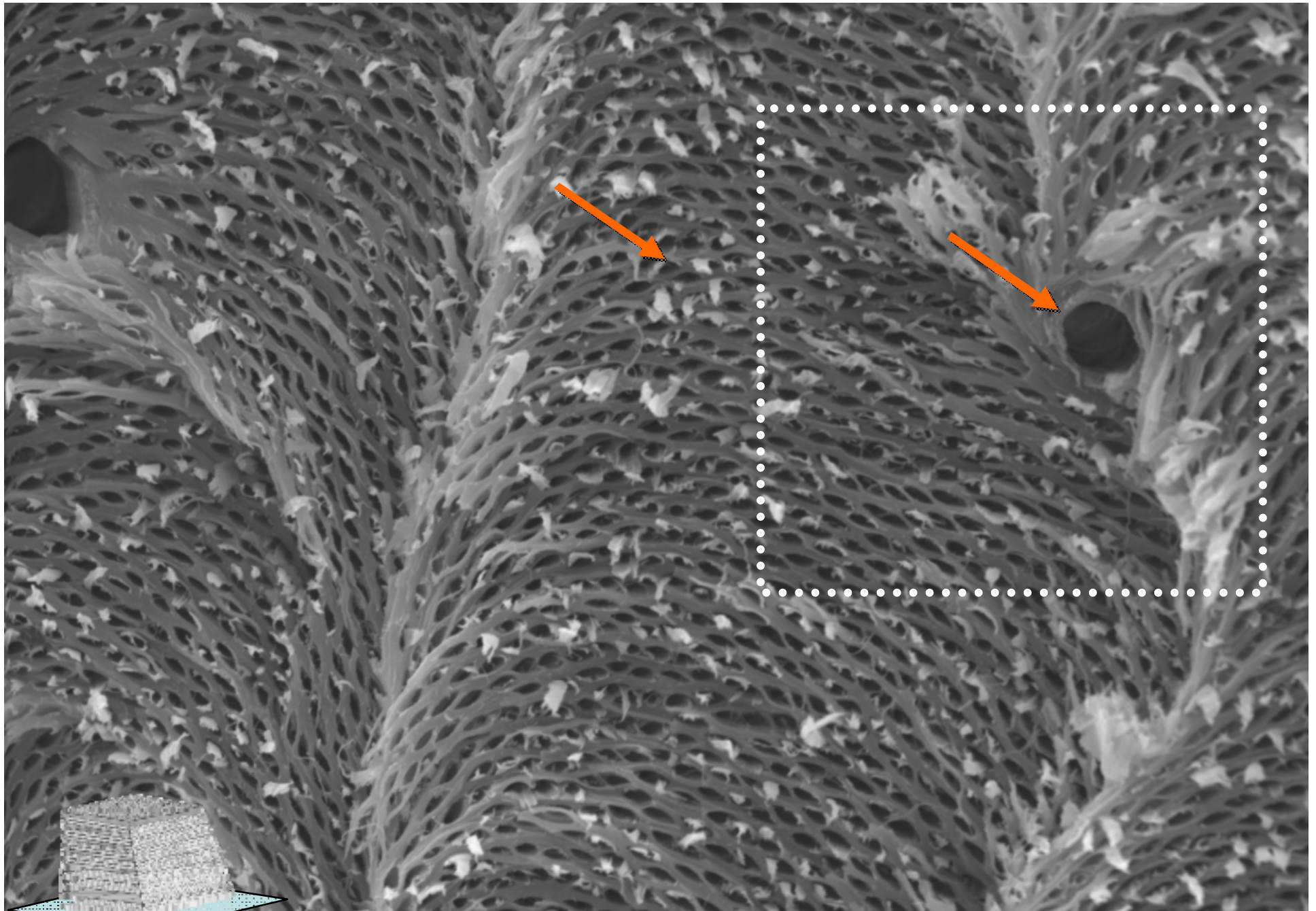
┌ 10 μm ┐

SEM: Lobster endocuticle, untreated



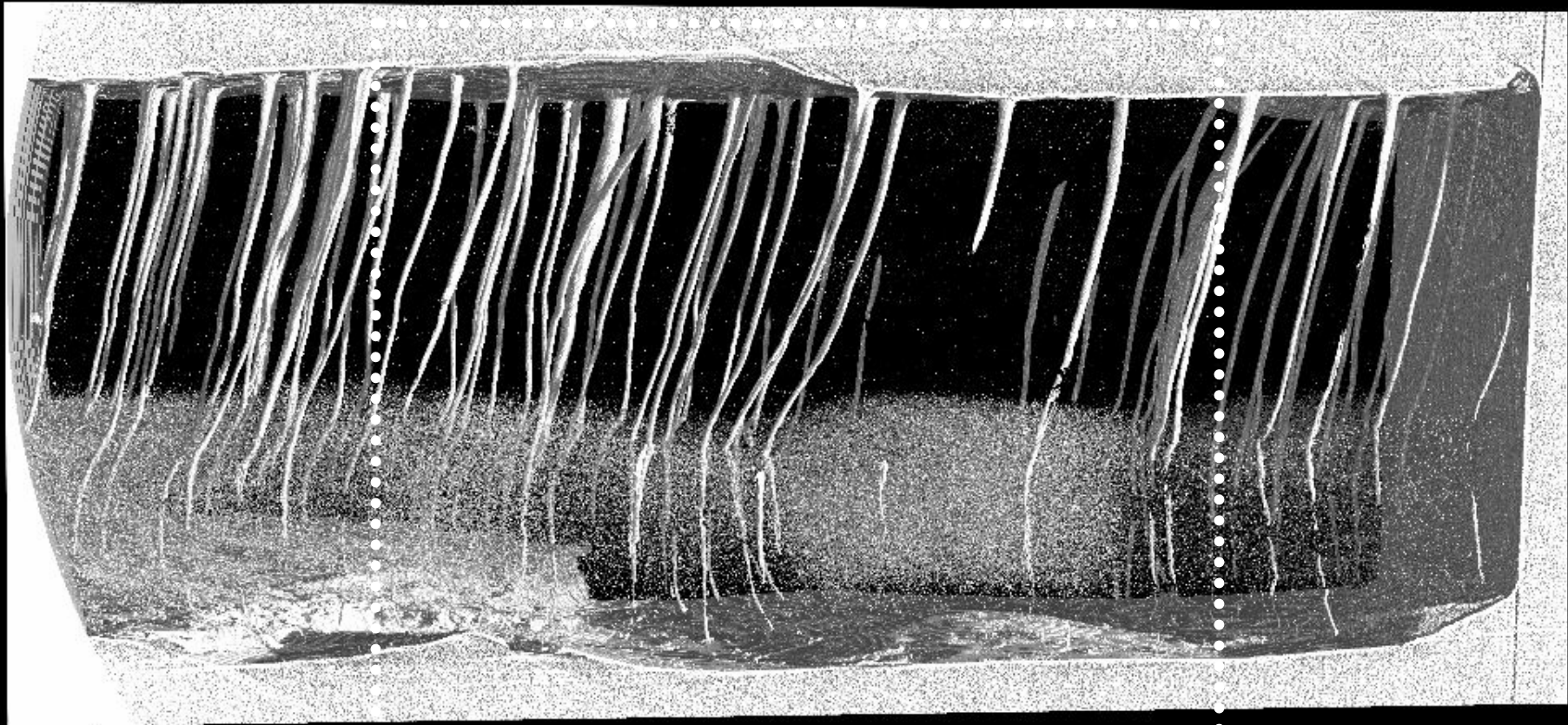






— 20 μm —

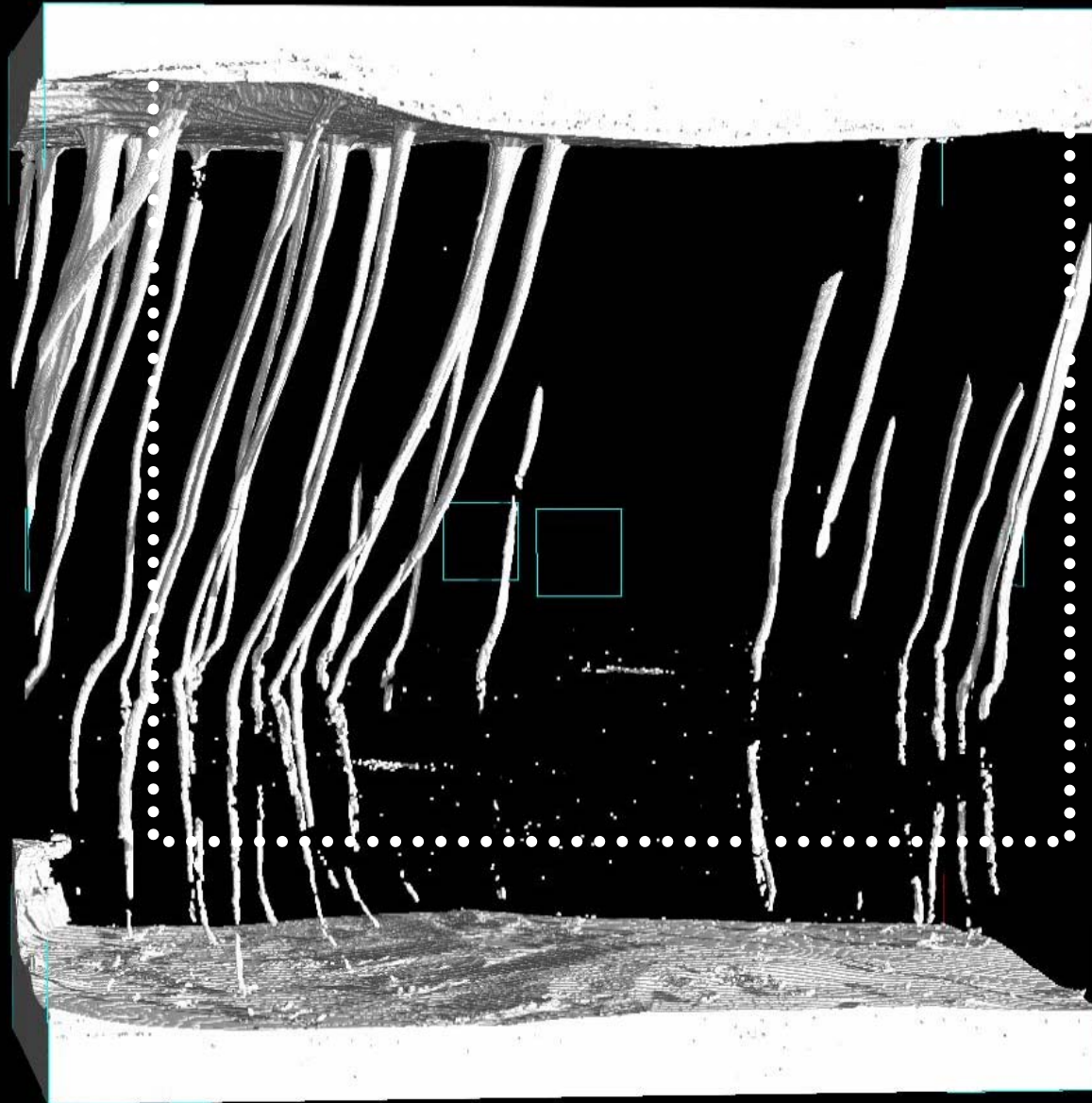
X-ray tomography, cuticle, horseshoe crab



