



# Crystal Plasticity and Fresh Lobster

Dierk Raabe

Lecture given at BAM Berlin, Germany on 23. August 2006

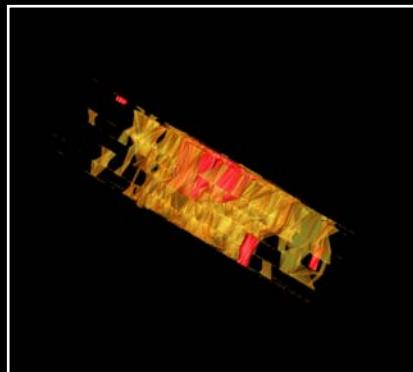
Roters: crystal mechanics

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

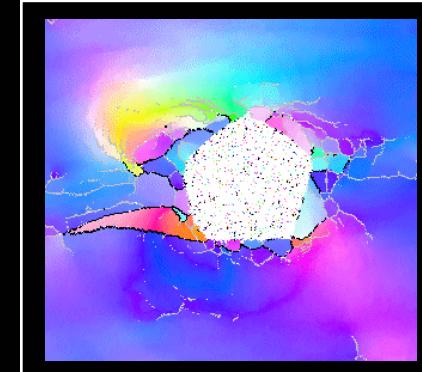
Zaefferer, Bastos, Konrad: 3D Microscopy



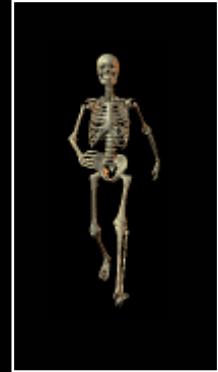
new steels



3D electron  
microscopy



complex  
microstructures



biomaterials  
biological materials

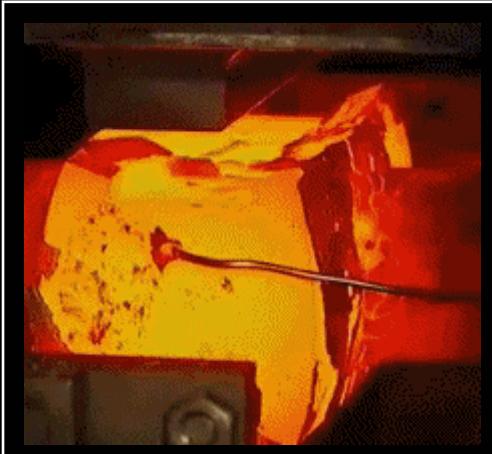


## Department for Microstructure Physics and Metal Forming

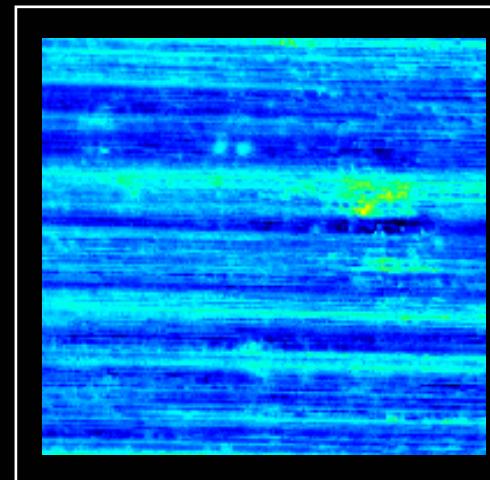
---

---

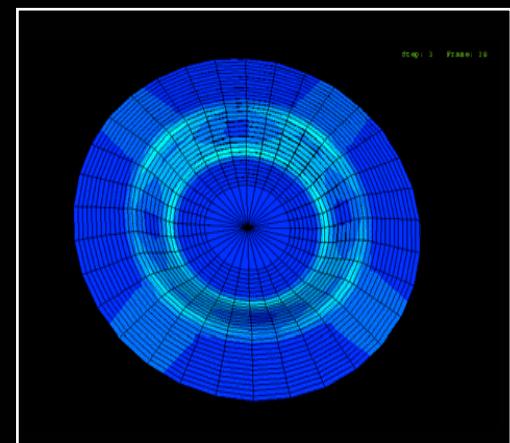
thermomechanical  
treatment



surface micro-mechanics



physics-based  
mechanics simulation



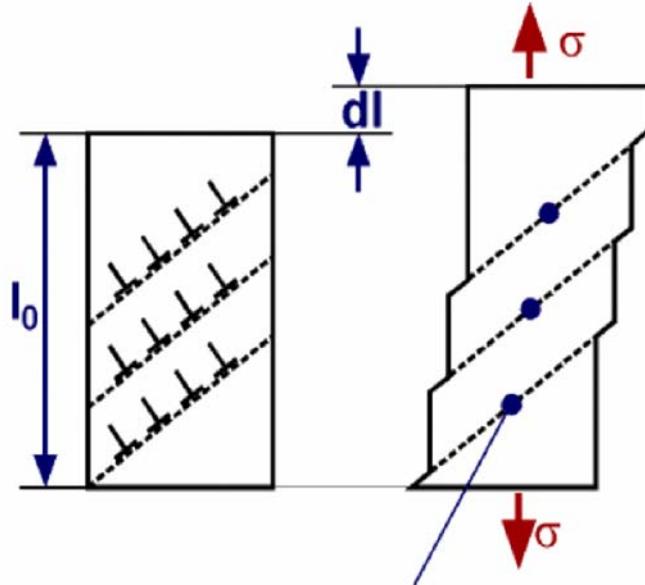


Mechanics of few crystals

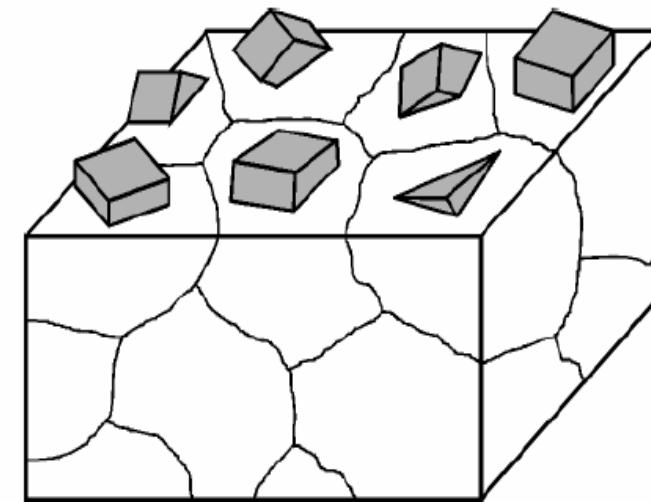
Mechanics of many crystals

3D electron microscopy

Chitin-composites



strain is the symmetric part of plasticity



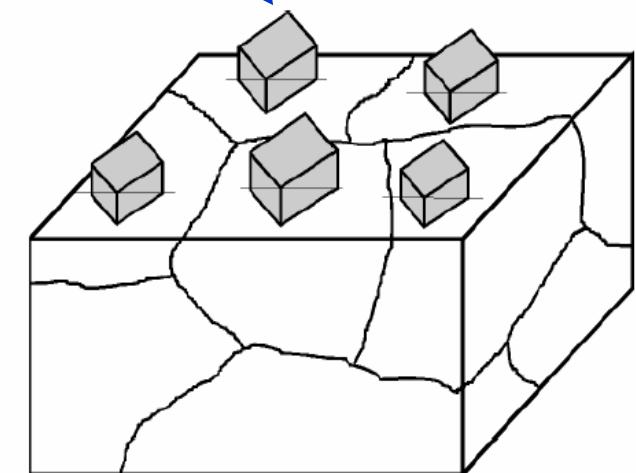
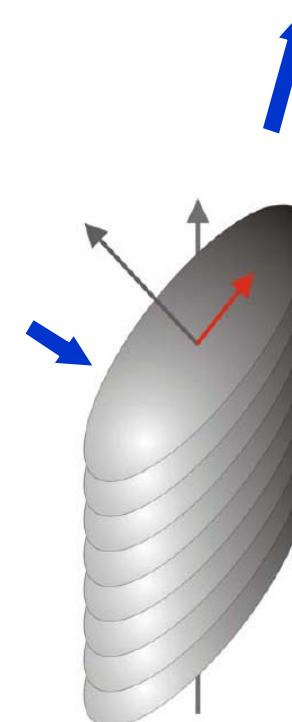
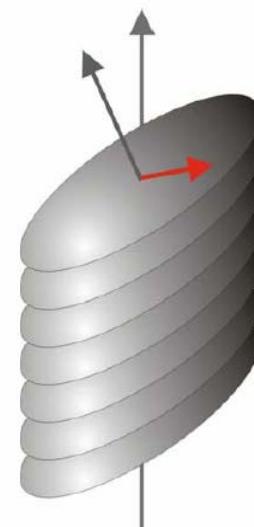
?

?



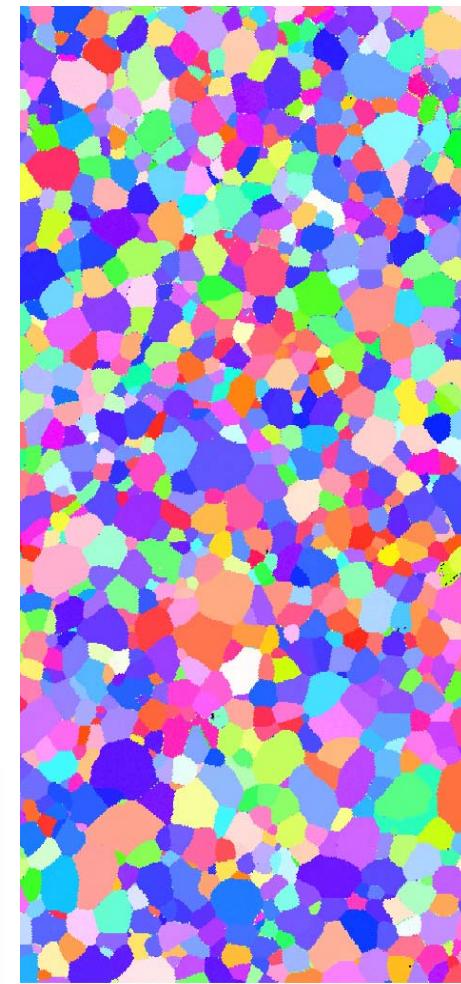
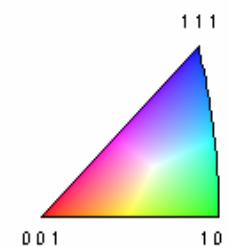
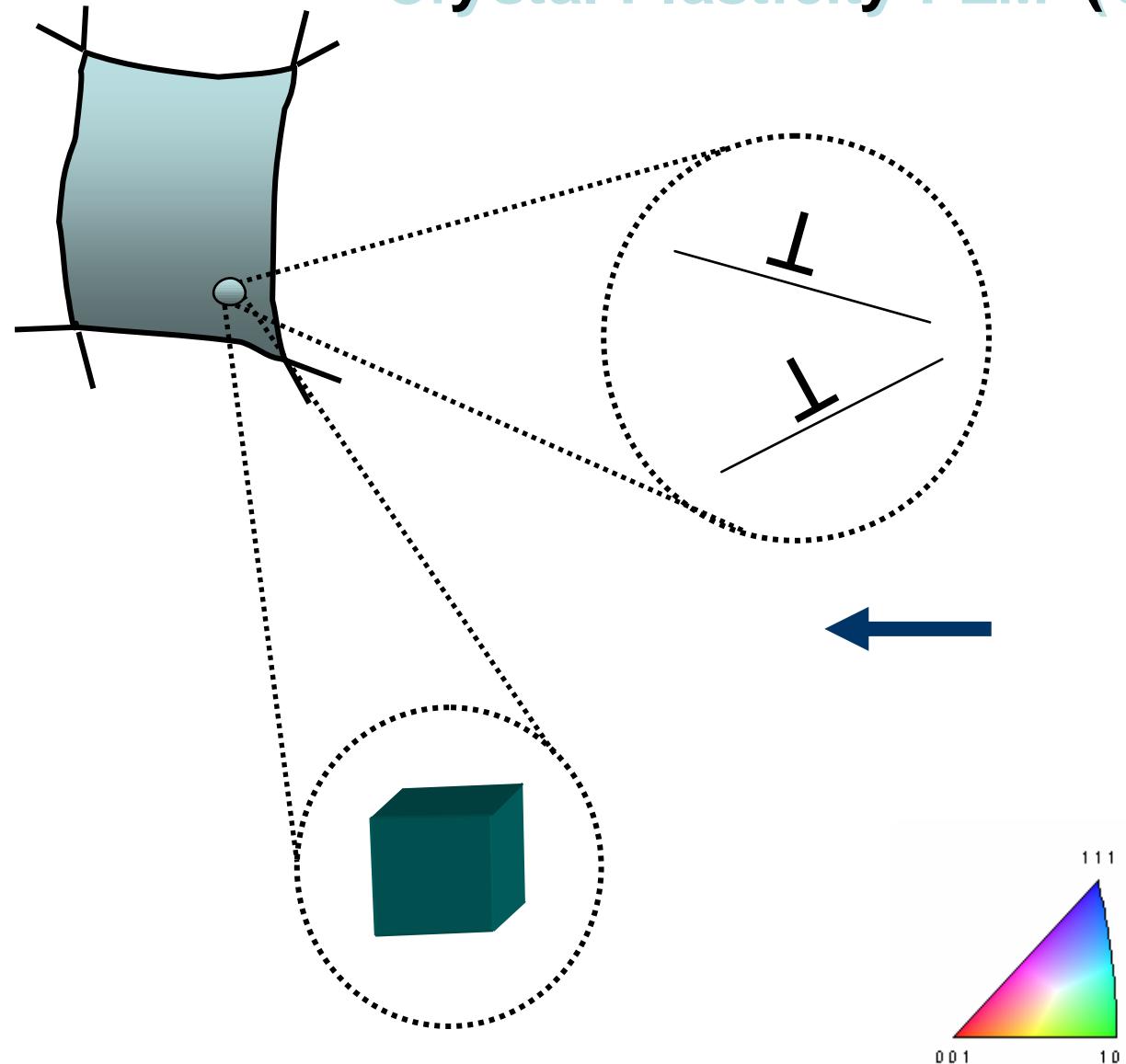
**Plastically stretched zinc single crystal.**