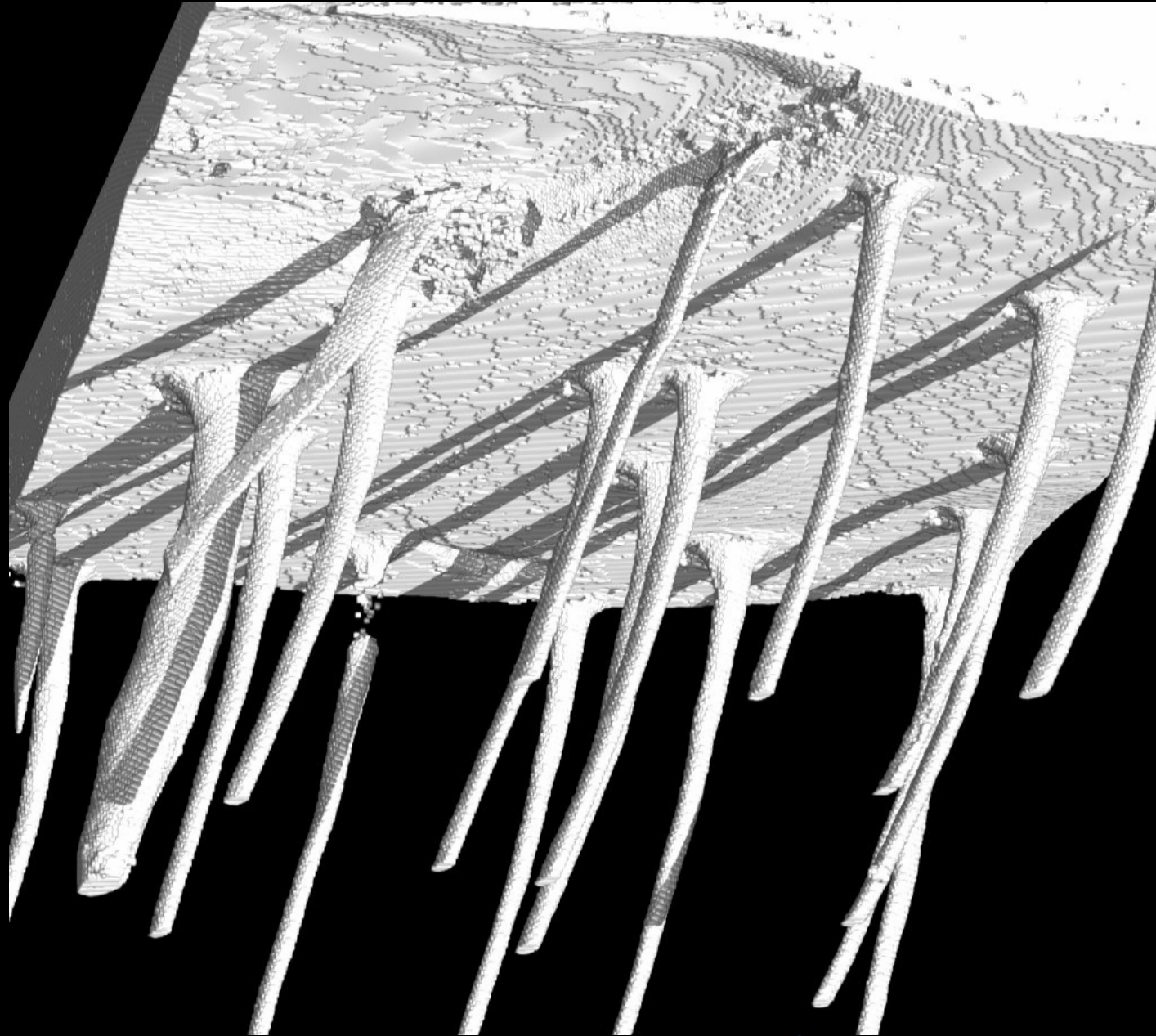
measurements at : HMI Berlin

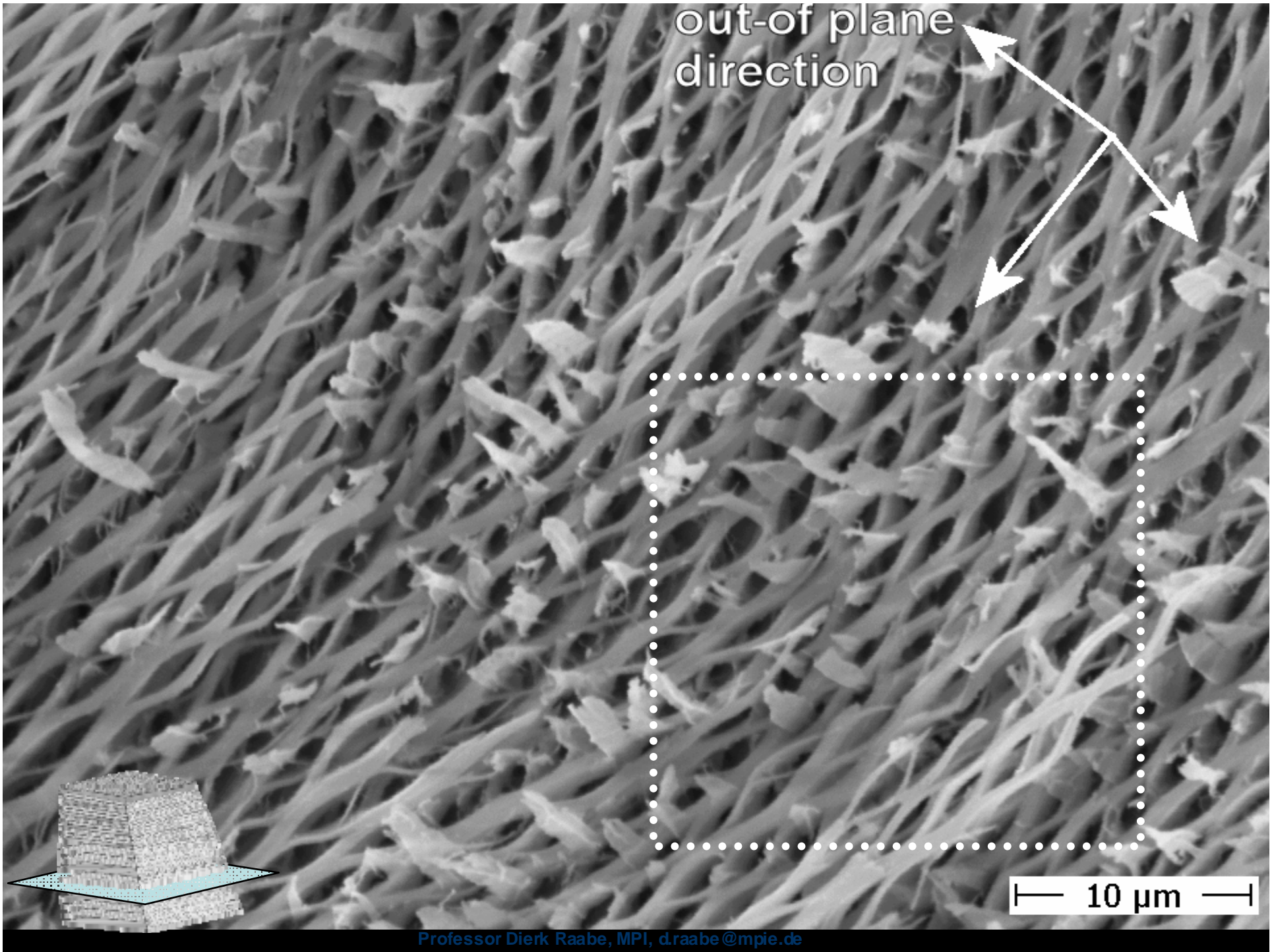
Professor Dierk Raabe, MPI, d.raabe@mpie.de

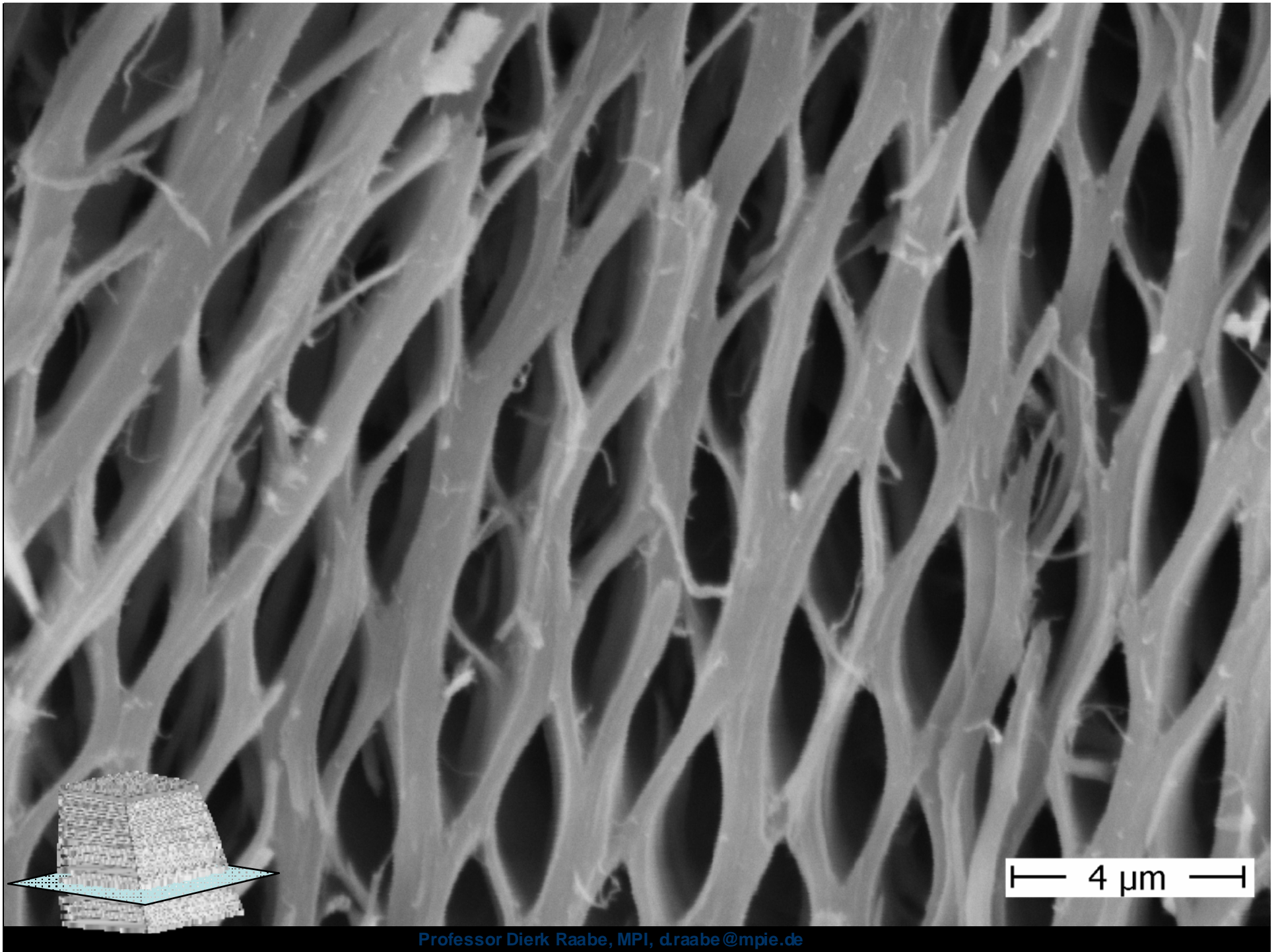
X-ray tomography, cuticle, horseshoe crab

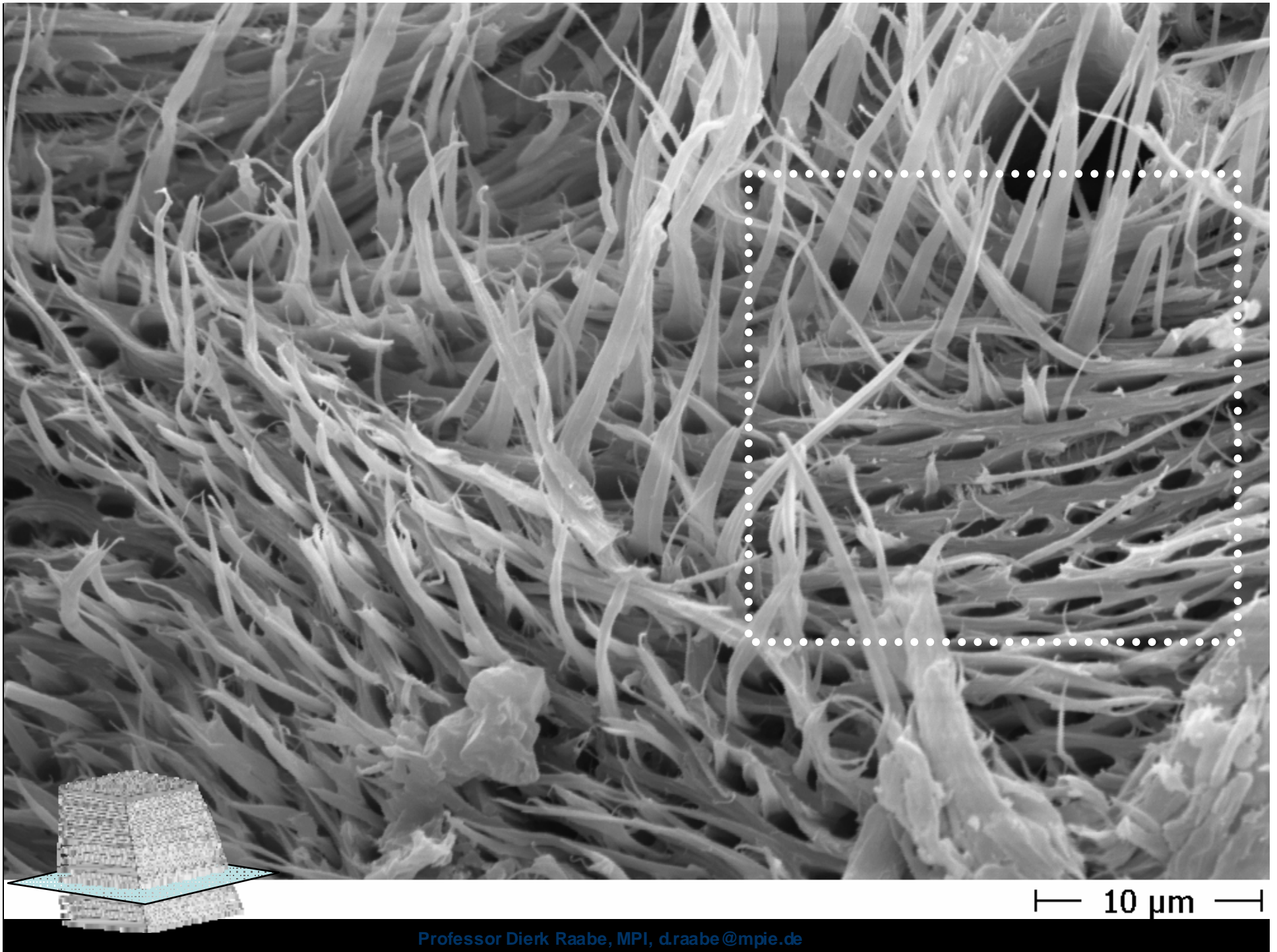


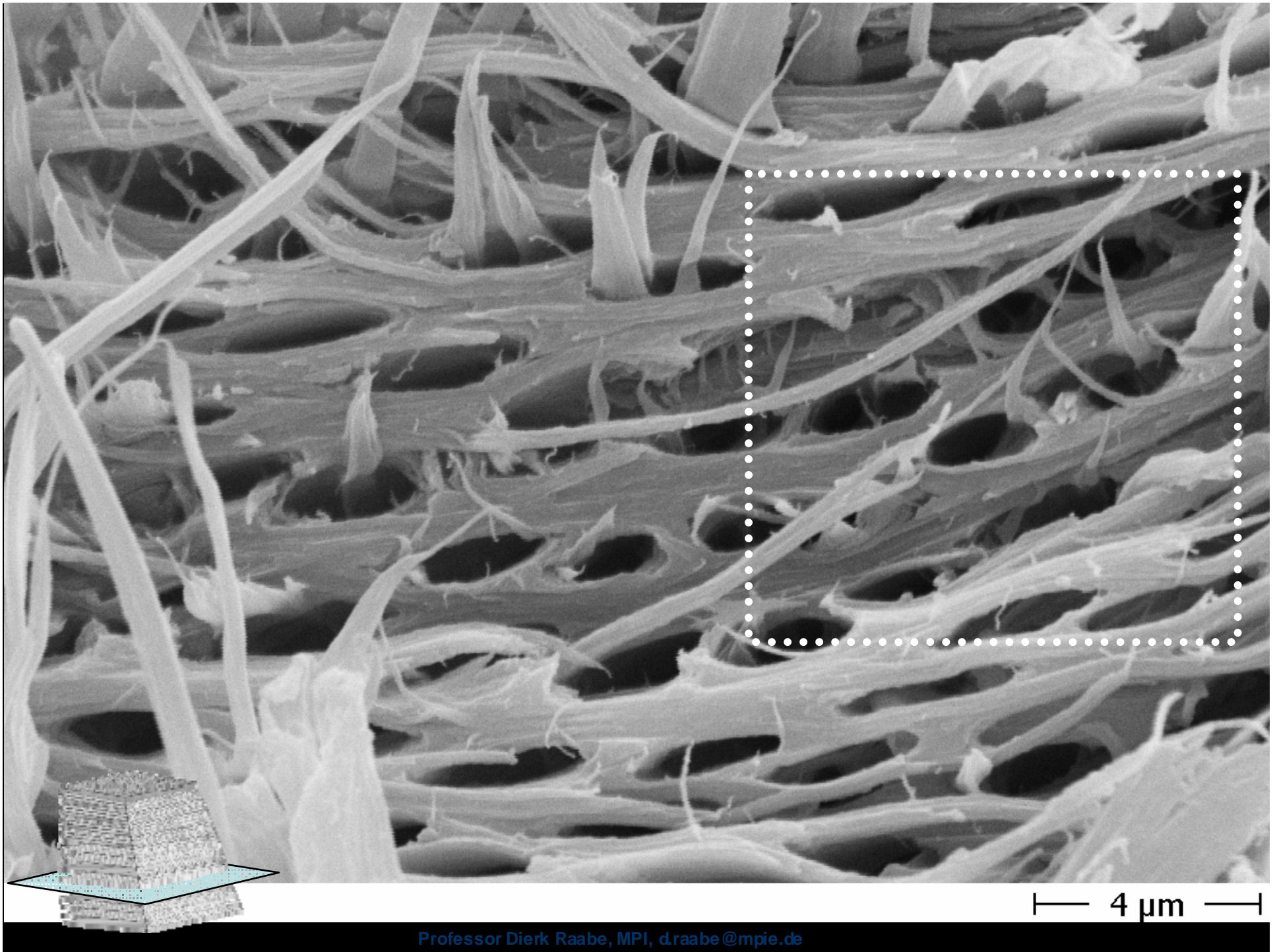
X-ray tomography, cuticle, horseshoe crab