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



70.00  $\mu\text{m}$  = 70 steps  
Prof. Dierk Raabe

# Crystal Plasticity FEM (include more physics)



Multiplicative Decomposition of the Deformation Gradient

**flow law**

constitutive reduction of DOF:

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

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

—— Phenomenological

$\dot{\gamma}_\alpha(\tau_\alpha, \rho, \theta)$

—— Dislocation density laws

$\mathbf{F}^*$  : elastic and rotation deformation gradient

$\mathbf{F}$  : total deformation gradient

$\mathbf{F}_p$  : plastic deformation gradient

$\mathbf{L}_p$  : plastic velocity gradient

$\mathbf{L}_e$  : elastic velocity gradient

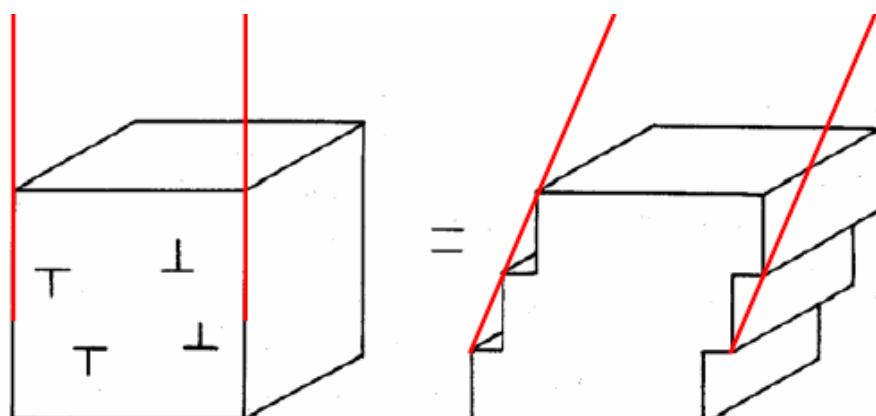
Definitions:

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

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

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

$$\mathbf{L}_p := \mathbf{F}_e \tilde{\mathbf{L}}_p \mathbf{F}_e^{-1}$$



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

# physics-based constitutive laws

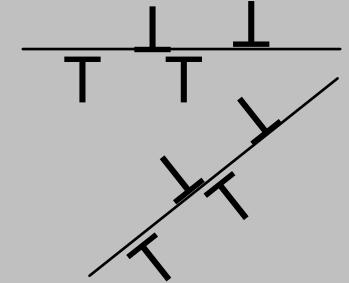


1

1. set  
internal  
variables

dyadic flow law based on dislocation rate theory

Taylor, Kocks, Mecking, Estrin,....

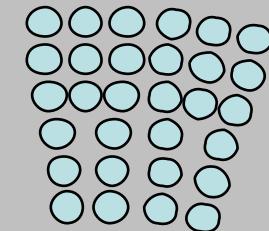


2

2. set  
internal  
variables

plastic gradients,  
size scale and orientation gradients (implicit)

Nye, Ashby1, Kröner,....

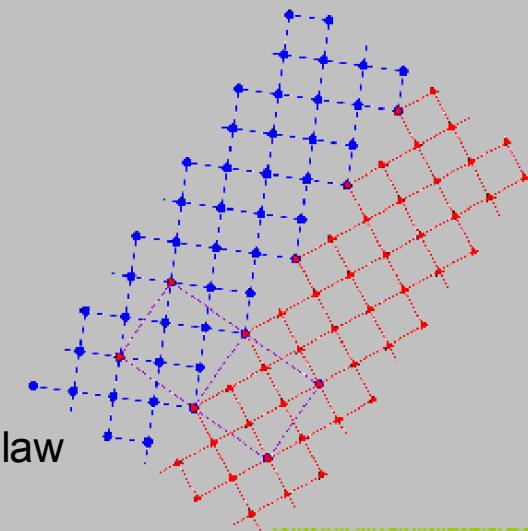


3

3. set  
internal  
variables

grain boundaries

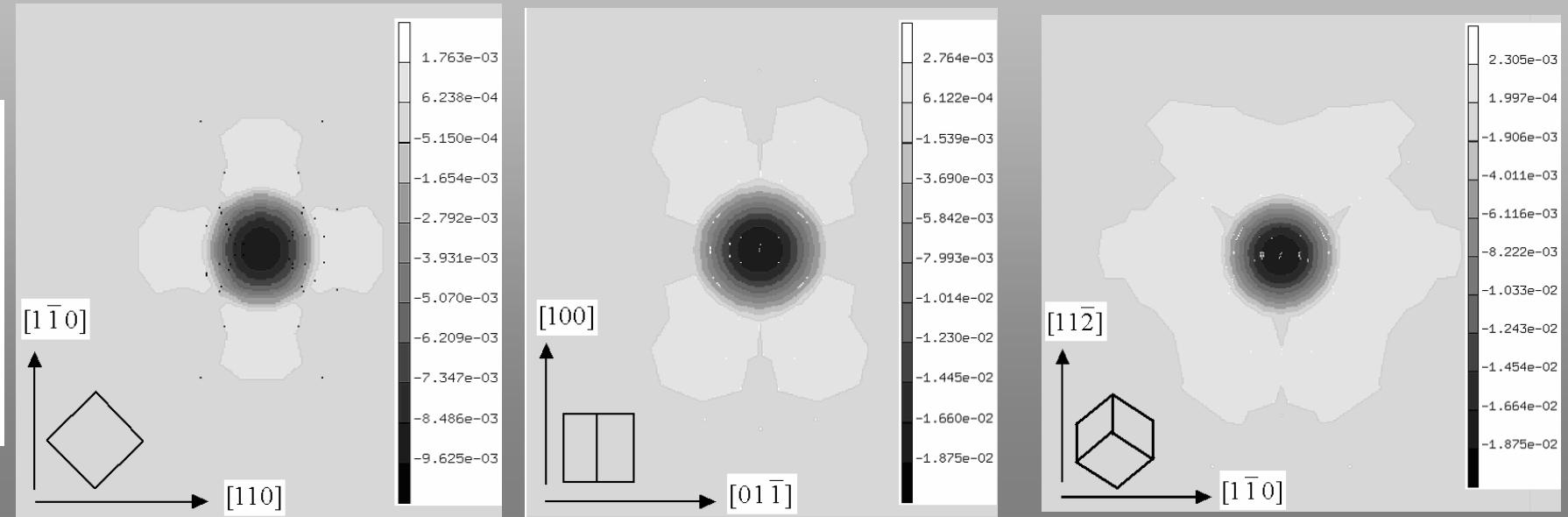
activation concept:  
energy of formation upon slip penetration: conservation law