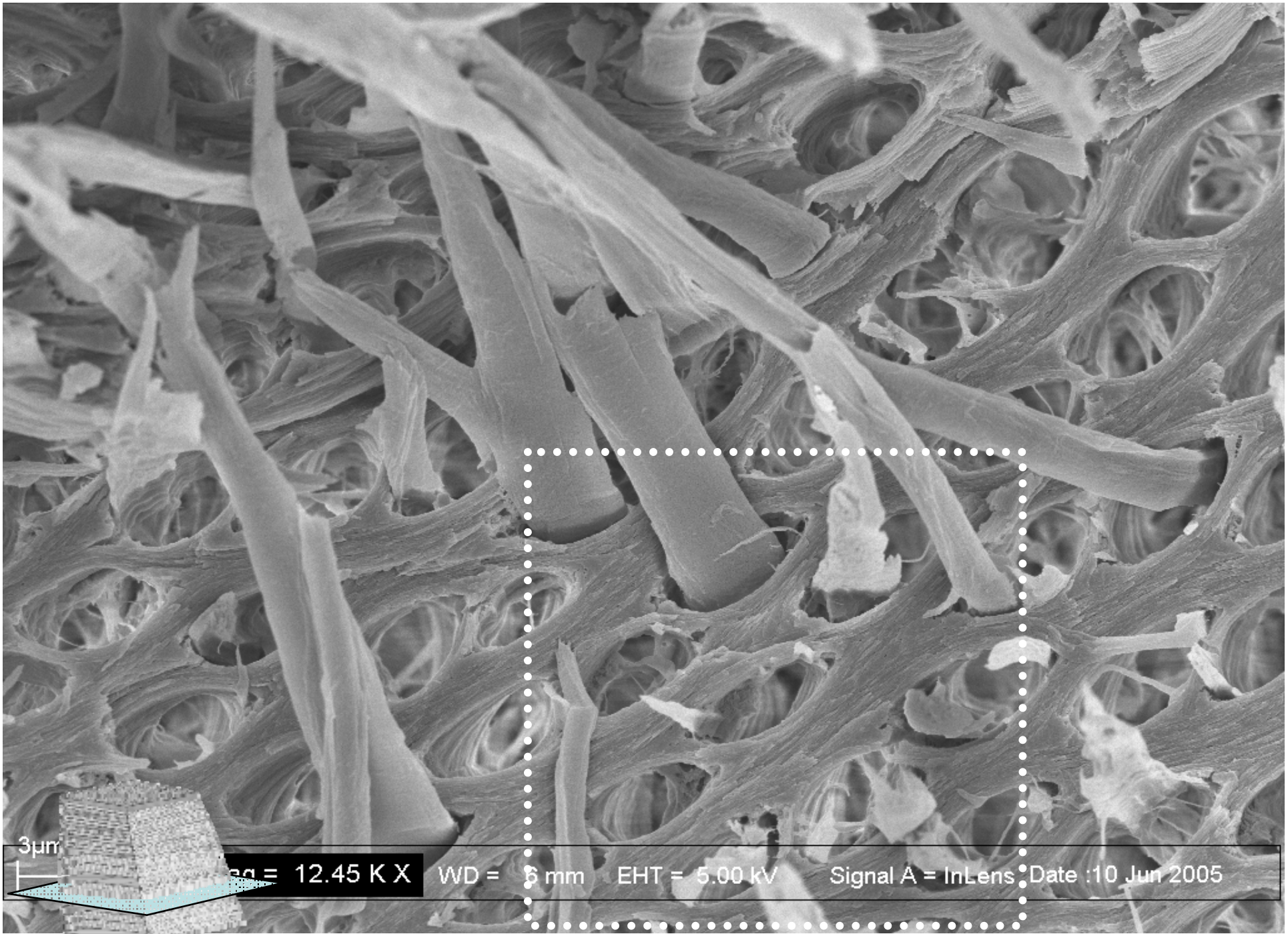


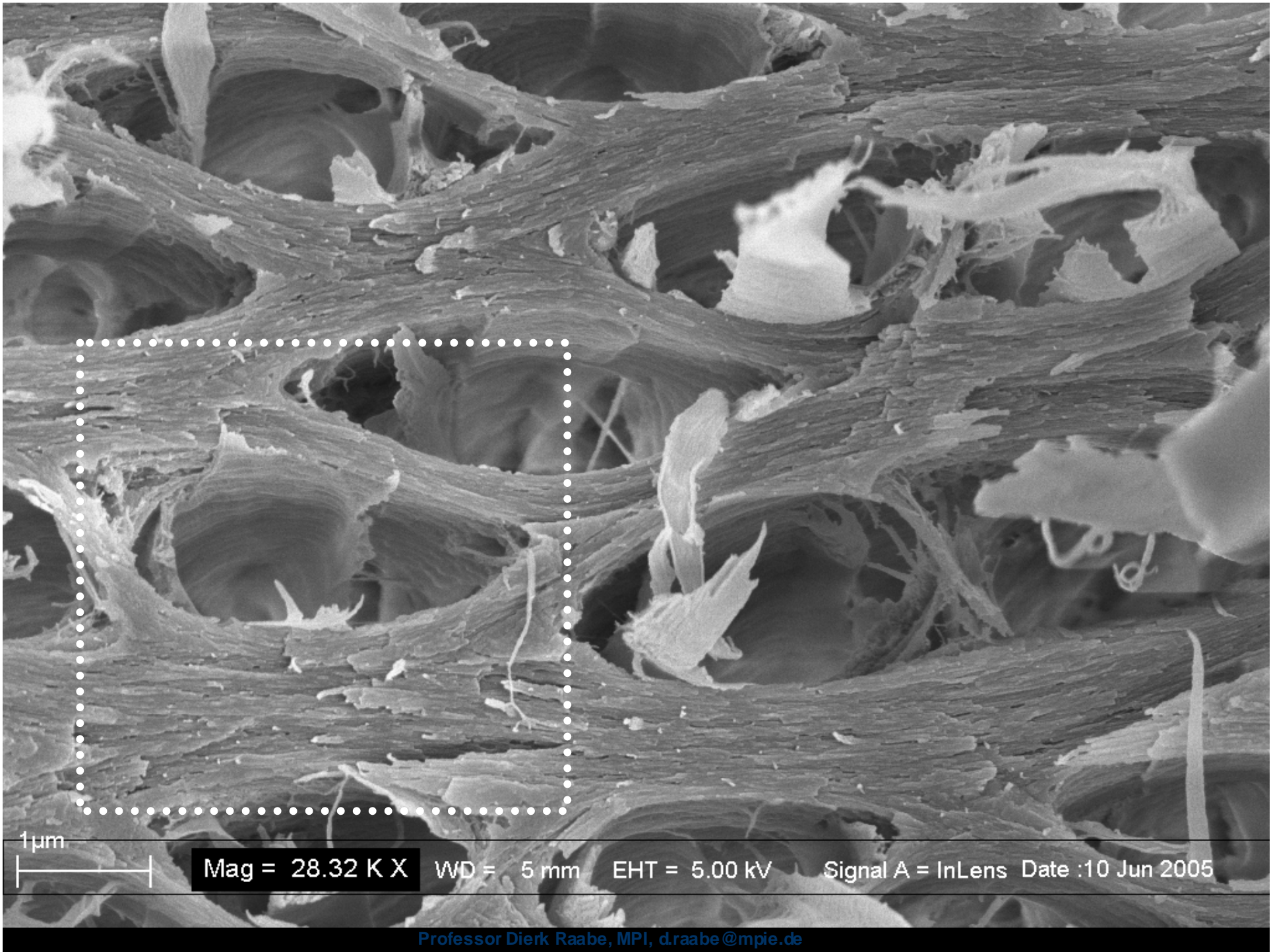


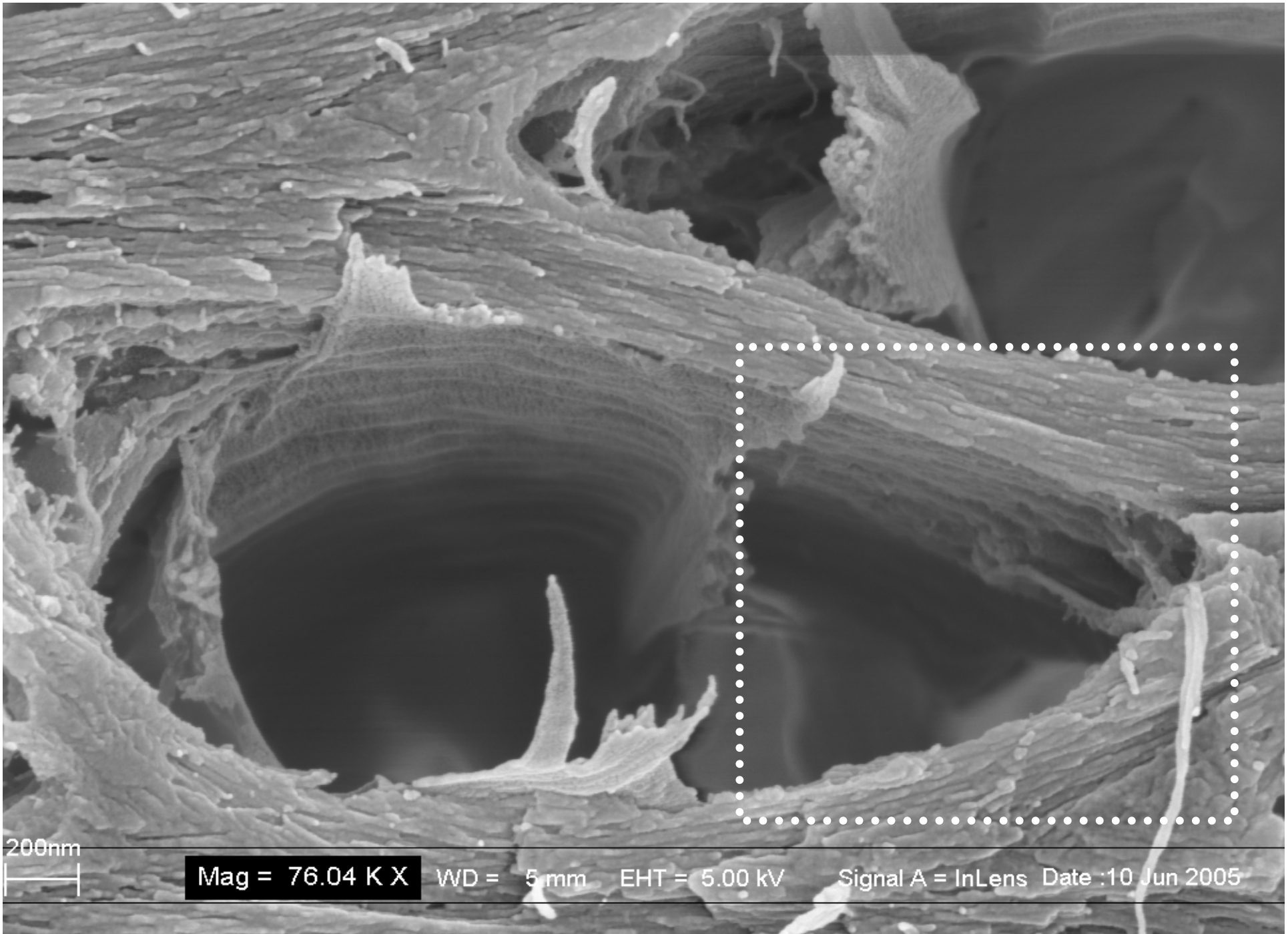










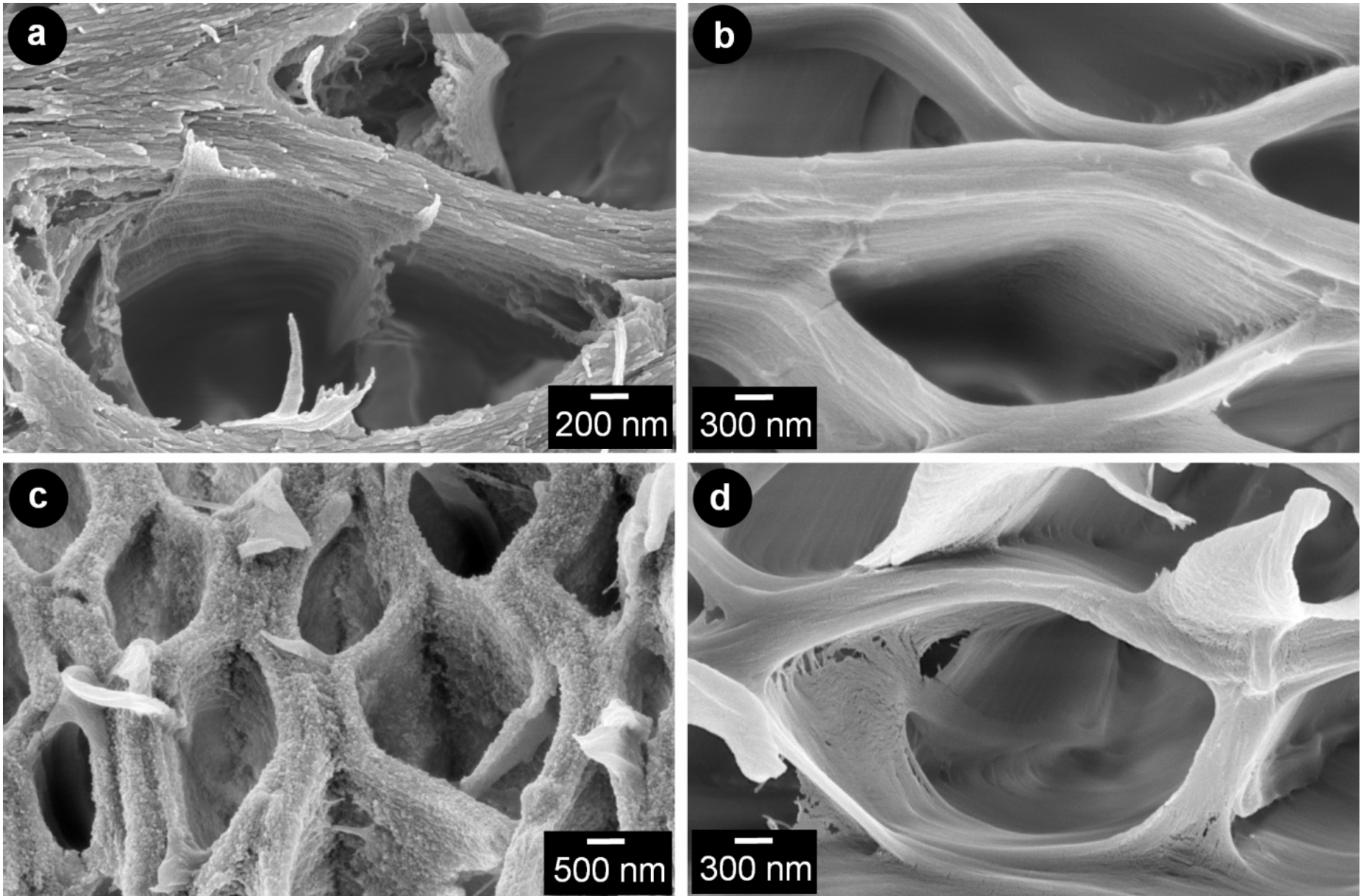




100nm

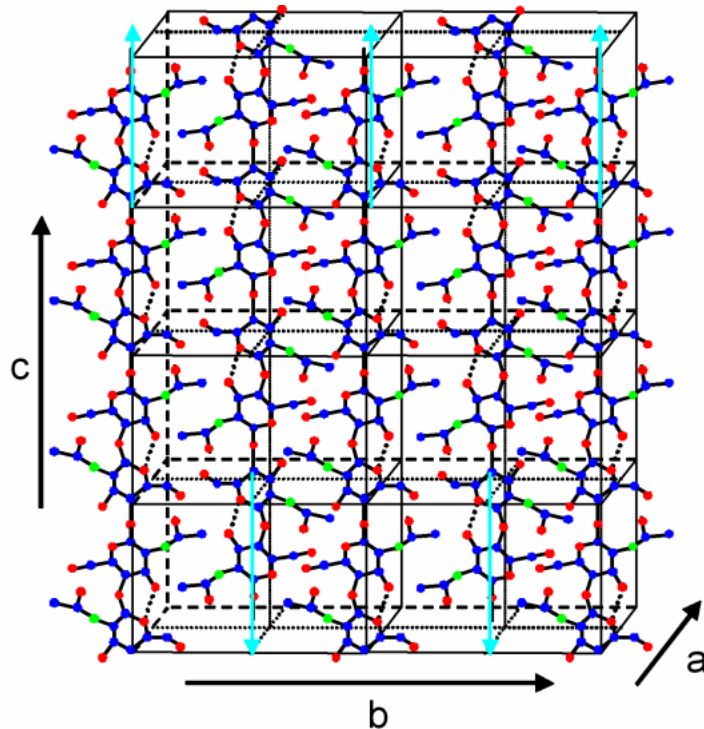


Mag = 133.31 K X WD = 5 mm EHT = 5.00 kV Signal A = InLens Date :9 Jun 2005

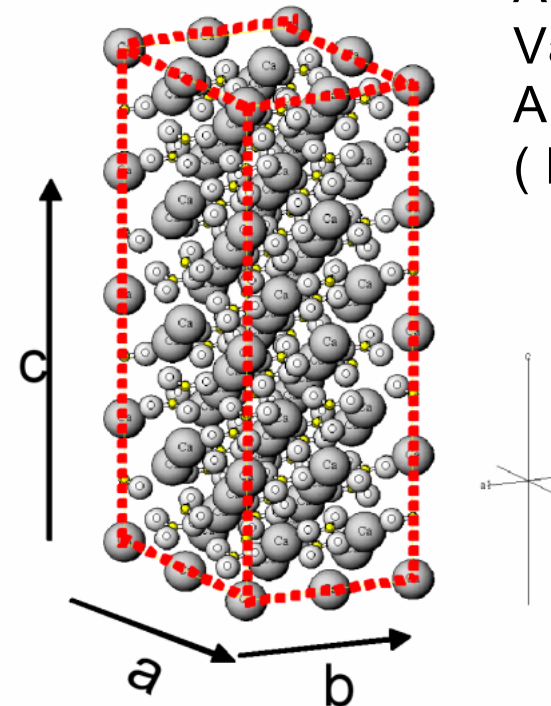


(a) Untreated cuticle, (b) decalcified cuticle (EDTA, 0.15M), (c) deproteined cuticle (NaOH, 1M) and (d) decalcified and deproteined cuticle (EDTA, 0.15M + NaOH, 1M).

Phases and crystallography in crustaceans



CC (calcite)
ACC
Vaterite
Aragonite
(Mg !)



- Density: 1,41 gm/cm³
- Lin. absorption coef : 3700 μm^{-1} (@14 KeV(~ 1 Å))
- Orthorhombic **a= 4.74 Å, b= 18.86 Å, c= 10.32 Å** (Takai et al, 1992)
- Space group: P222 (# 16 @ITC)
- Point group: 222

- Density: 2,71 gm/cm³
- Lin. Absorption Coef. : 200 μm^{-1} (@14 KeV(~ 1 Å))
- Hexagonal , **a=b=4,989 Å, c=17.062 Å** (Maslen et al. 1993)
- Space group: R -3 2/c (#167 @ITC)
- Point group: -3 2/m

X-ray wide angle diffraction, lobster



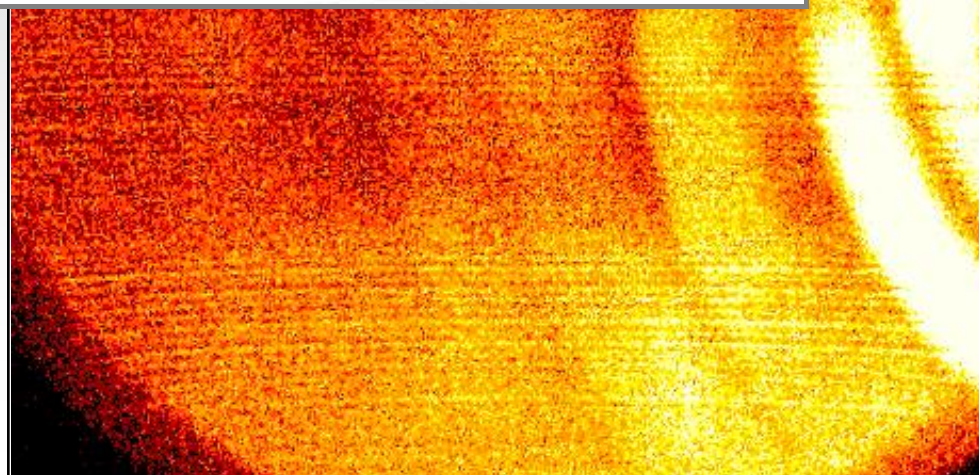
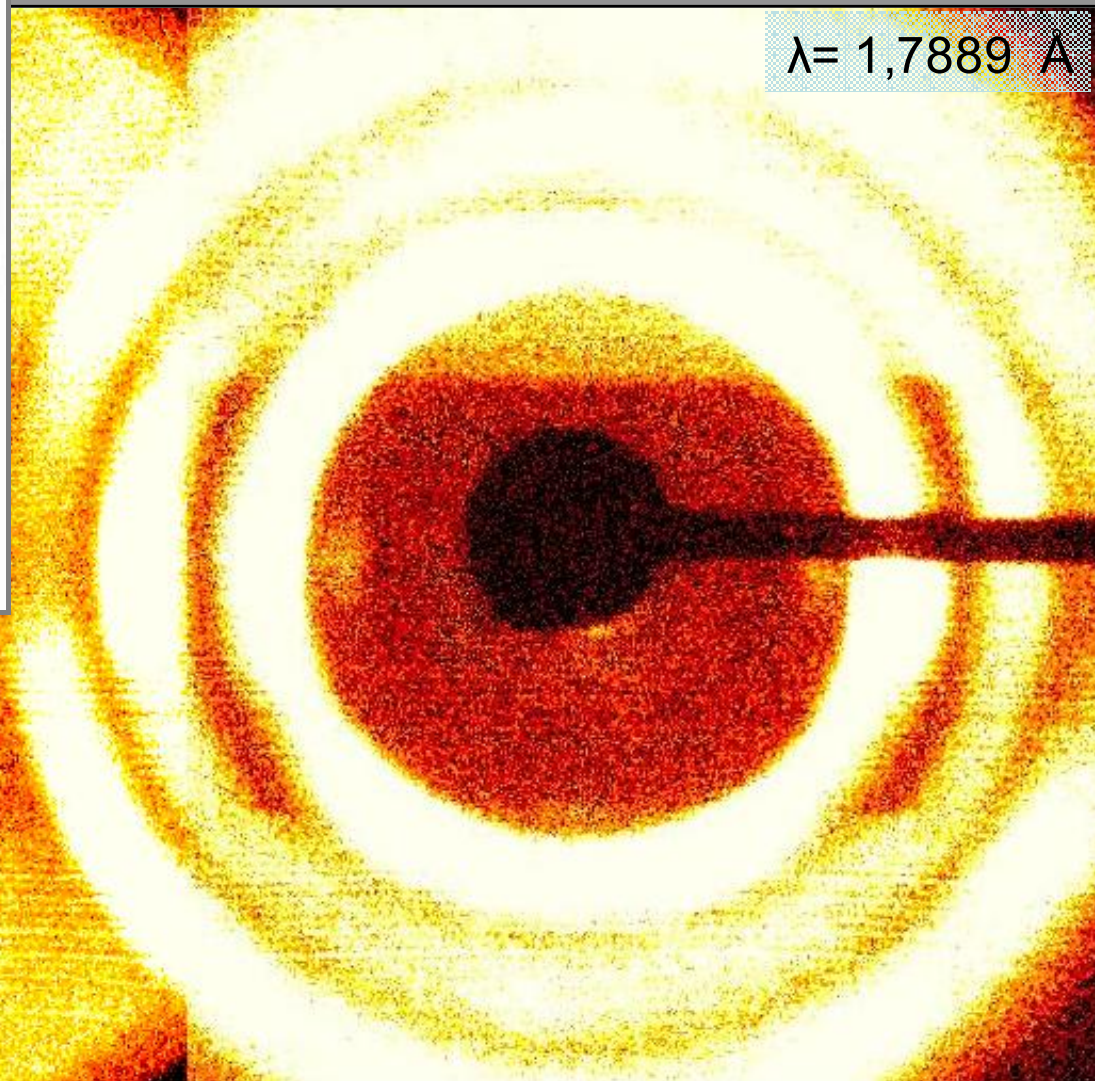
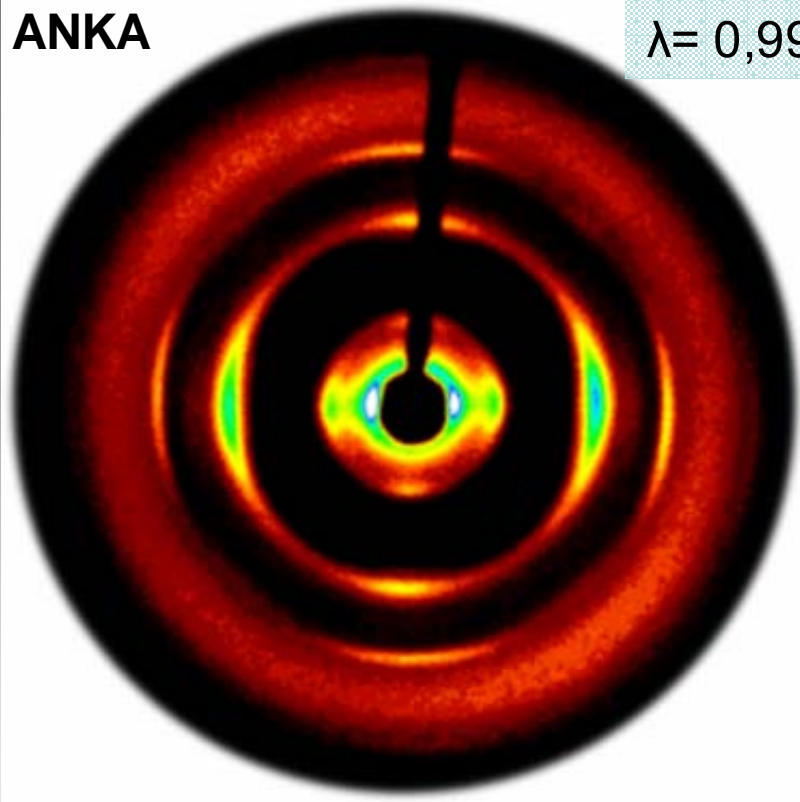
ANKA