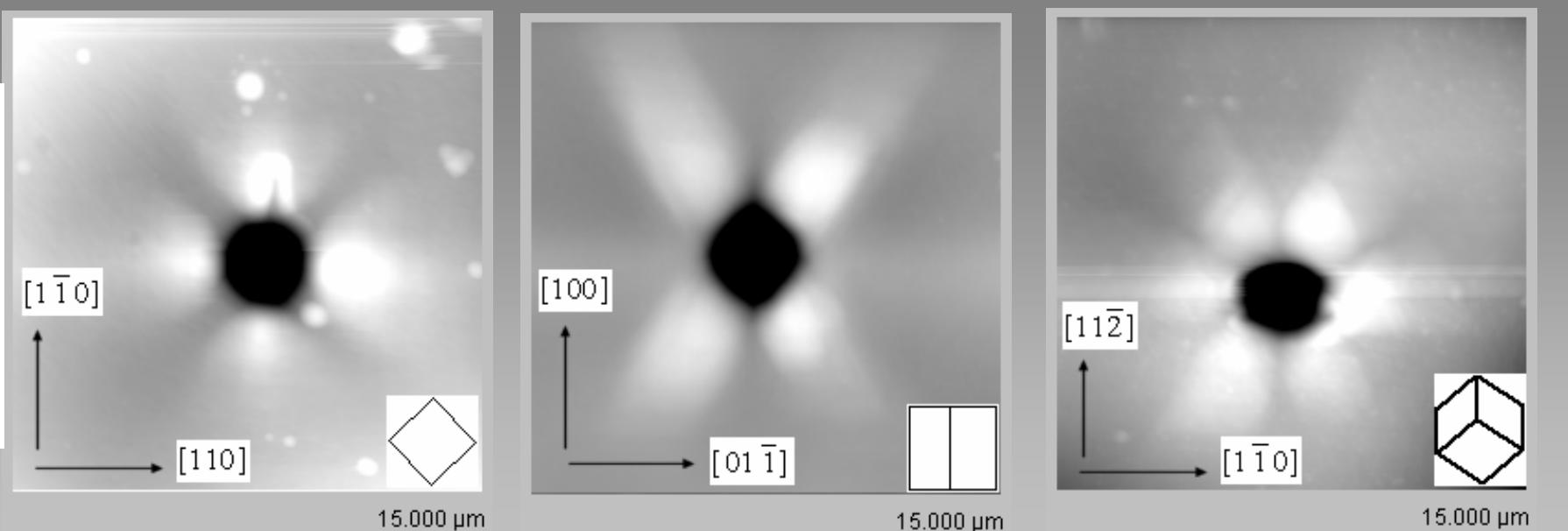
# Nanoindentation - 2D



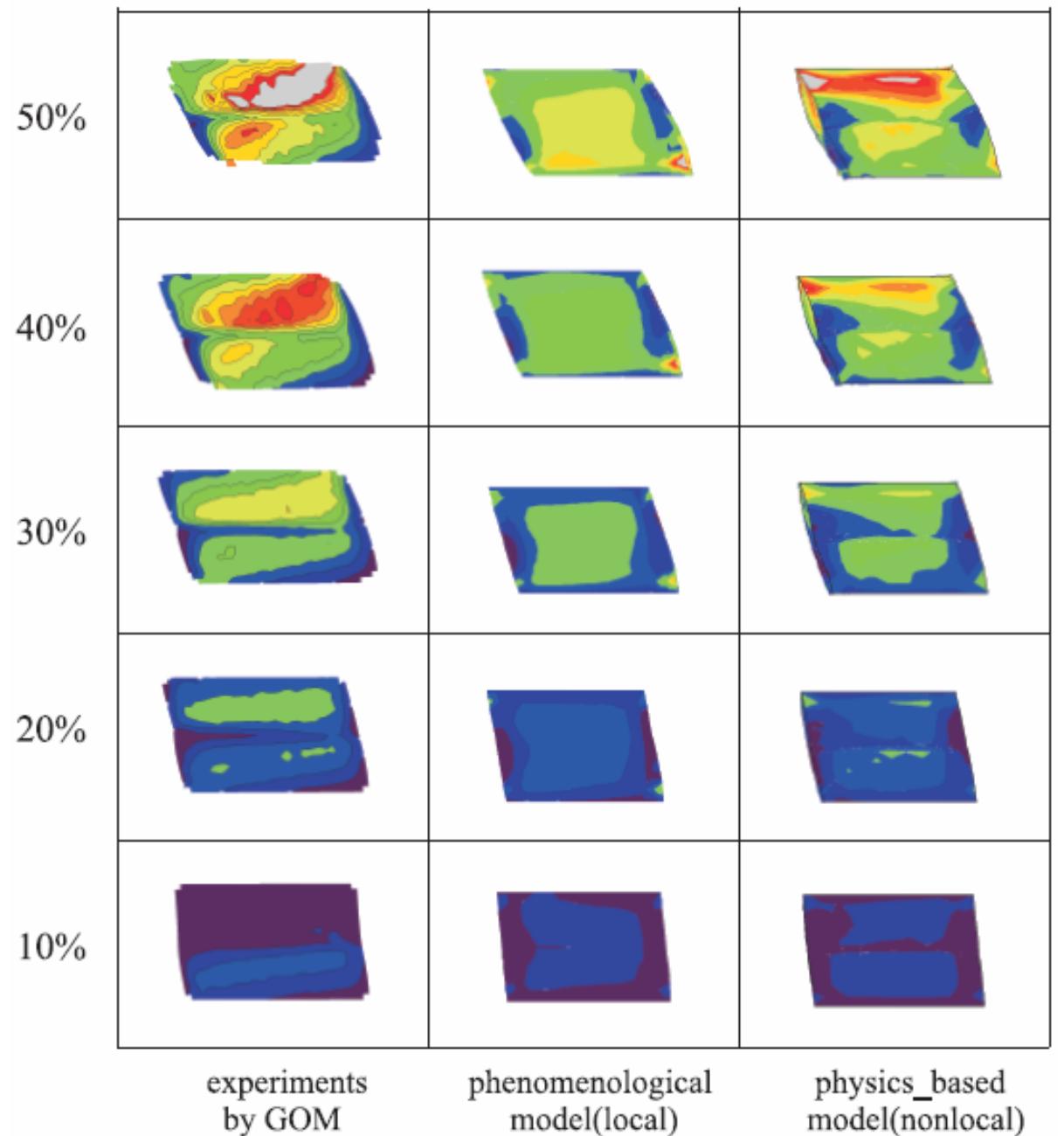
simulation



experiment



# Bicrystals



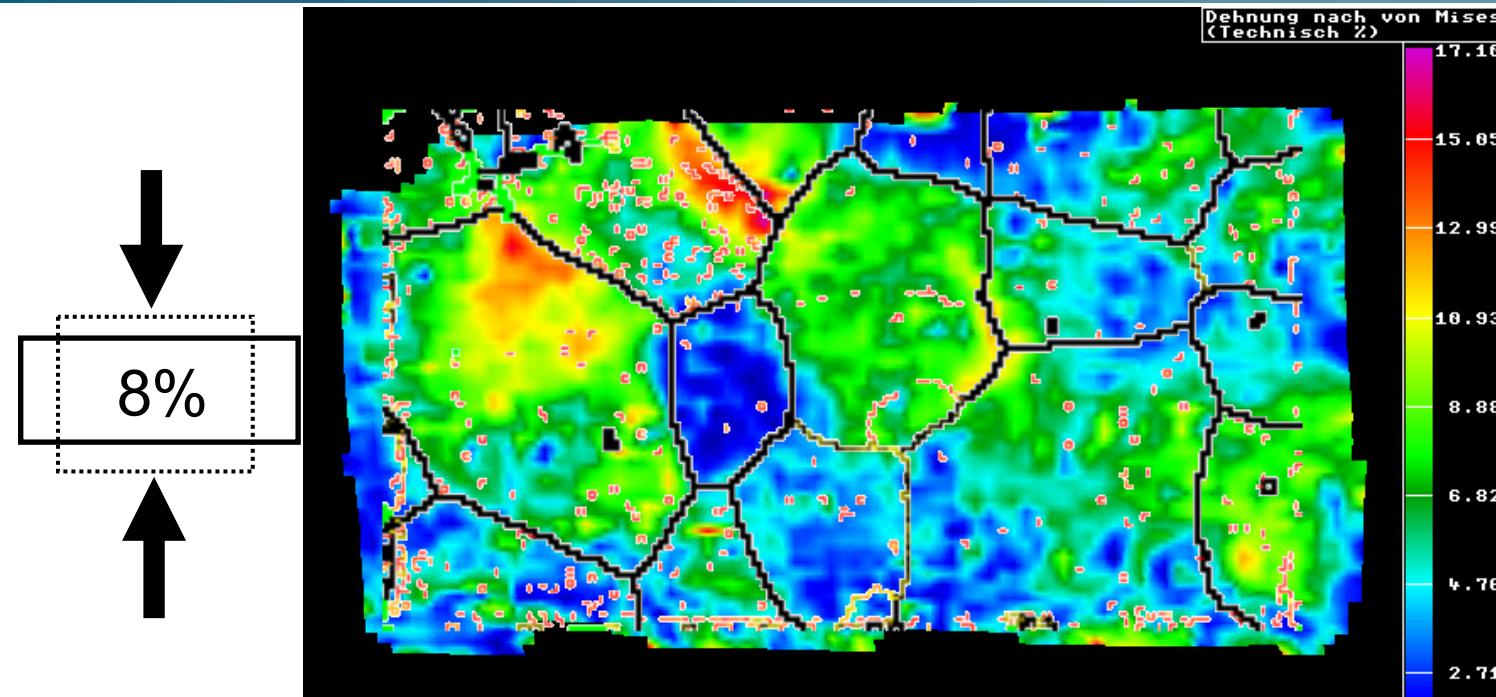
grain boundary mechanics

7.4°  
v. Mises  
Aluminium

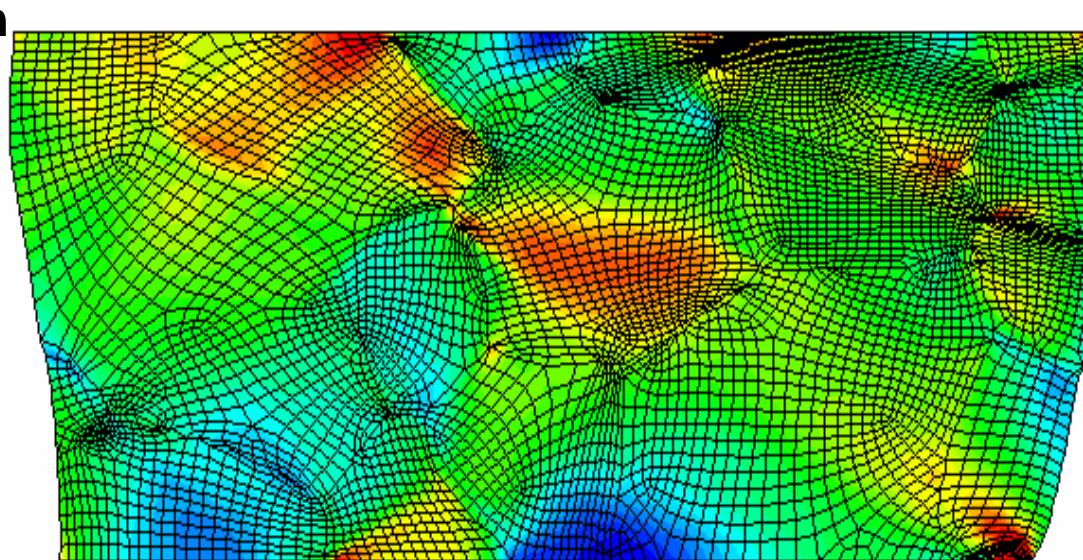
A. Ma,  
F. Roters  
D. Raabe

Prof. Dierk Raabe

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



Experiment  
(DIC, EBSD)  
v Mises strain





Mechanics of few crystals

Mechanics of many crystals

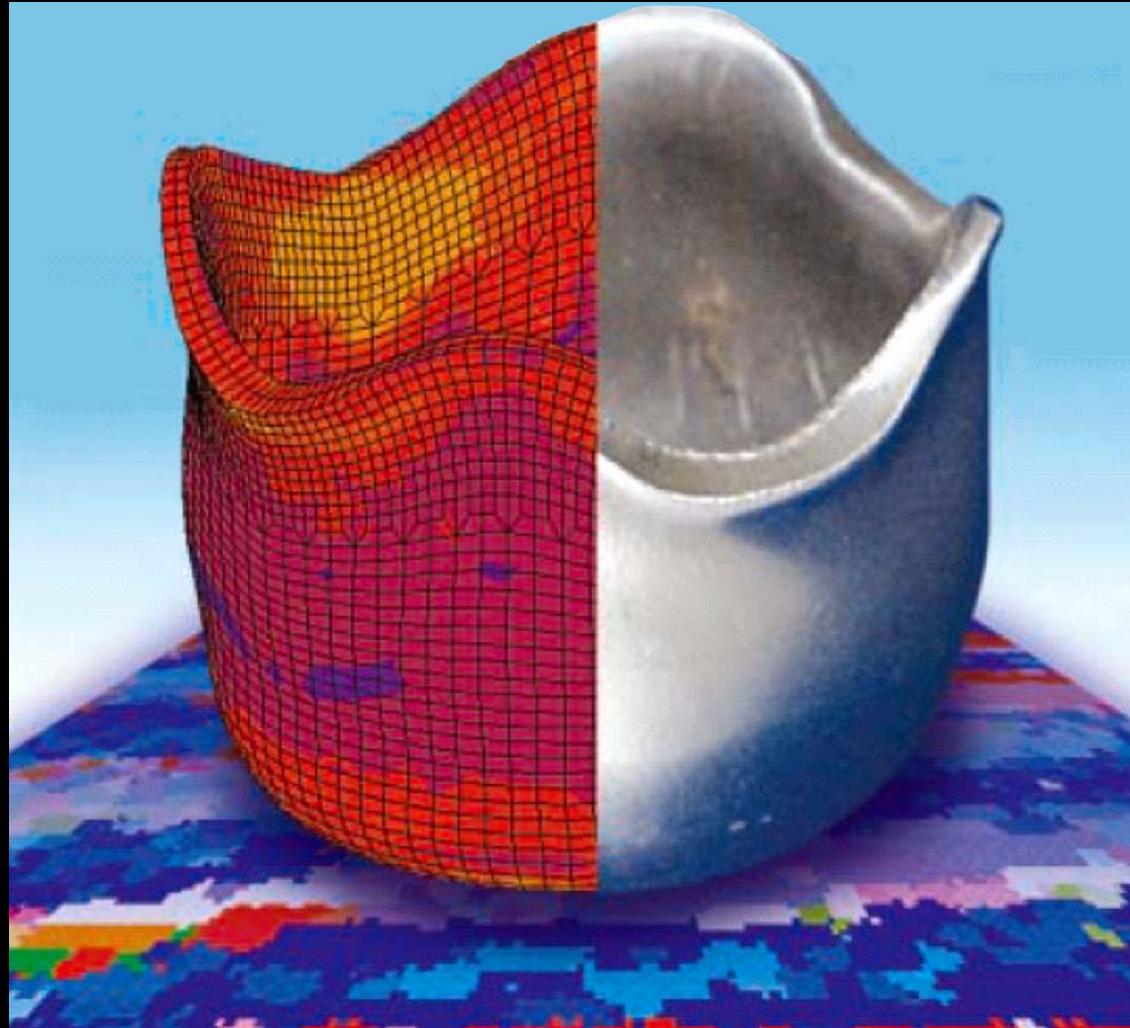
3D electron microscopy

Chitin-composites

# Crystal Mechanics FEM (large scale)



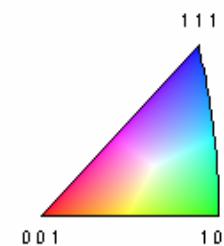
many crystals ( $10^{10}$ )