$\lambda = 0,99955 \text{ \AA}$

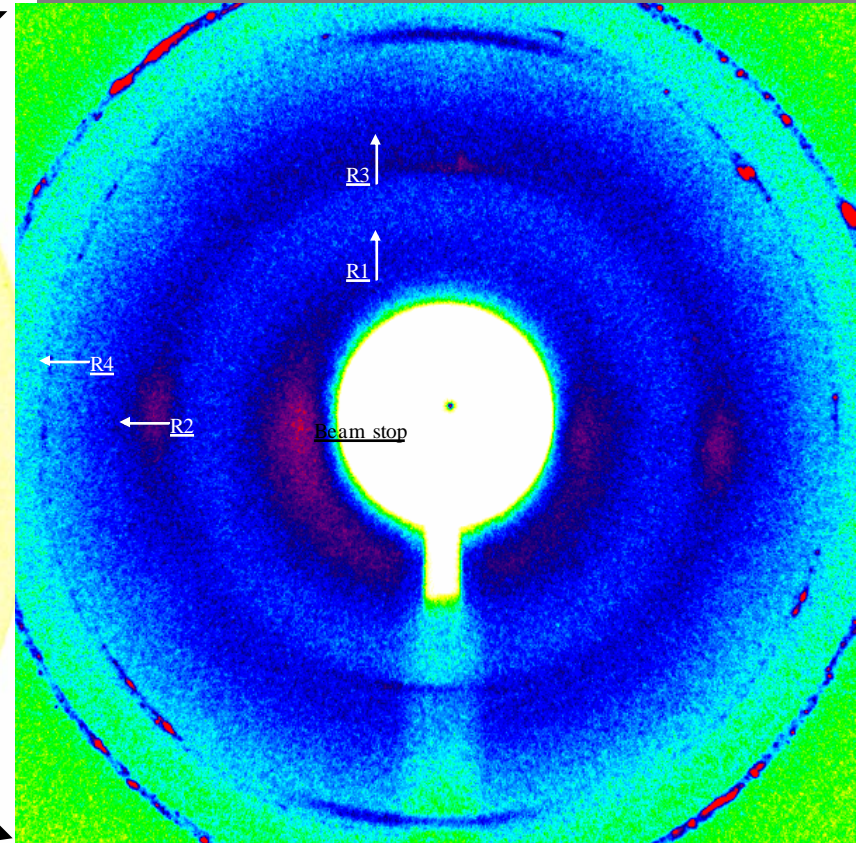
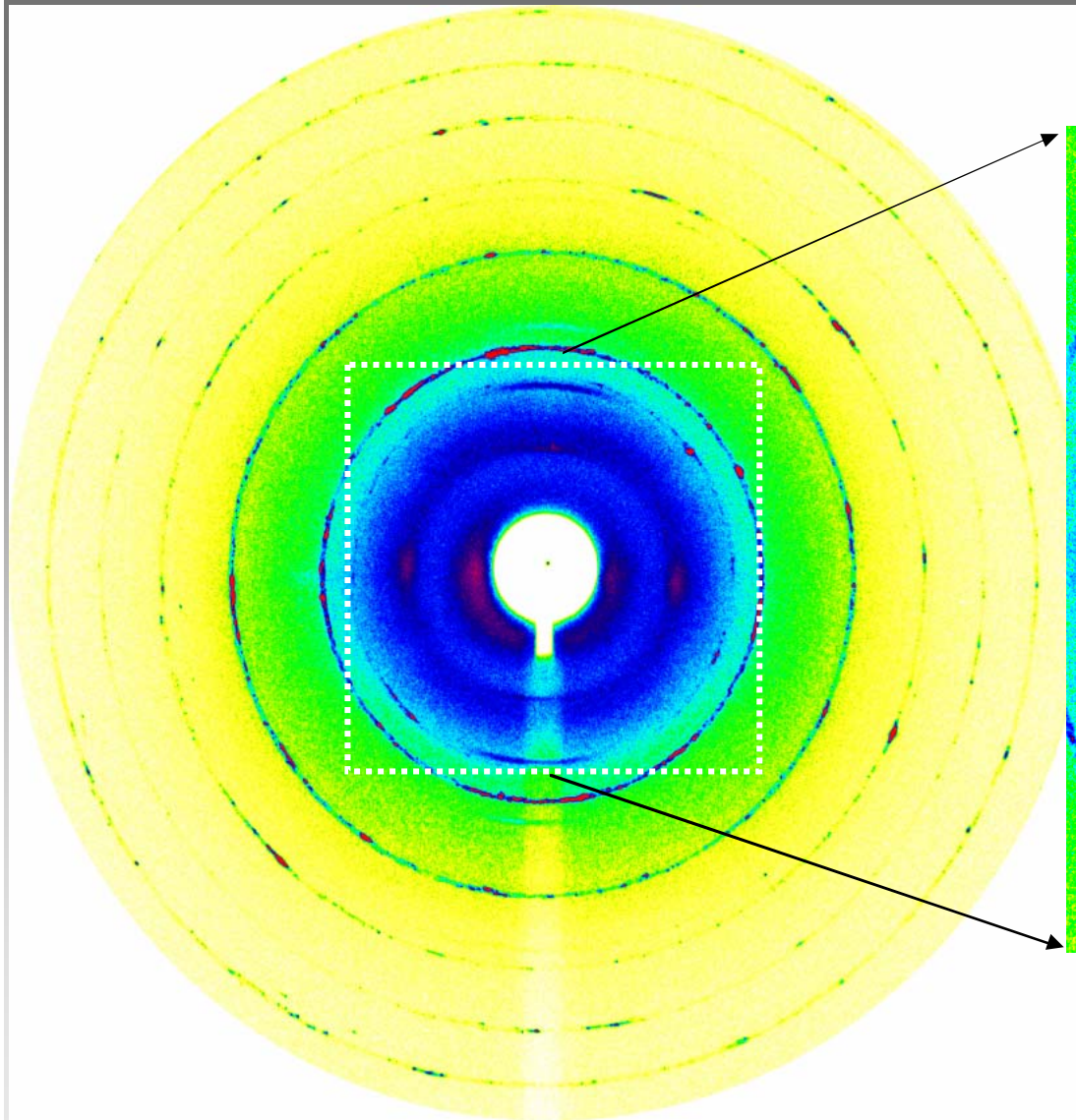
very strong chitin textures

Co-target

$\lambda = 1,7889 \text{ \AA}$



Synchrotron x-ray, wide angle, lobster

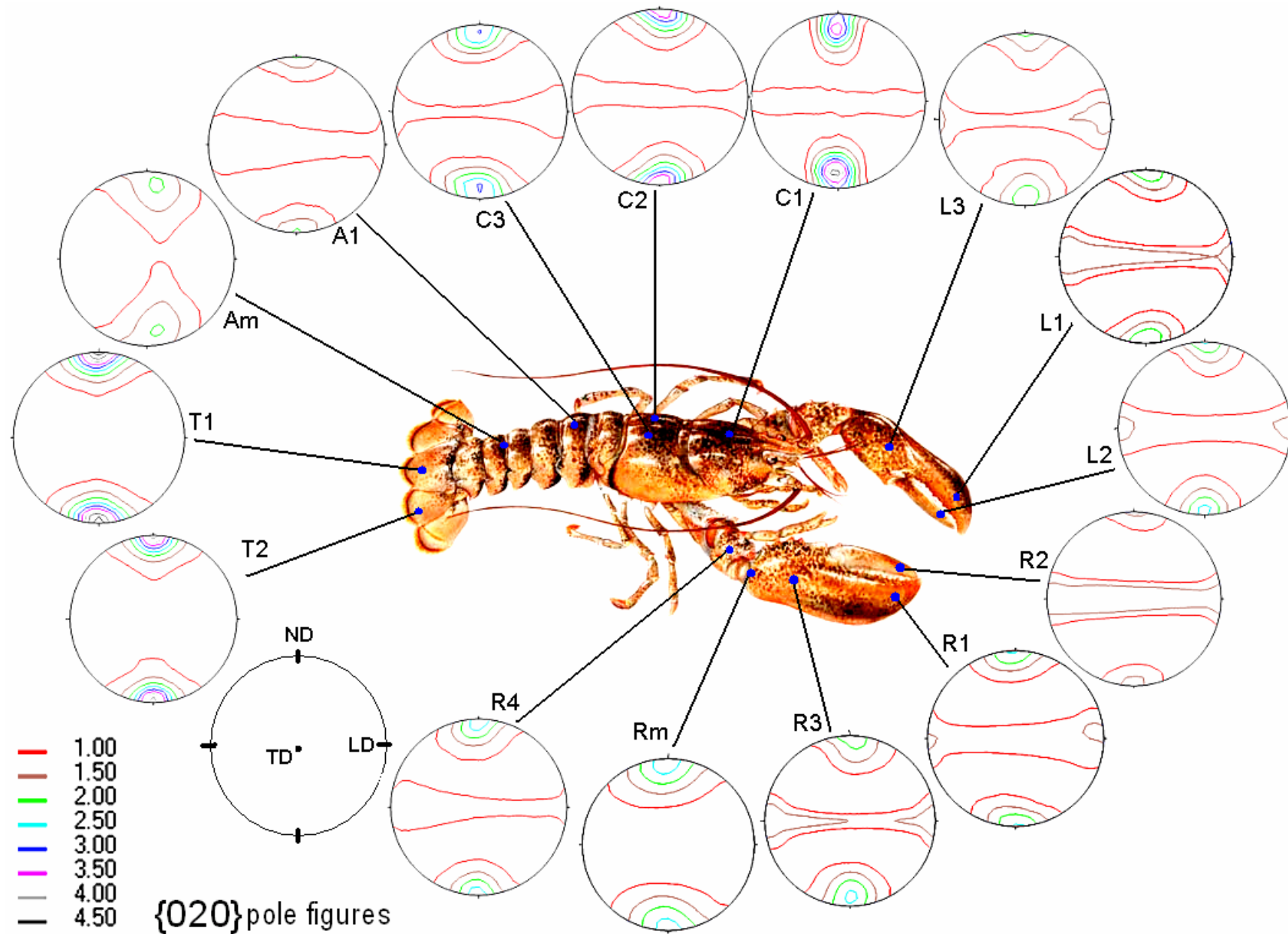


very strong chitin textures
clusters of calcite ?

DESY (BW5), $\lambda=0.196 \text{ \AA}$.