# 10 billion grains



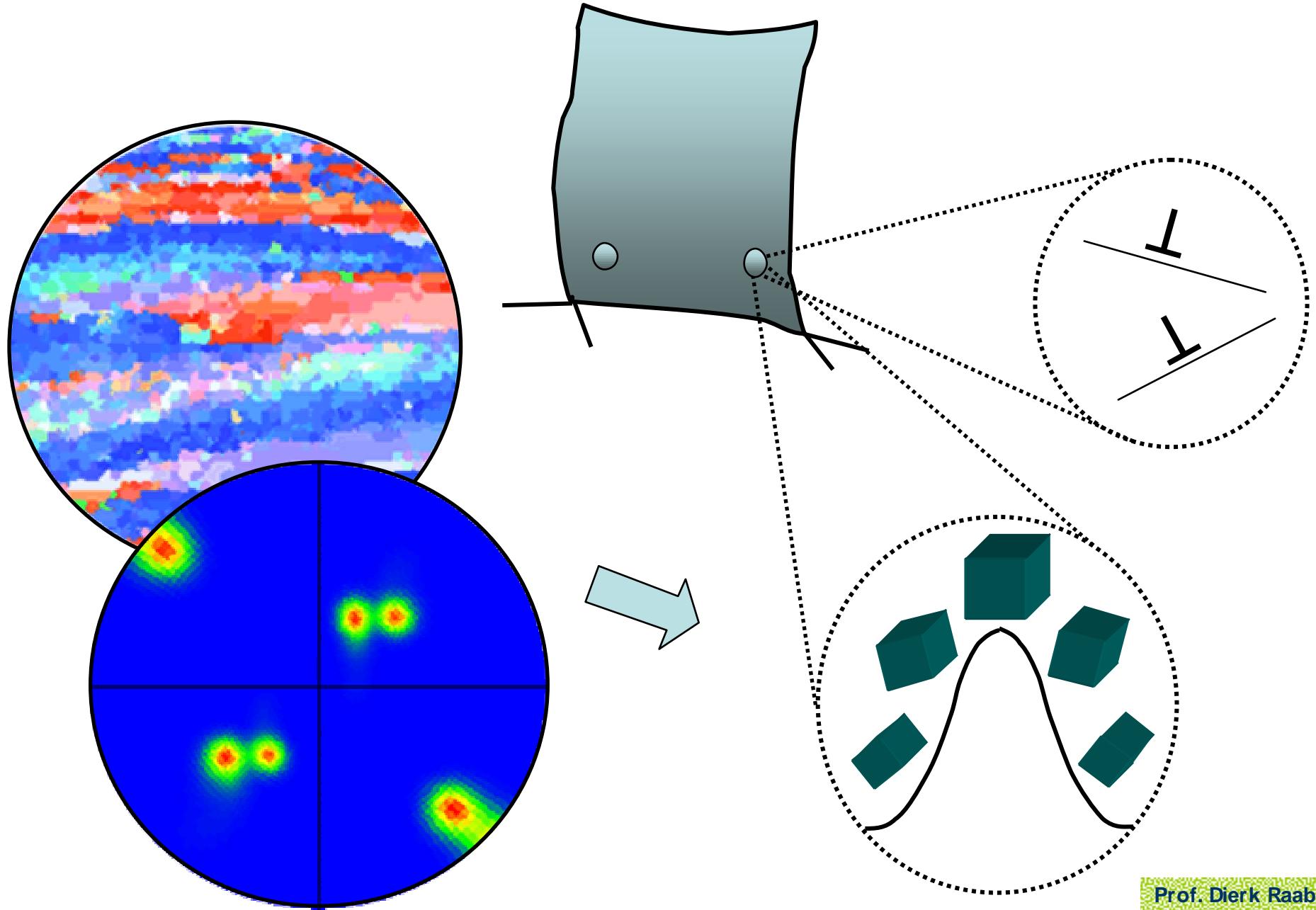
too many  
grains

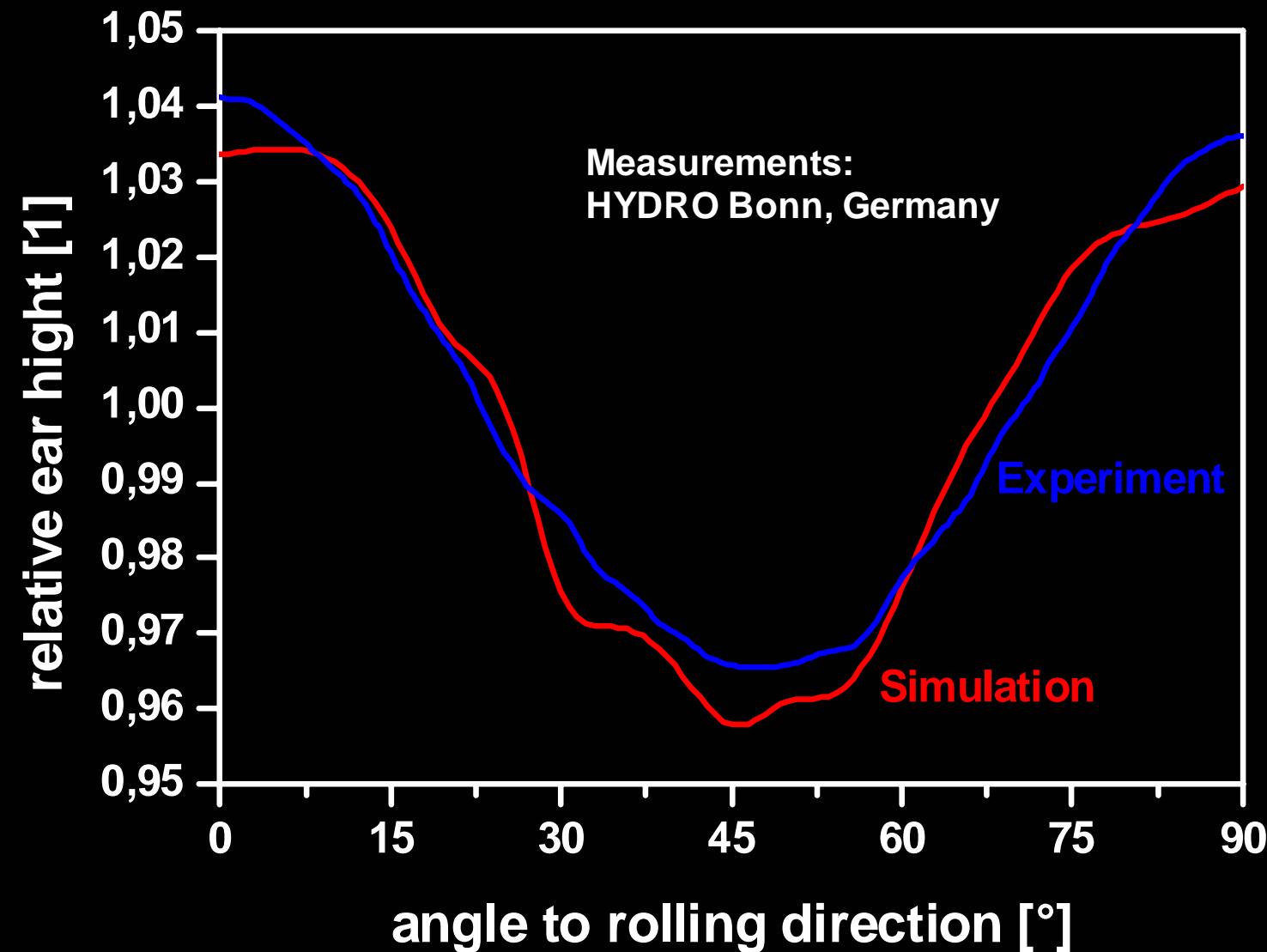


70.00  $\mu\text{m}$  = 70 steps

Prof. Dierk Raabe

# Using spherical functions in FEM







**Biomedical parts, implant devices**

**Small mechanical and electronic parts**

**Automotive**

**Structural aerospace and turbines**

**Numerical laboratories**

**Homogenization theory**

**Micromechanics and damage**



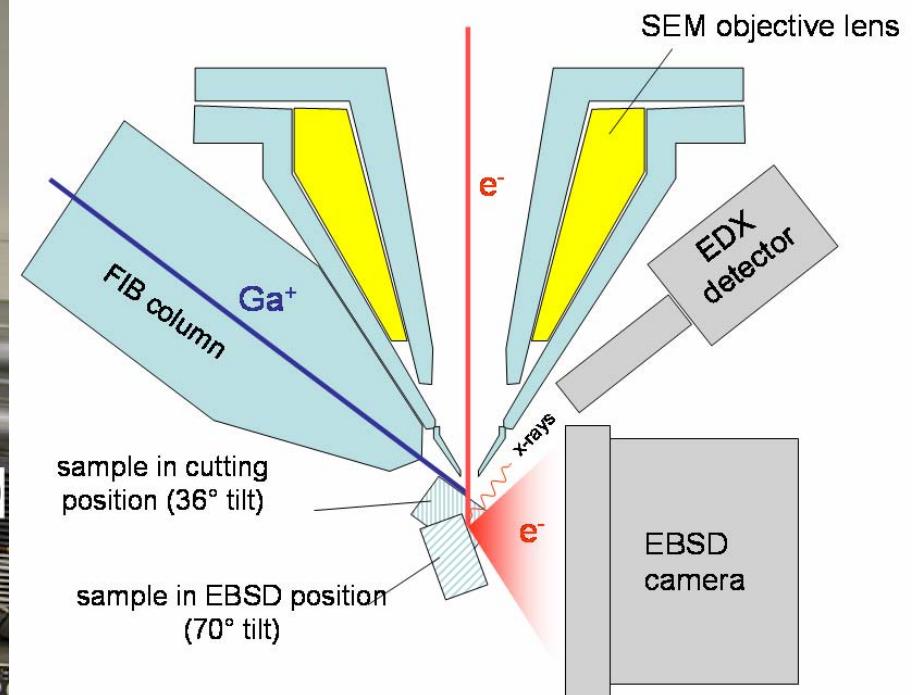
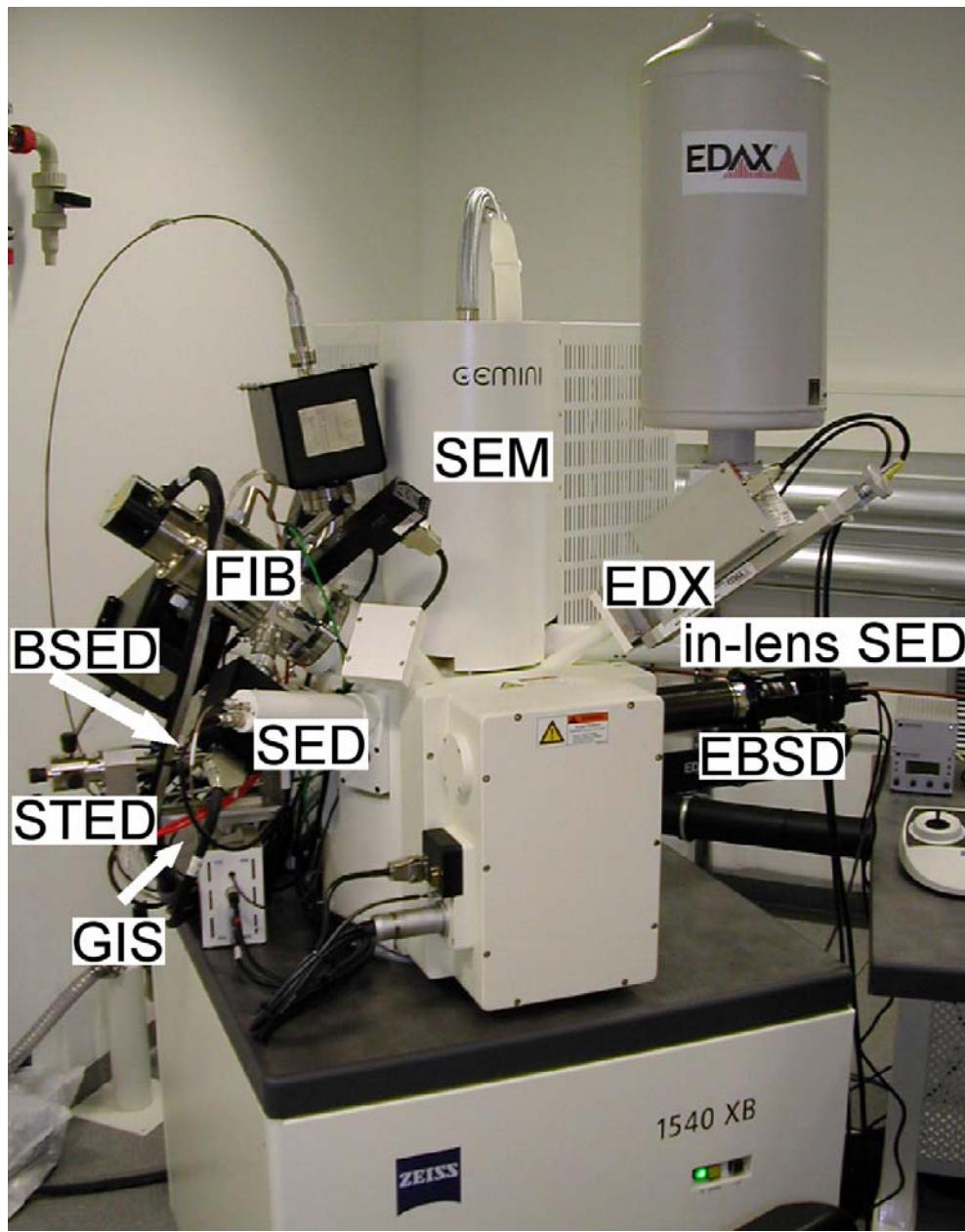
## Mechanics of few crystals

## Mechanics of many crystals

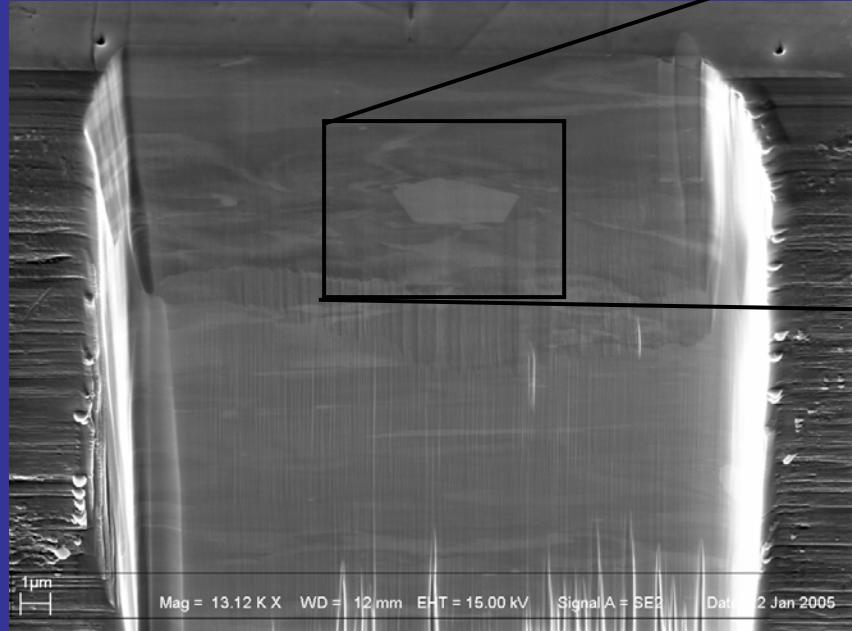
### 3D electron microscopy

## Chitin-composites

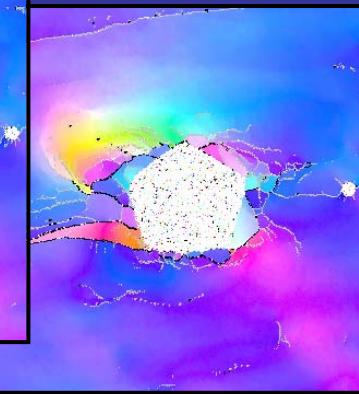
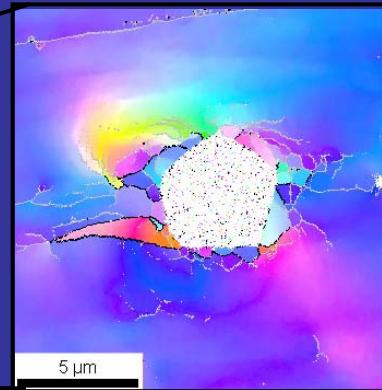
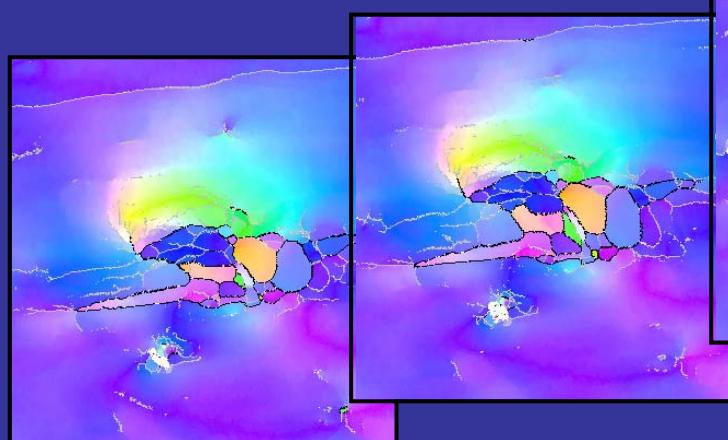
# 3D electron orientation microscopy



# 3D electron orientation microscopy



SE-image



Measurements:  
Joachim Konrad

300 nm spacing

# 3D electron orientation microscopy

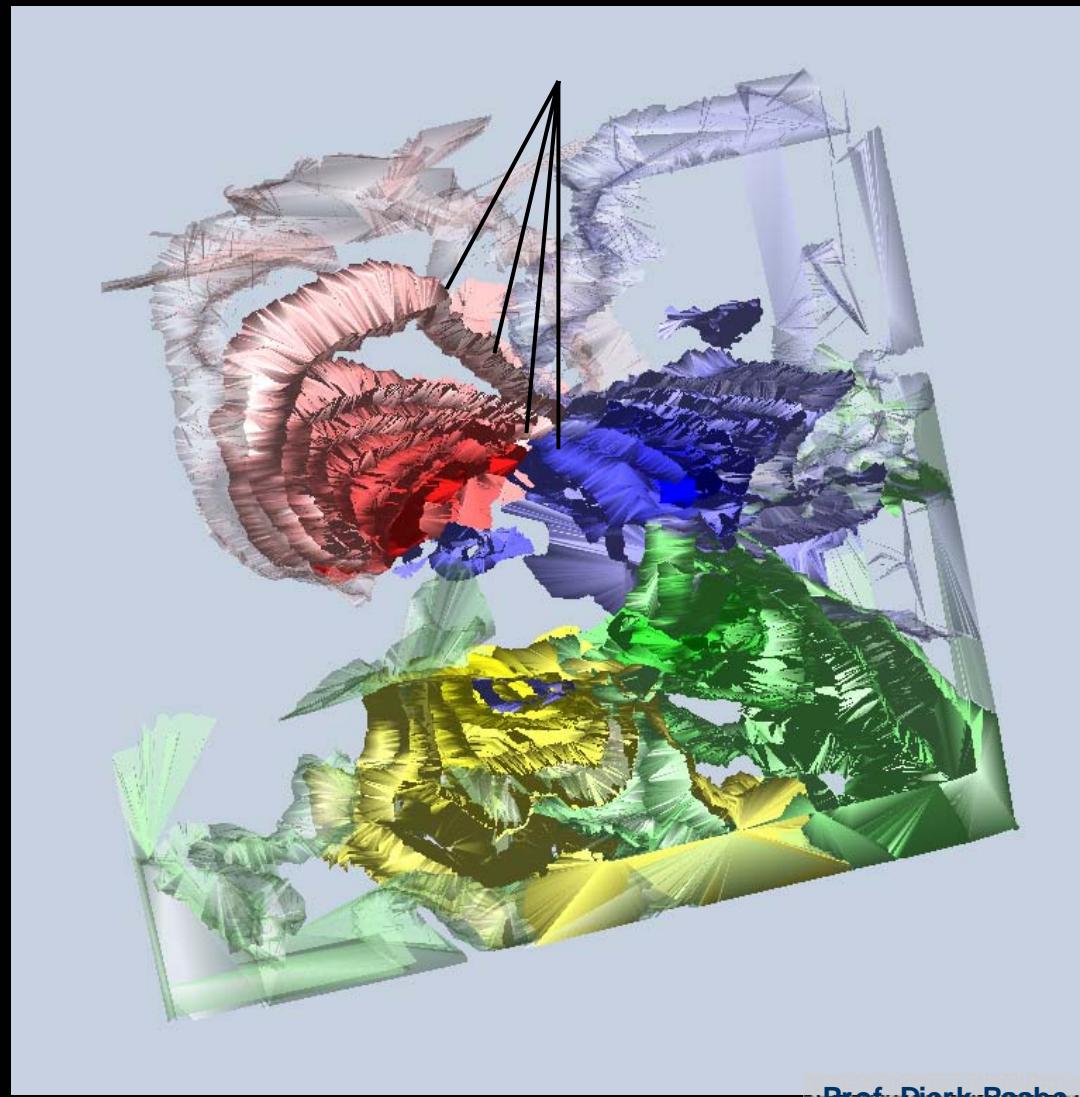


5° misorientation steps from shell to shell

Measurements:  
Joachim Konrad

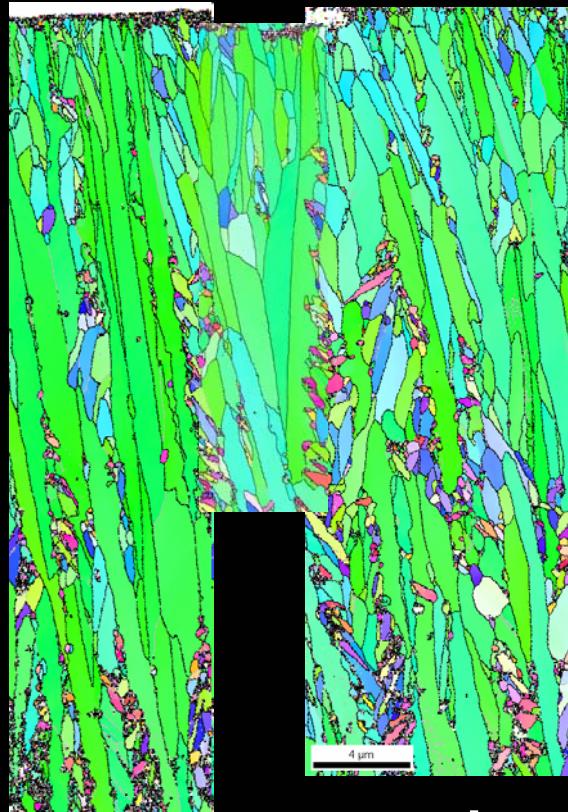
lattice rotations around Laves phase  
in  $\text{Fe}_3\text{Al}$