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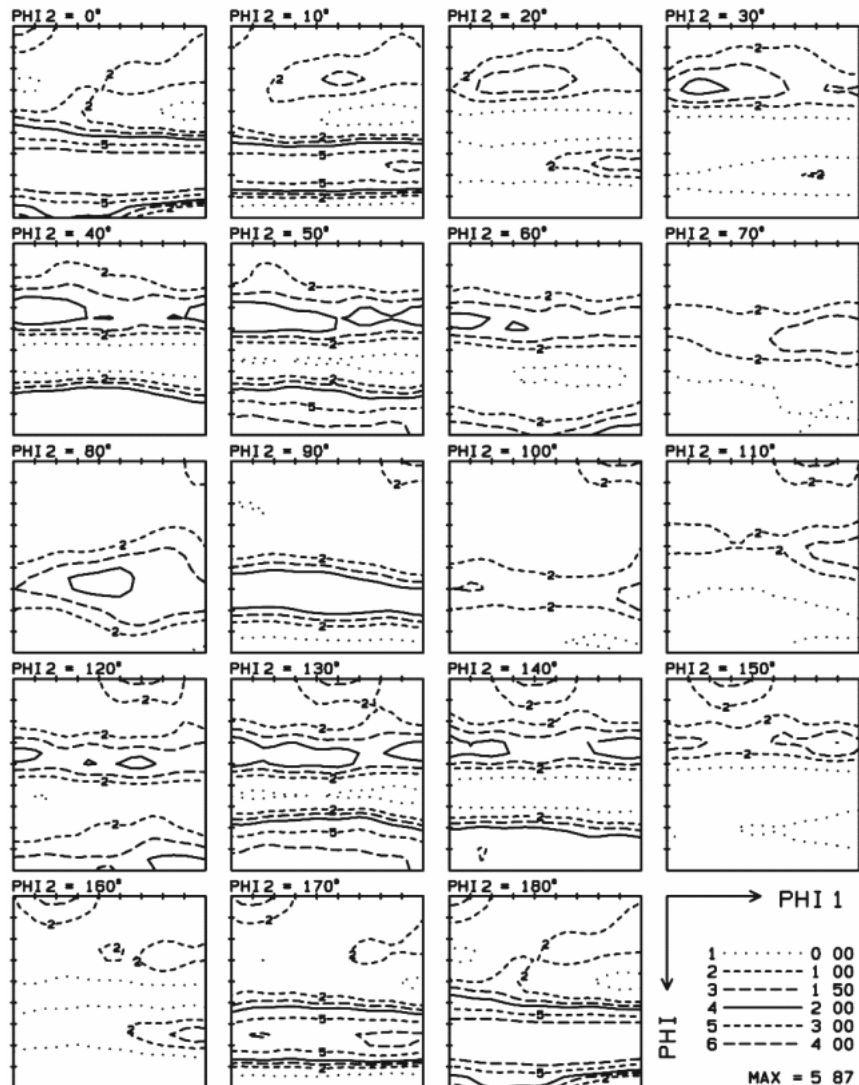
Smart design, local coordinate system



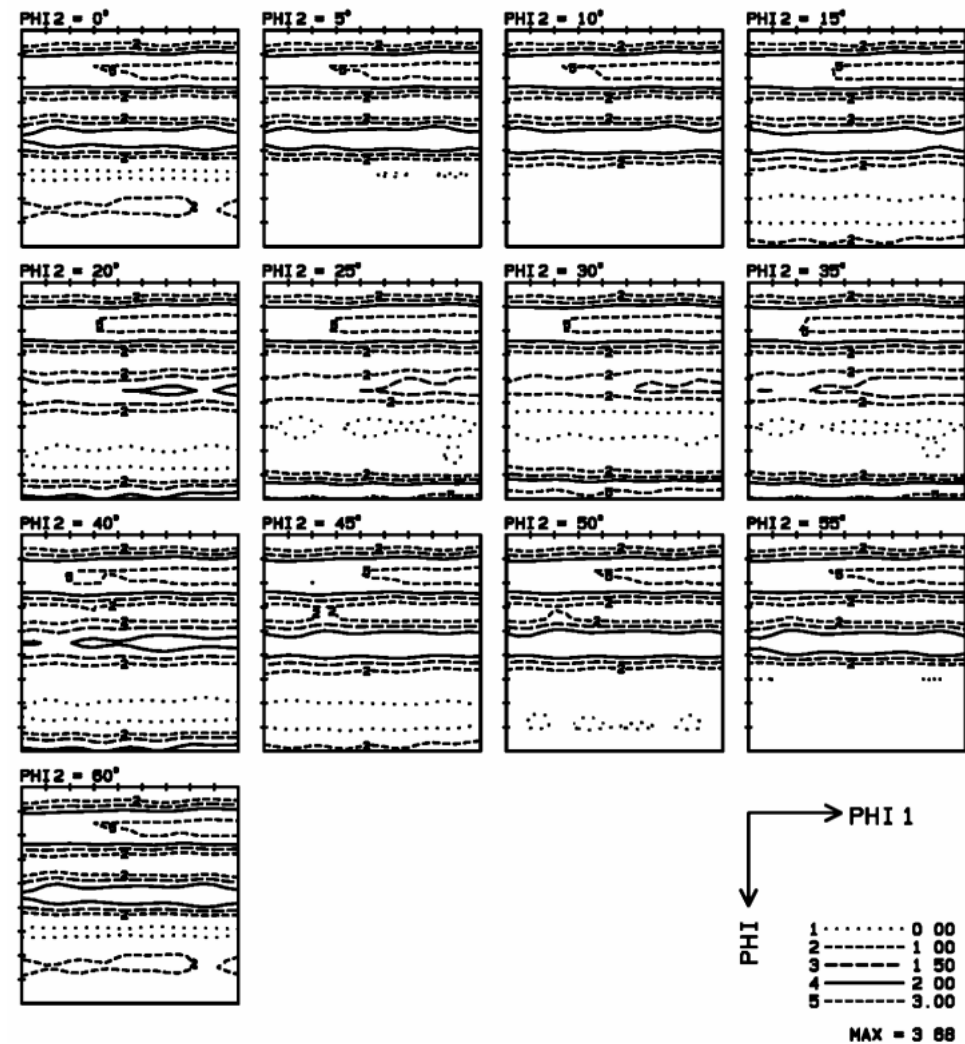
Structure and texture of chitin and calcite



ODF chitin

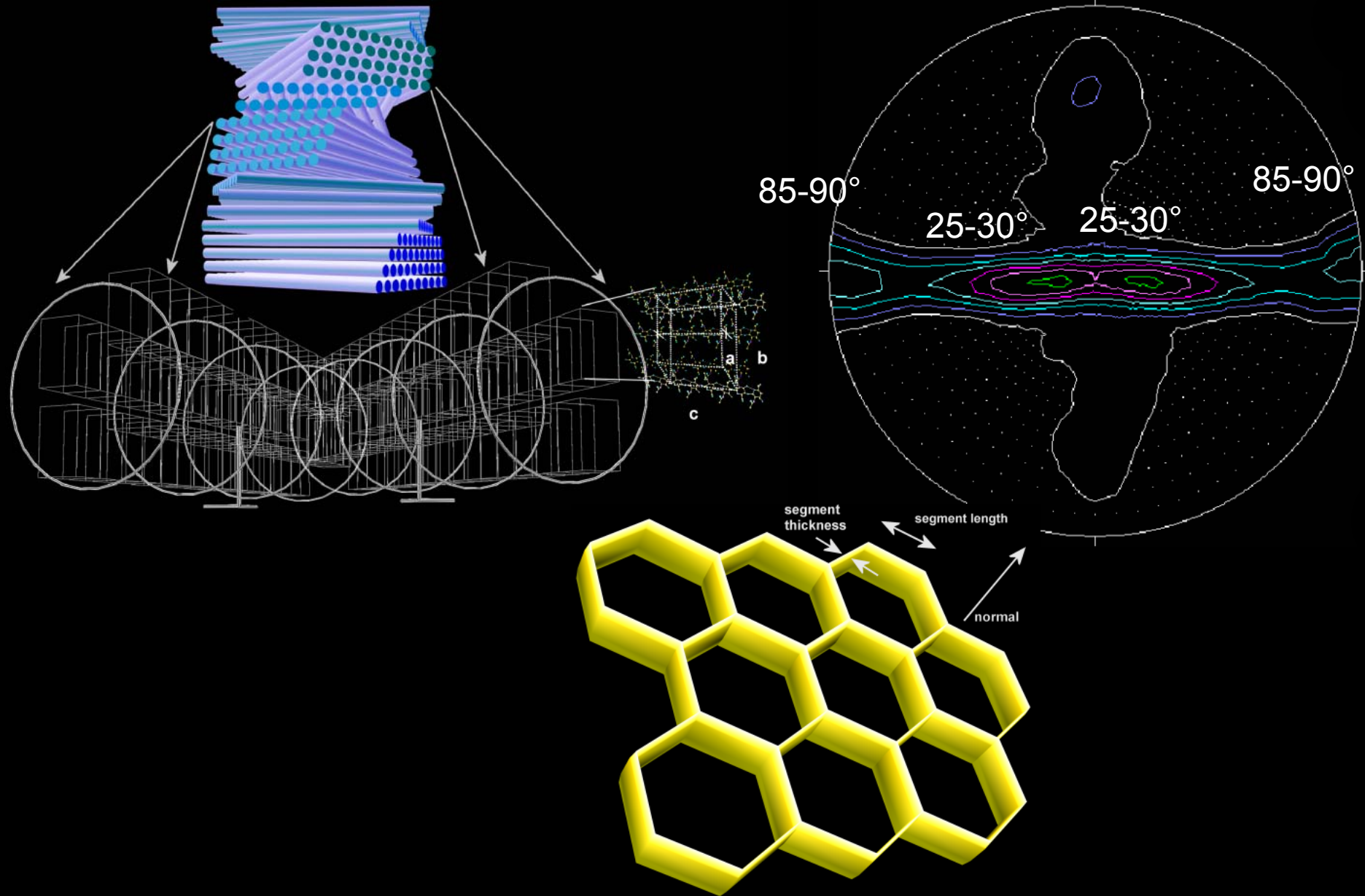


ODF calcite

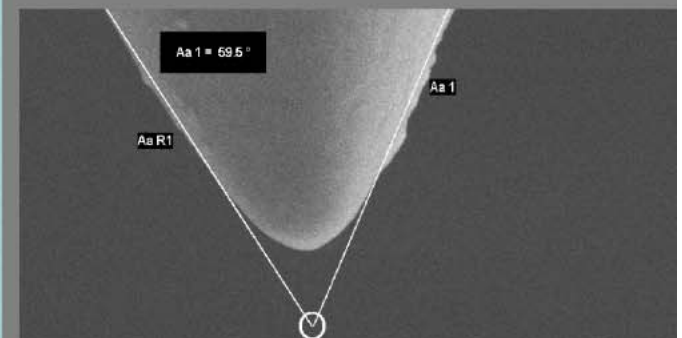
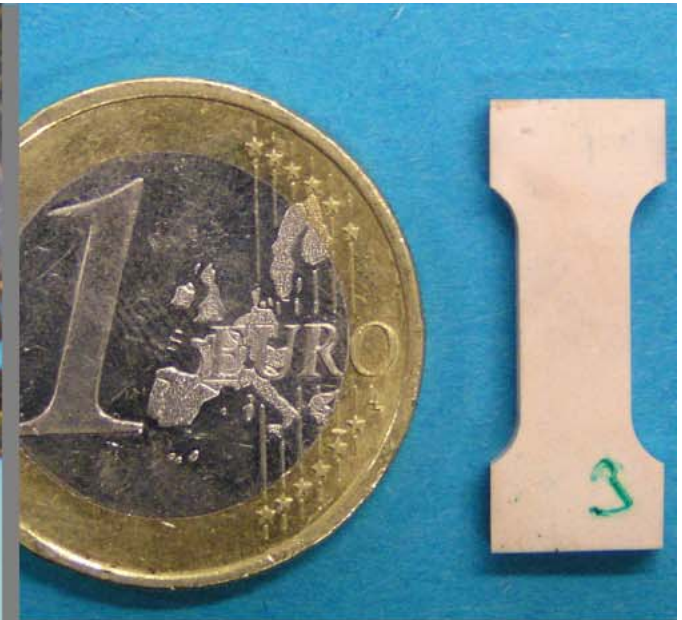