3D : EBSD, EDX, SEM, FIB

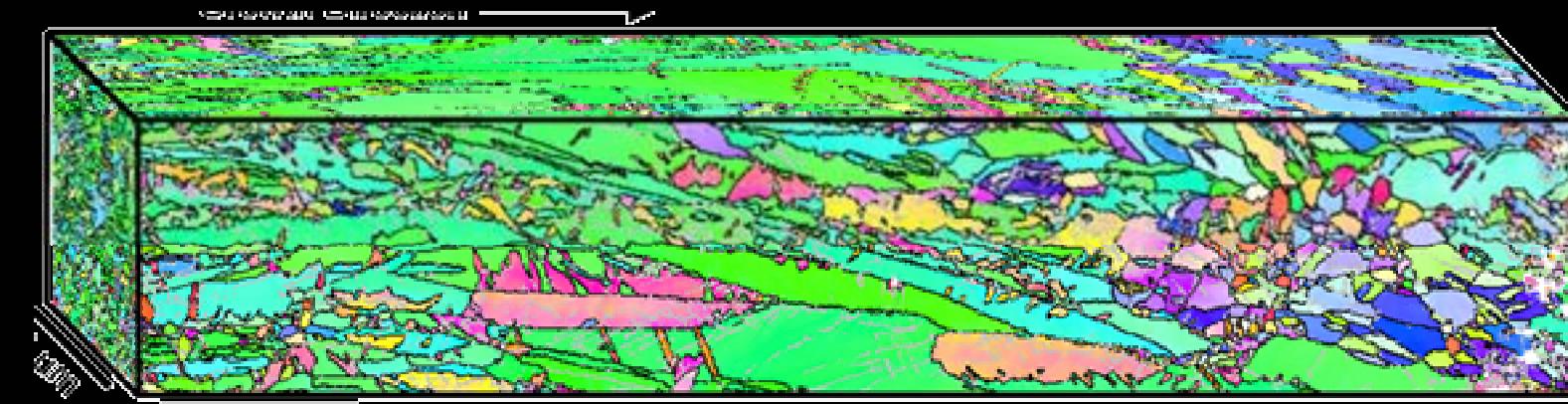


Prof. Dierk Raabe

# 3D electron orientation microscopy

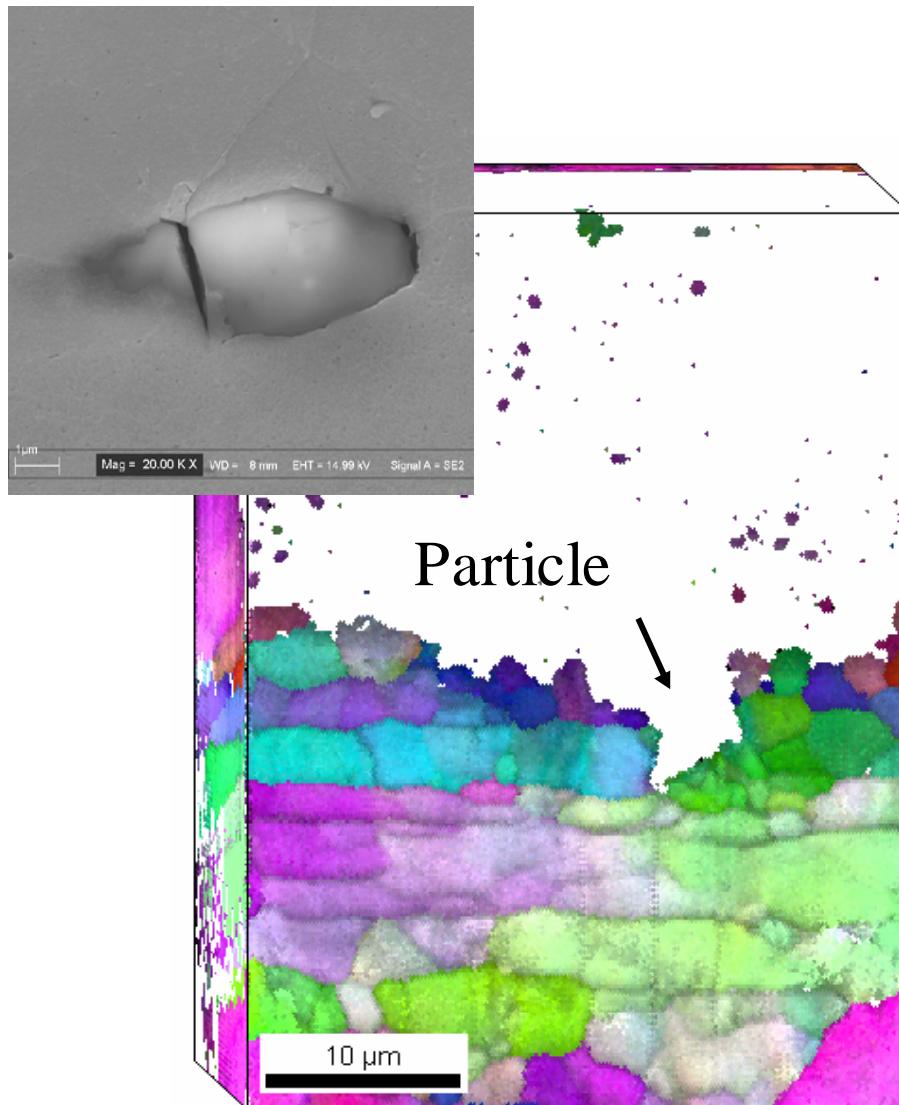


**cross view**



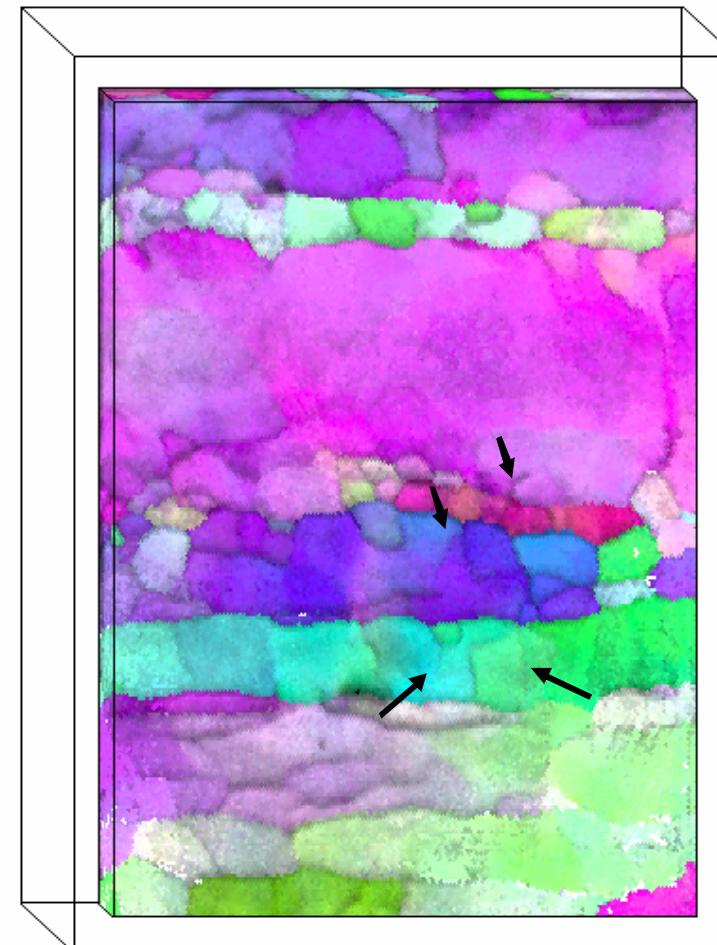
Prof. Dierk Raabe

# 3D electron orientation microscopy



50 nm step size in x,y,z

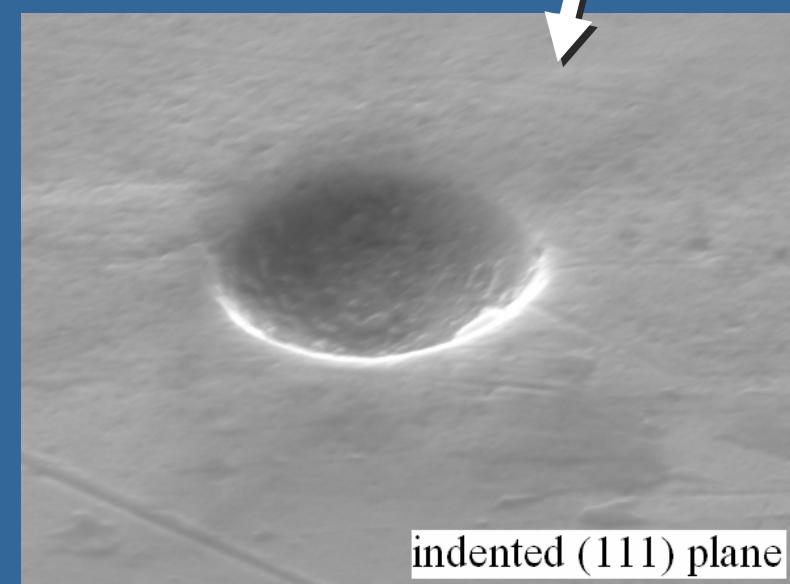
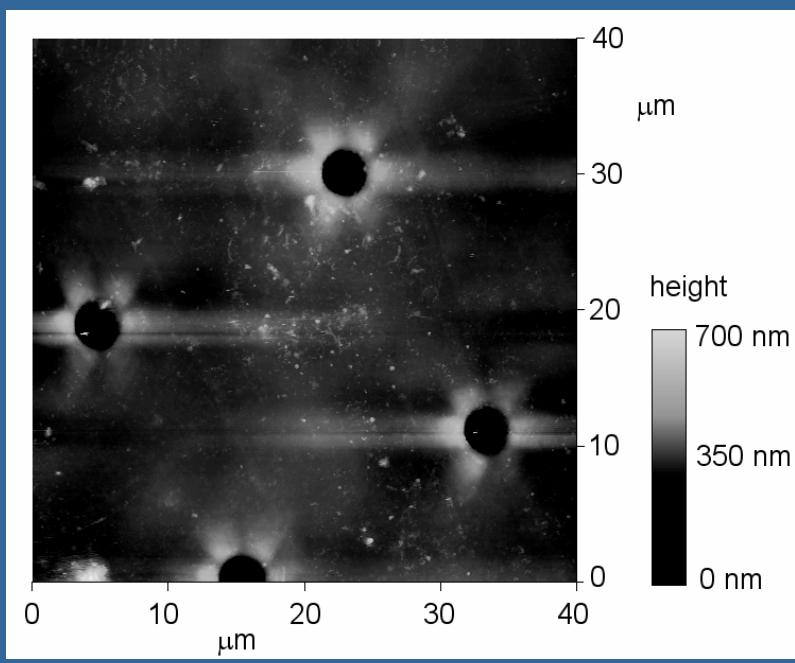
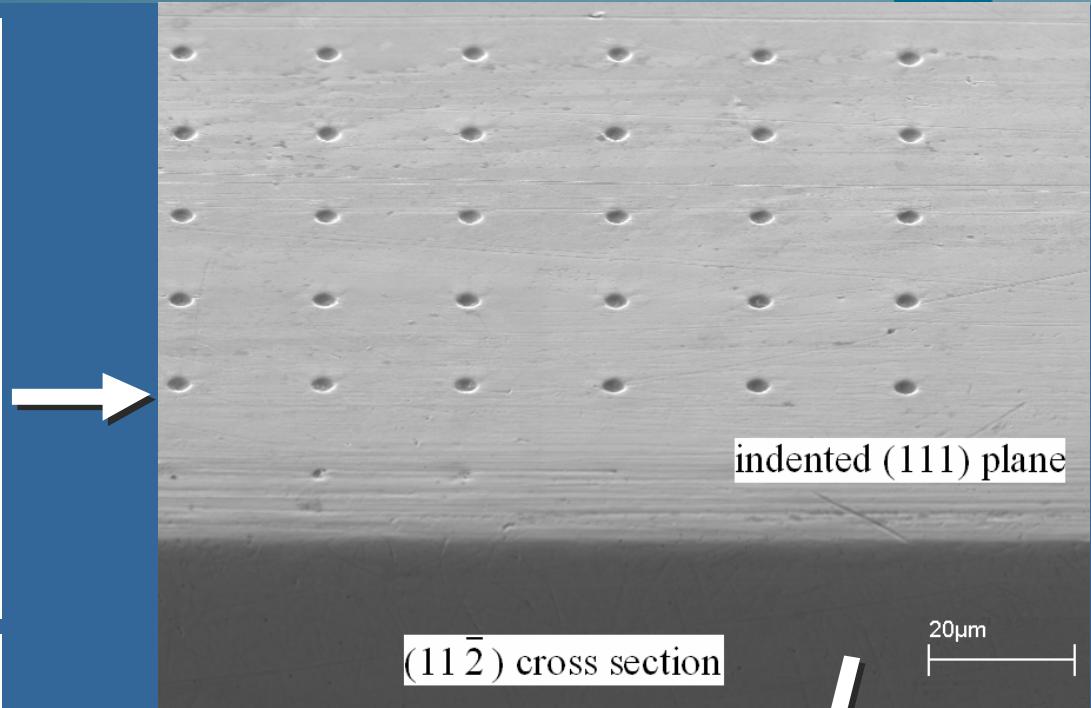
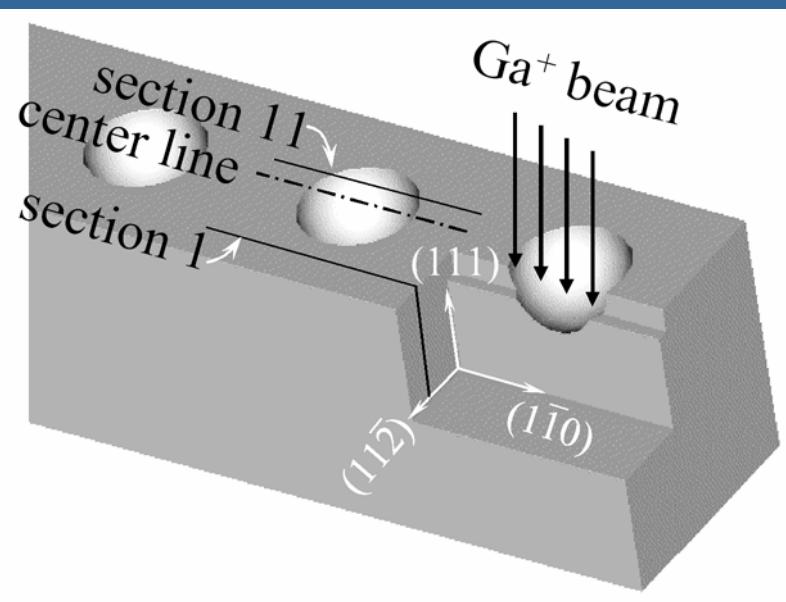
Measurements:  
Dr Hasso Weiland  
Dr Stefan Zaefferer