Structure and texture of chitin

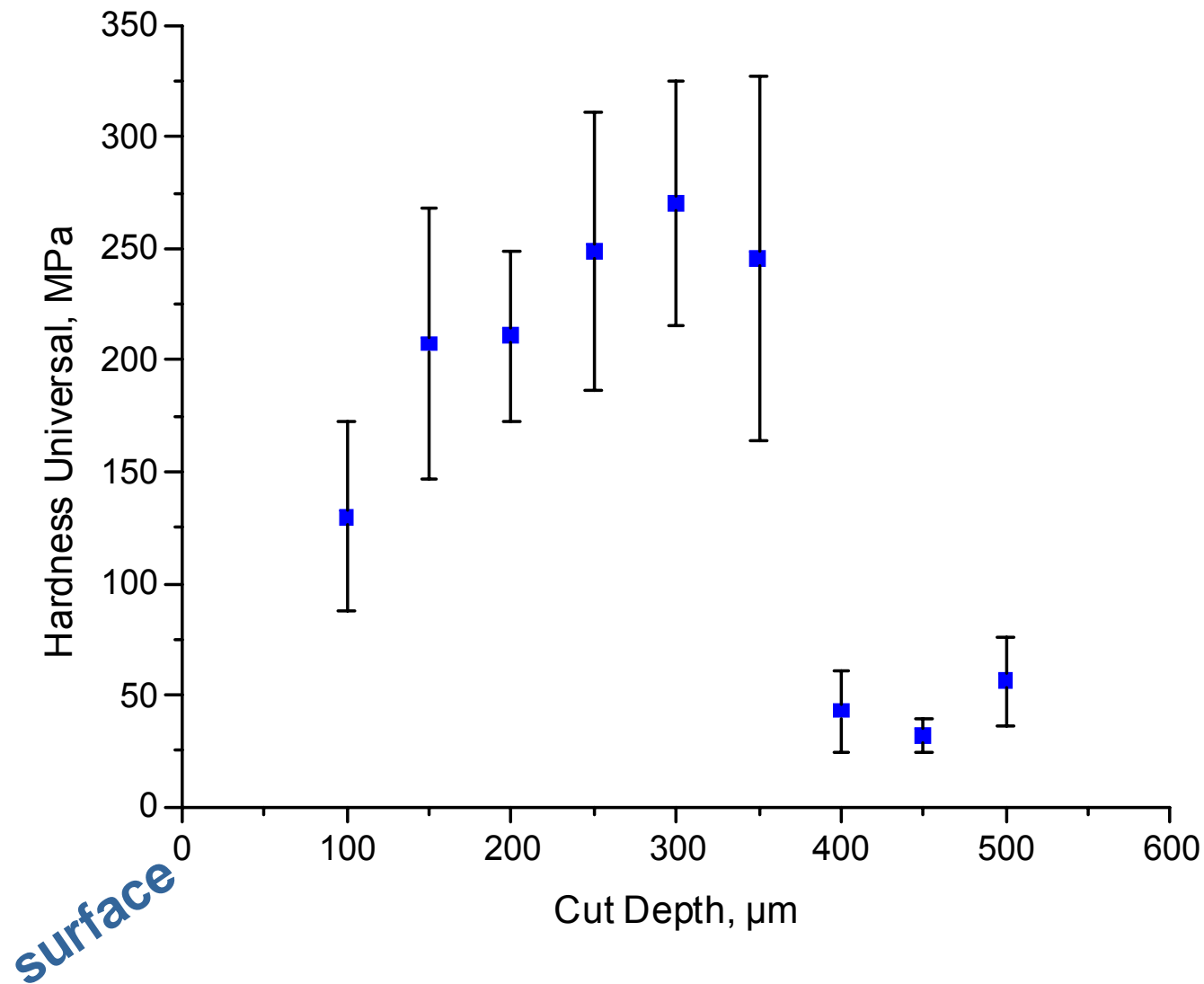


Tensile testing, Indentation

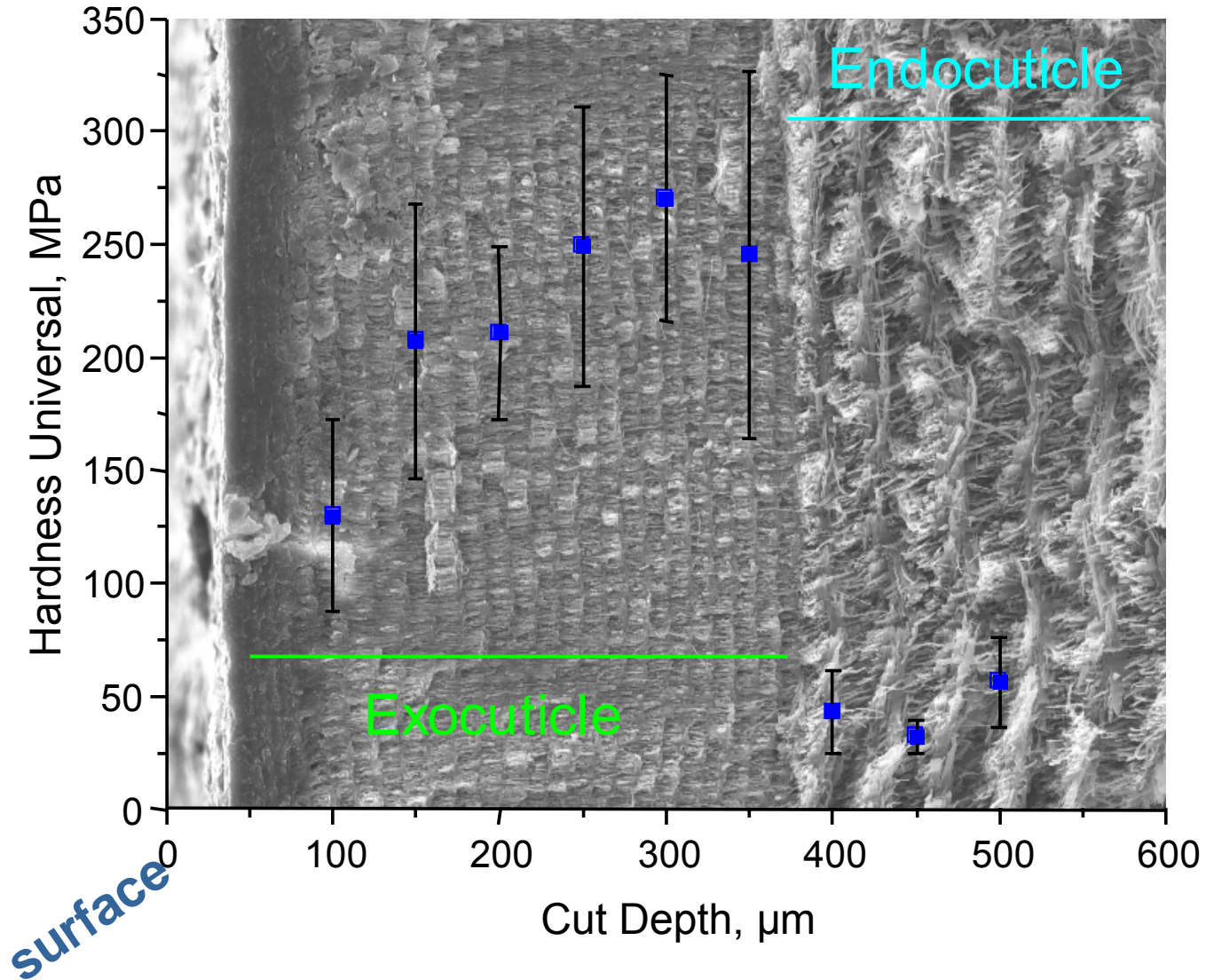




Hardness profile parallel to surface



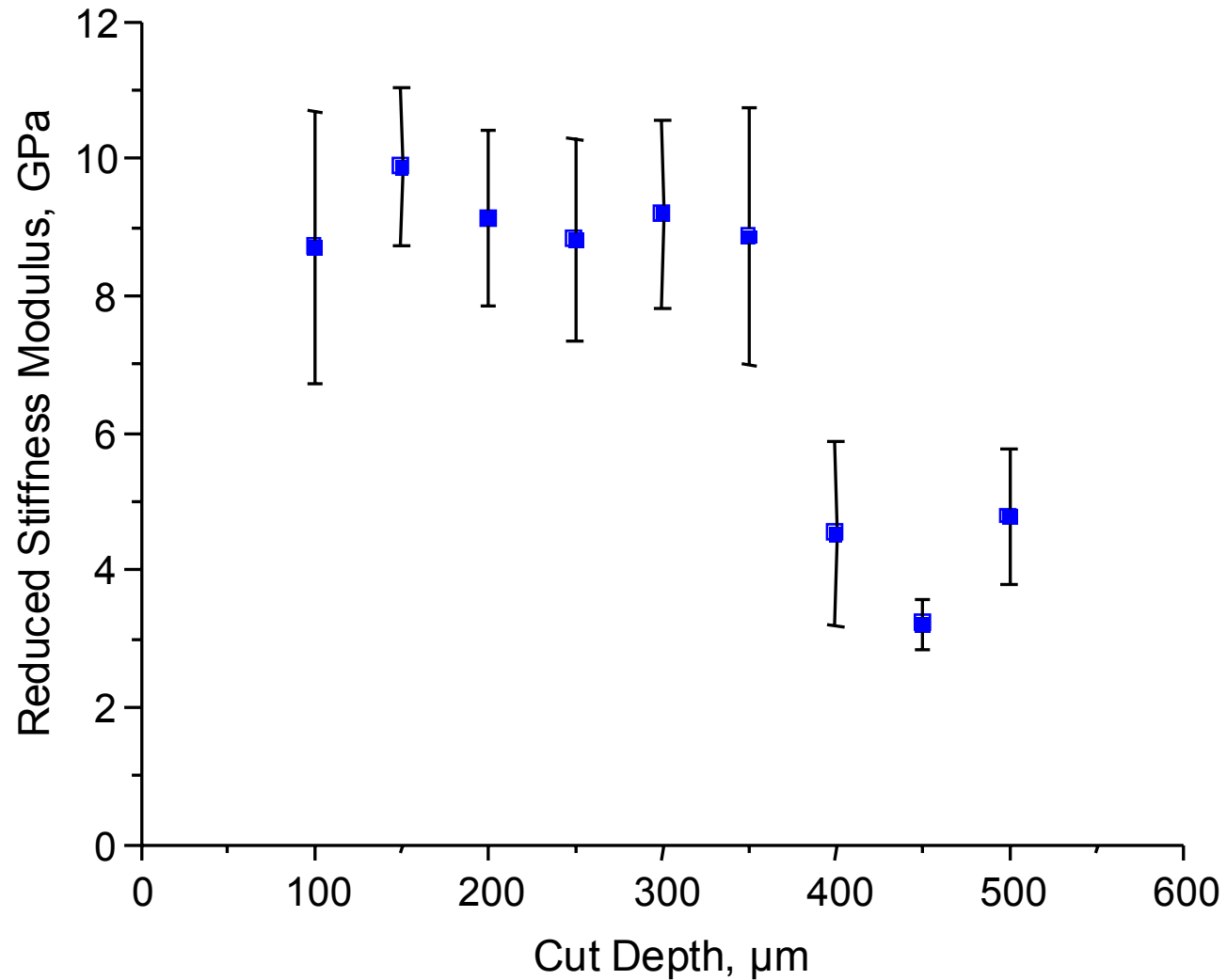
Hardness



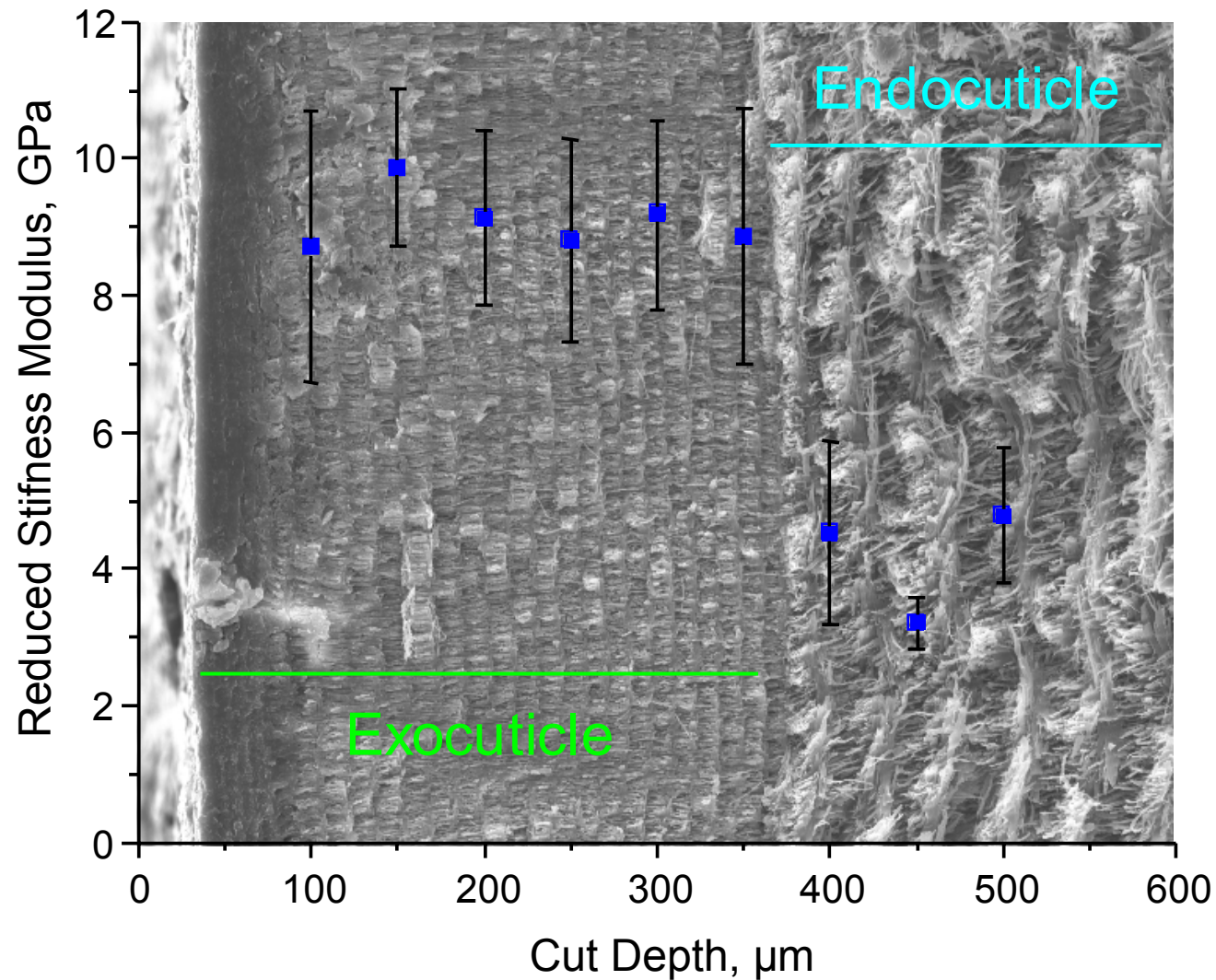
Micro-Indentation - stiffness



Reduced stiffness profile parallel to surface



Micro-Indentation - stiffness

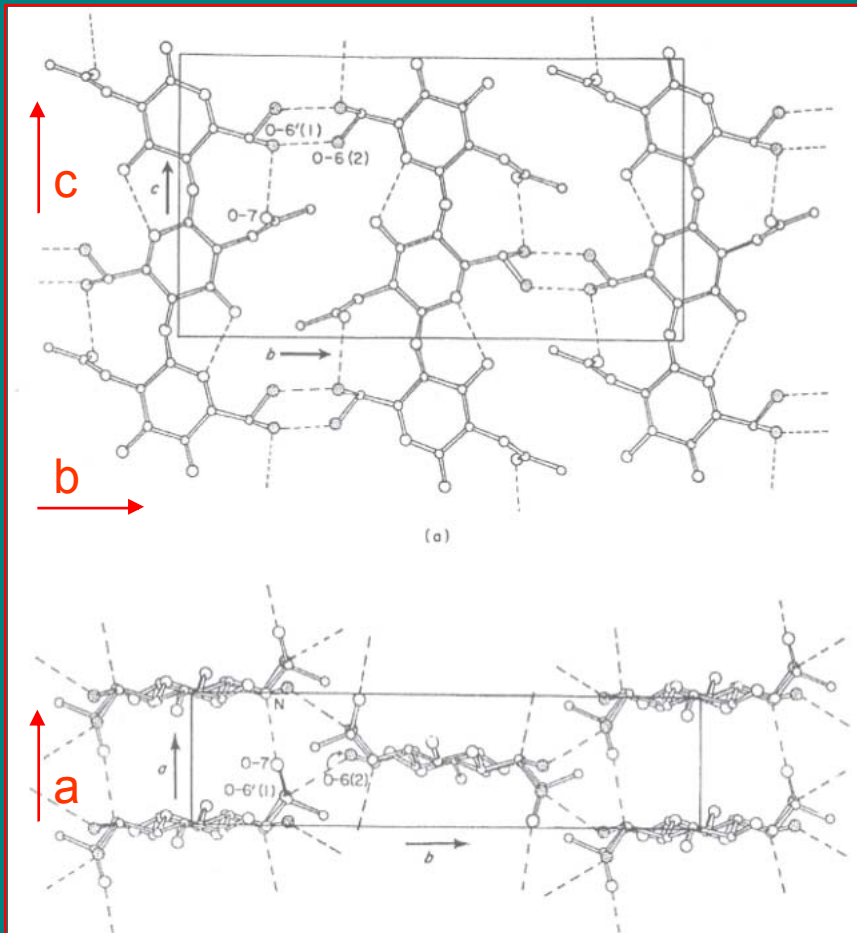


MD, LDF (Petrov, Limperakis, Neugebauer)



Searching the structure, checking available data

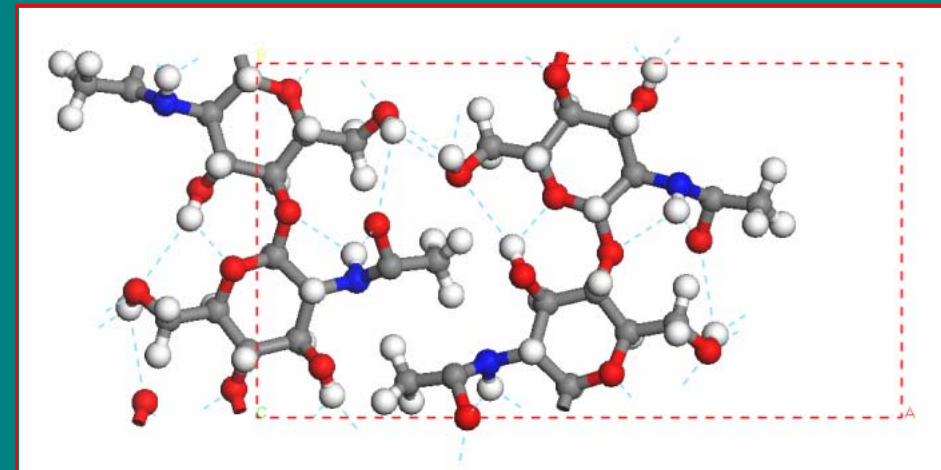
Ref: R. Minke and J. Blackwell, *J. Mol. Biol.* 120, 167 – 181 (1987).



Atomic geometry for atomic scale calculations?



conformational analysis with respect to potential energy and H-bond formation



find a stable atomic geometry of the α - chitin

400 Mio. years nanocomposites

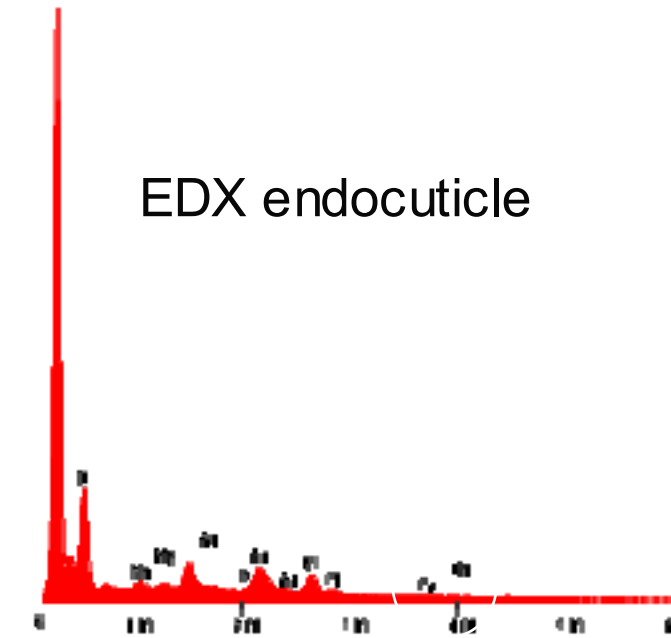


SEM: Horseshoe crab endocuticle, untreated

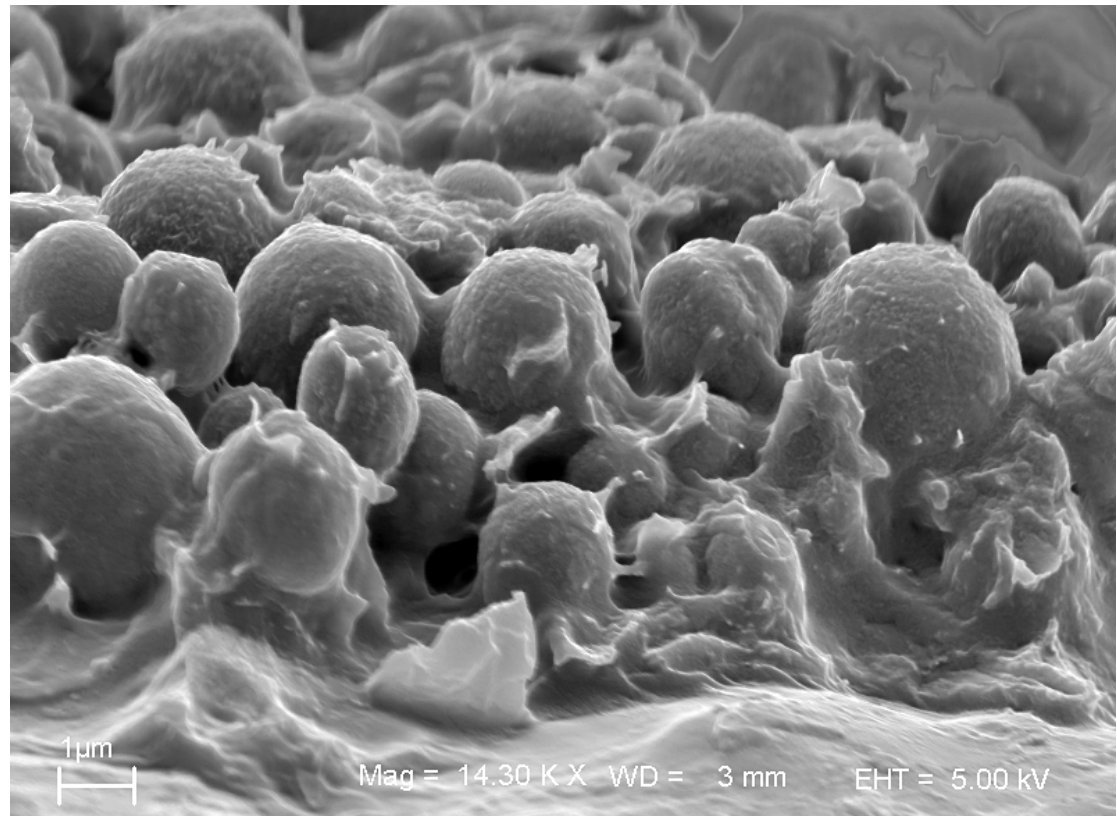
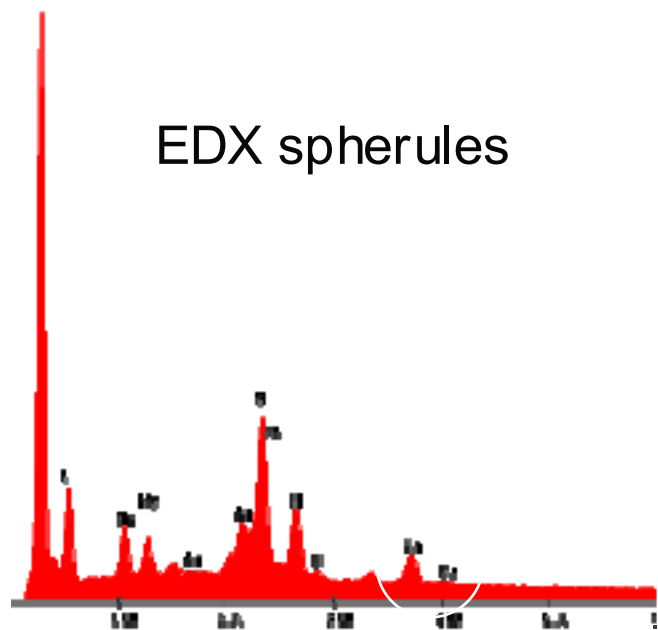


The spherules contain calcium, probably as CaCO_3

EDX endocuticle

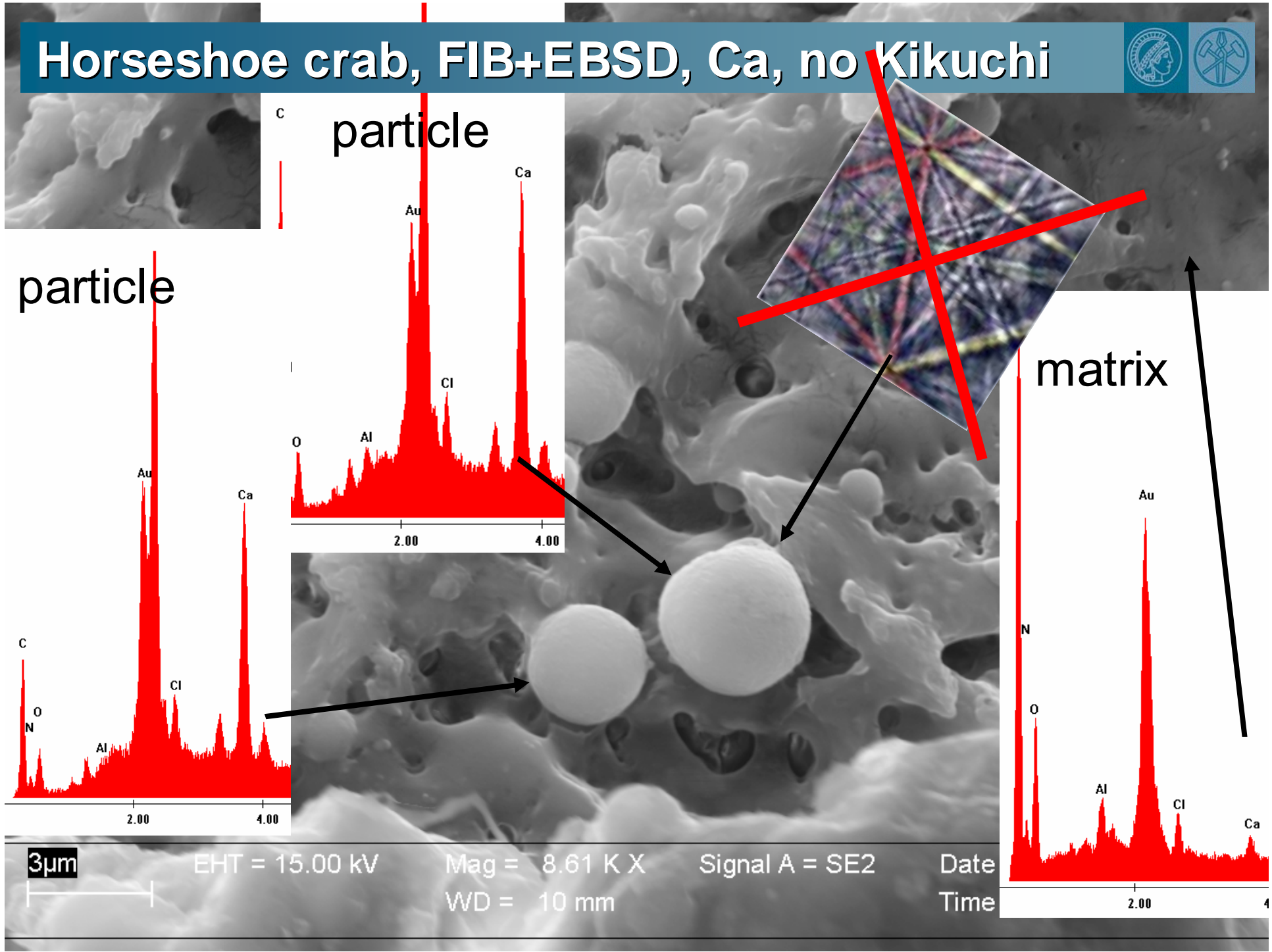


EDX spherules





Horseshoe crab, FIB+EBSD, Ca, no Kikuchi



!! Thanks !! to the team



Roters, Ma: crystal mechanics
Sachs, Romano, Al-Sawalmih, Fabritius: chitin-composites
Zaefferer, Bastos: 3D Microscopy
Neugebauer, Petrov, Limperakis: ab initio and MD