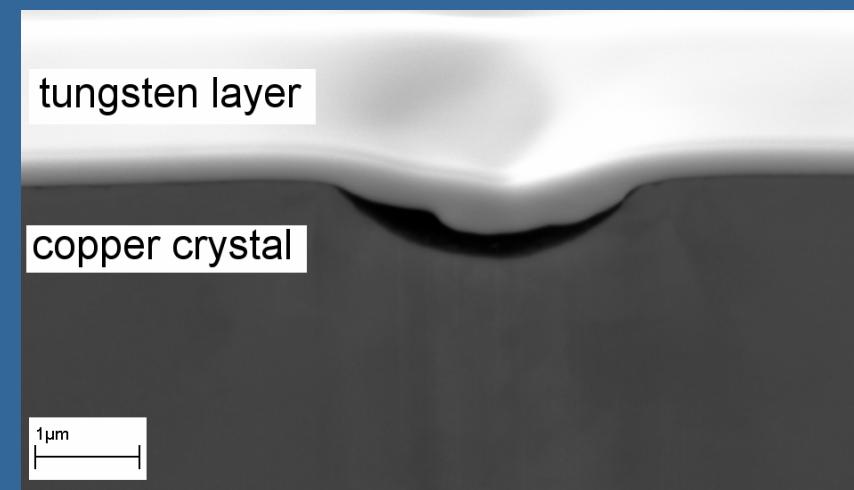
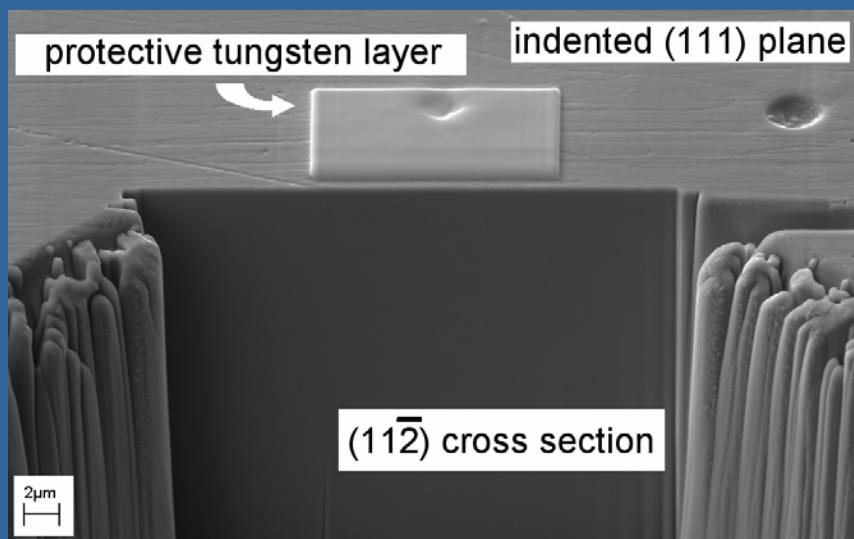
Matrix:  $(2 \ 5 \ 15)[5 \ -5 \ 1]$

Prof. Dieter Raabe

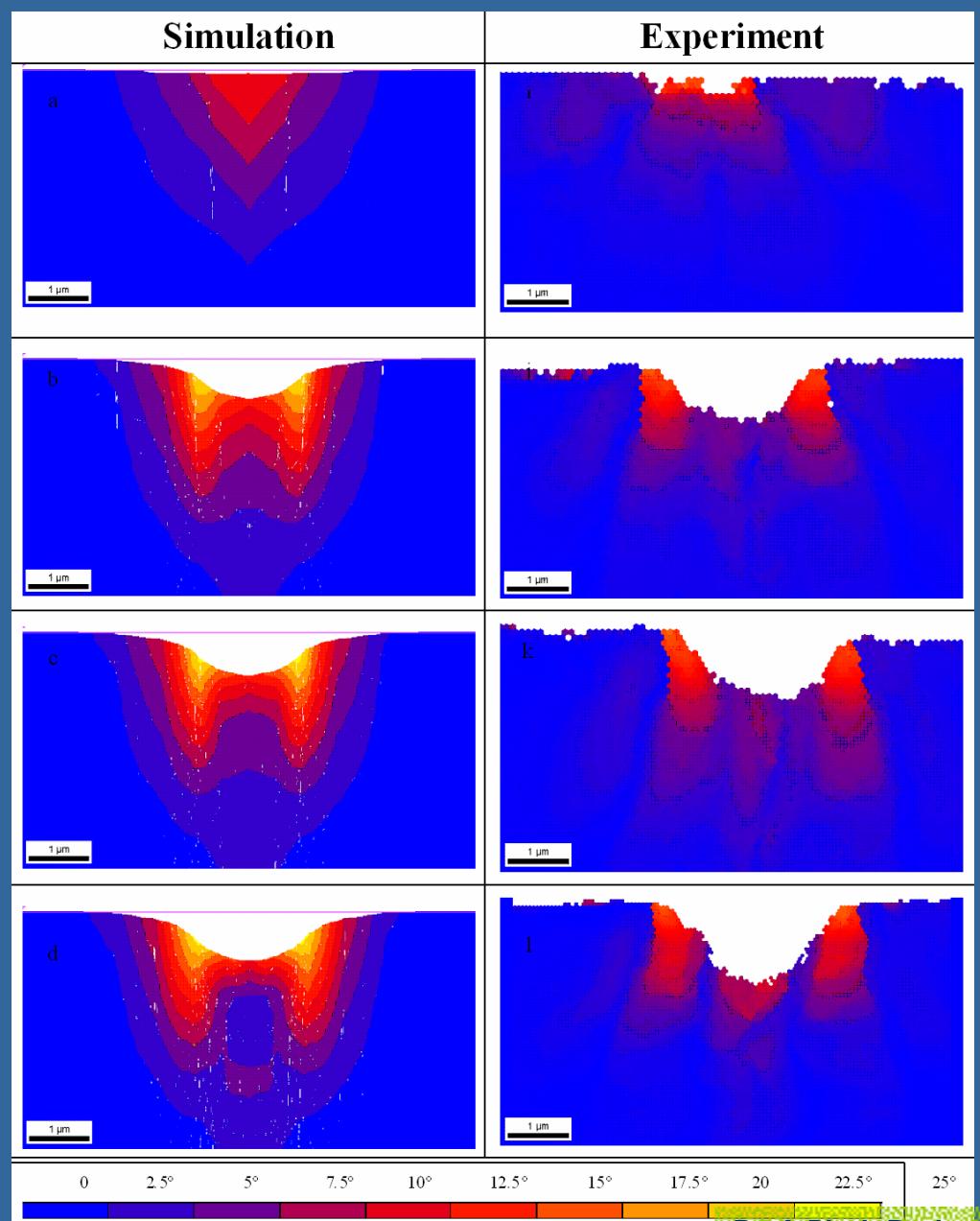
# Nanoindentation - 3D

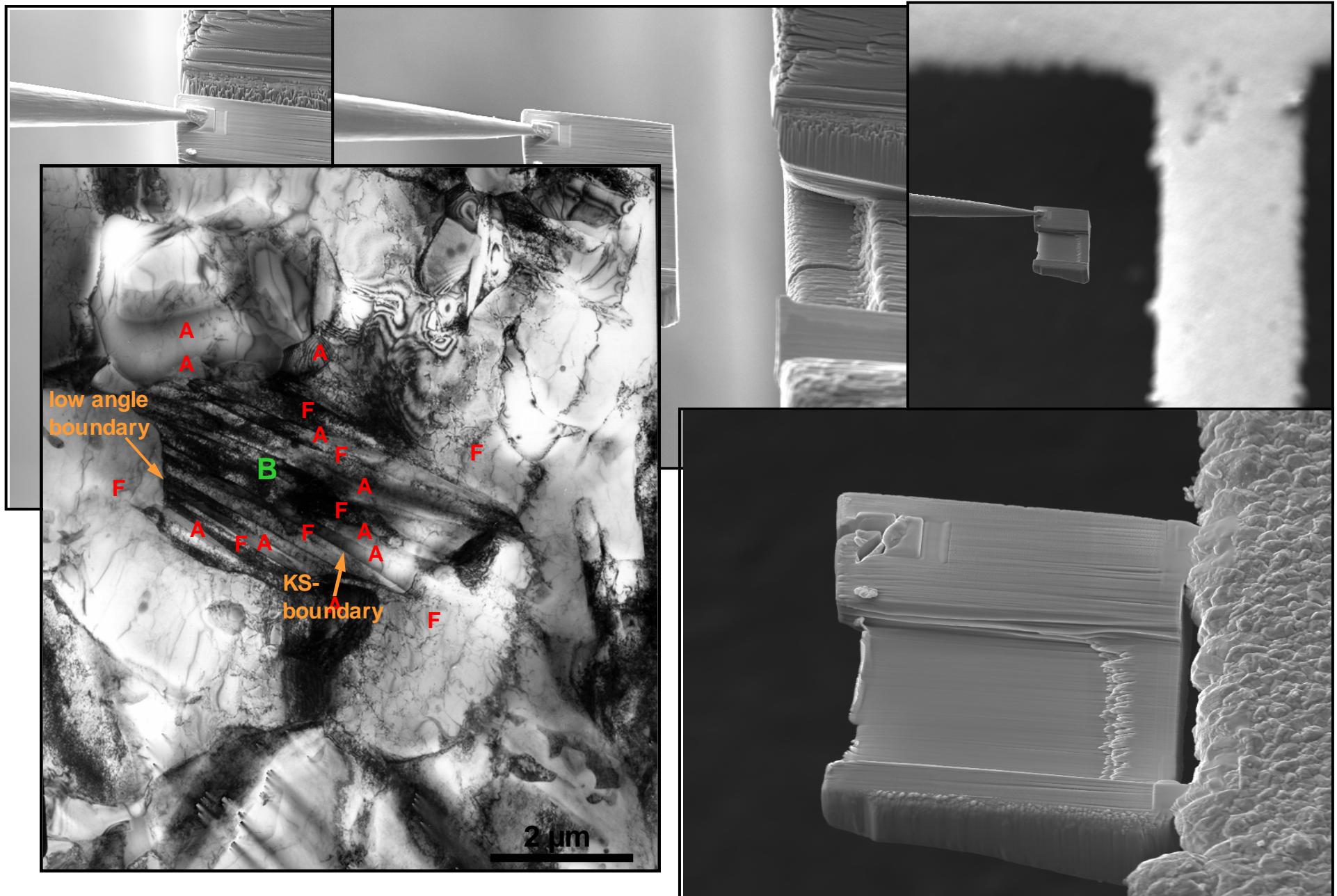


# Nanoindentation - 3D



absolute values of orientation change





## Multiphase Materials

Prof. Dierk Raabe



Mechanics of few crystals

Mechanics of many crystals

3D electron microscopy

Chitin-composites



## 1) structure, texture

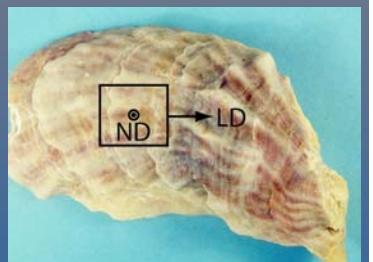
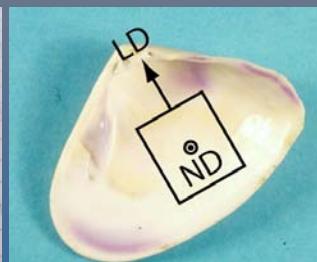
TEM, SEM, EBSD, EDX, FIB, X-ray (lab-scale), Synchrotron

## 2) properties

indentation, compression tests, tensile tests, photogrammetry

## 3) specimens

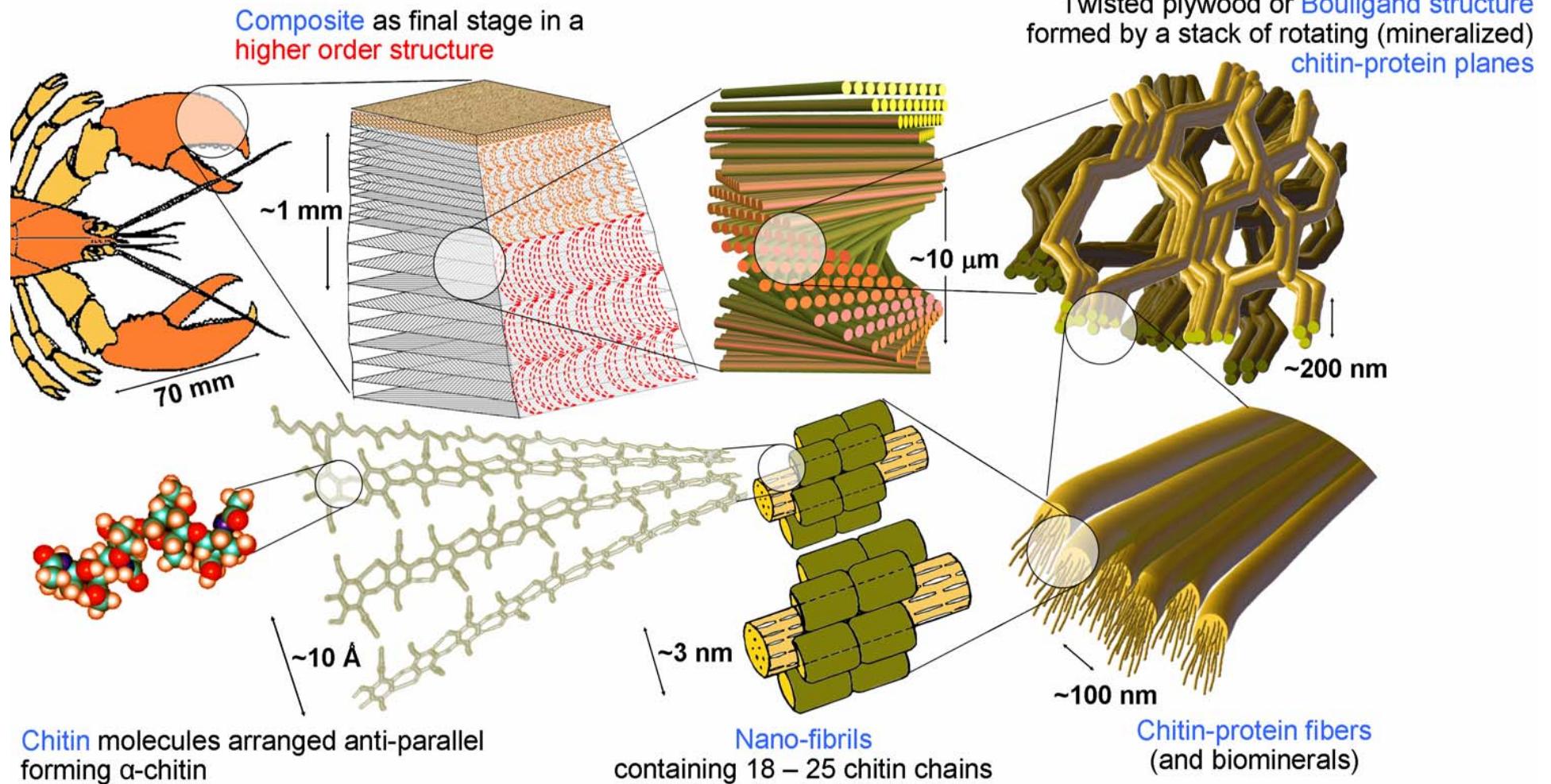
mineralized chitin-protein tissue

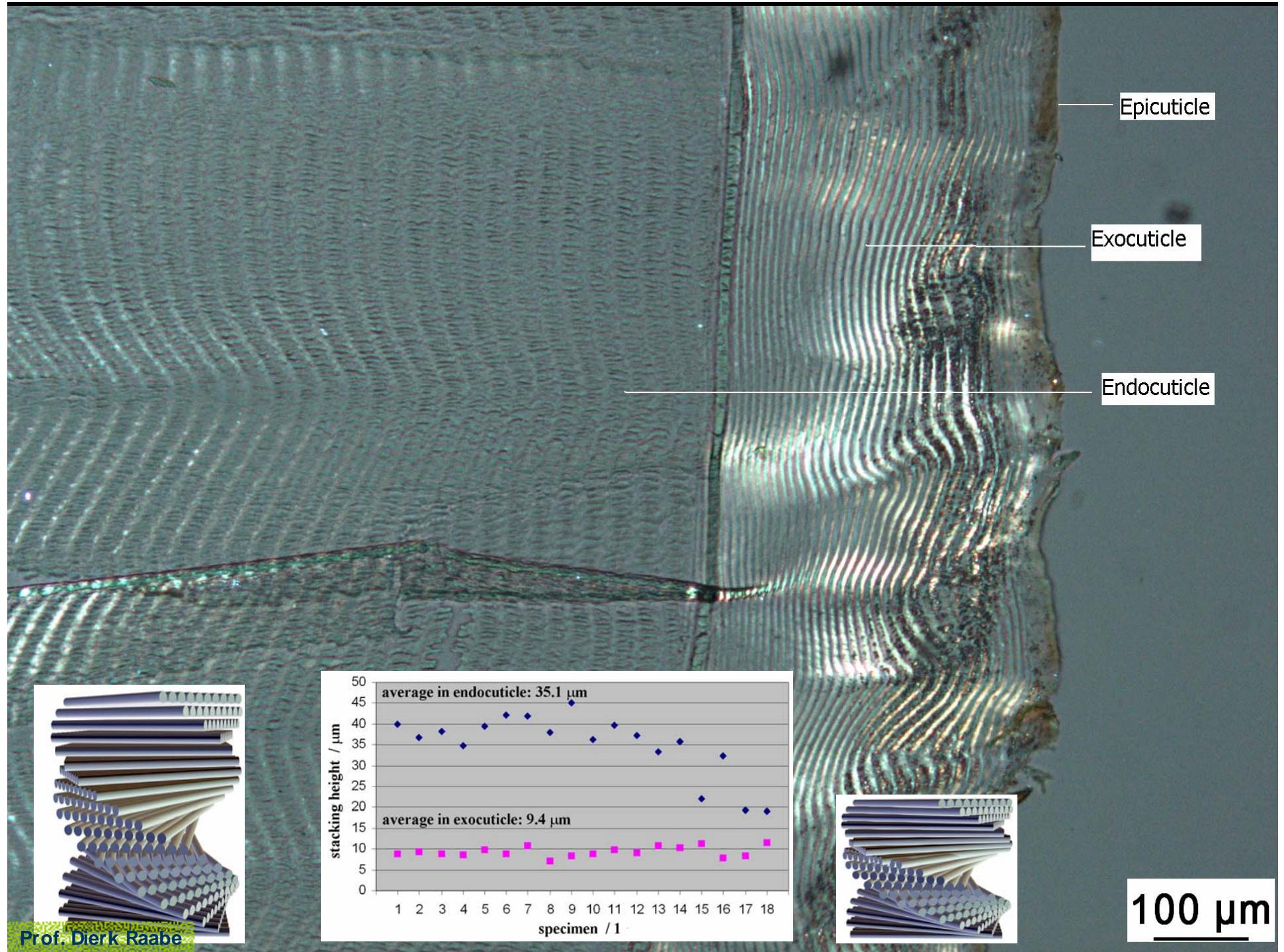


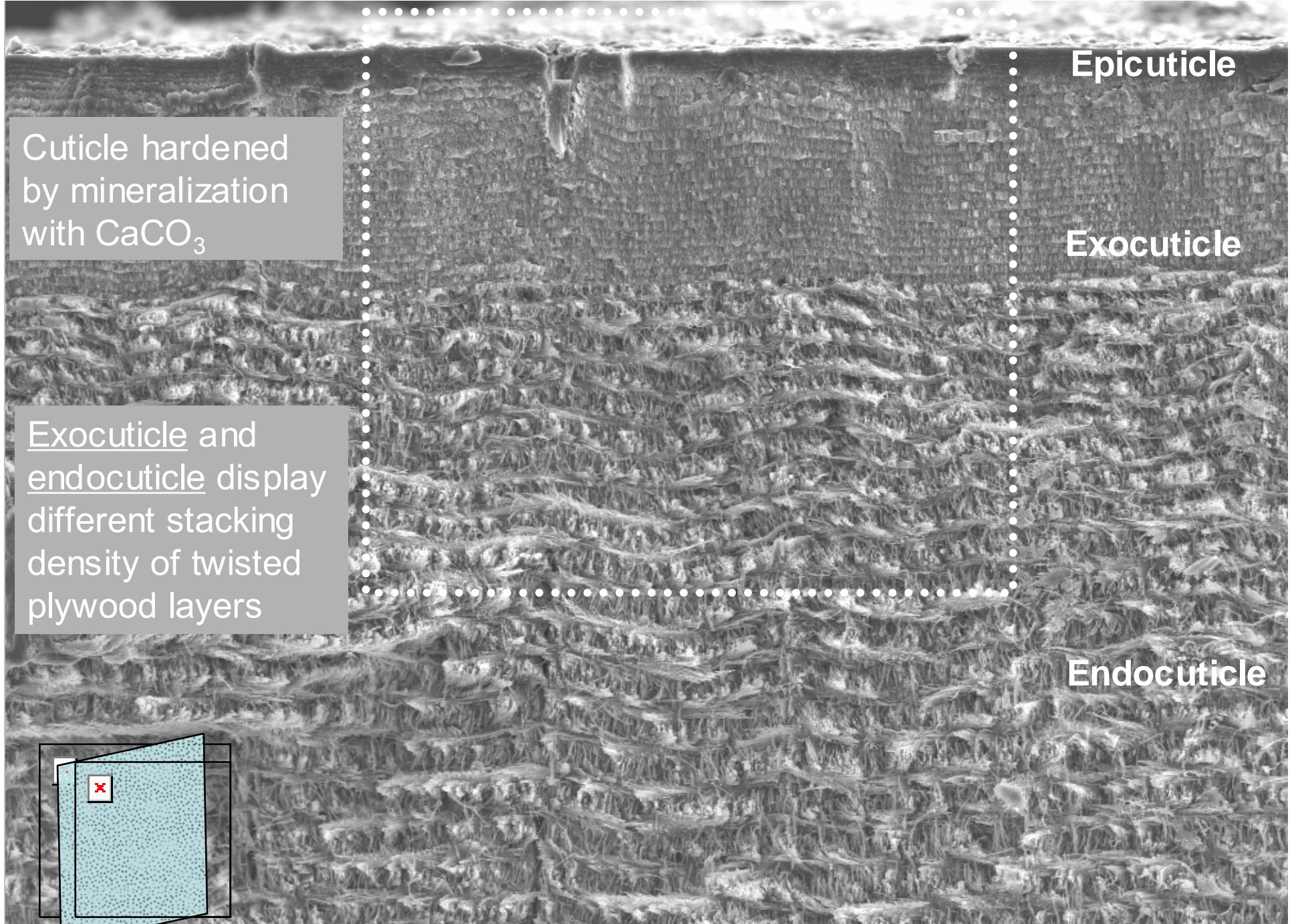
mineral content



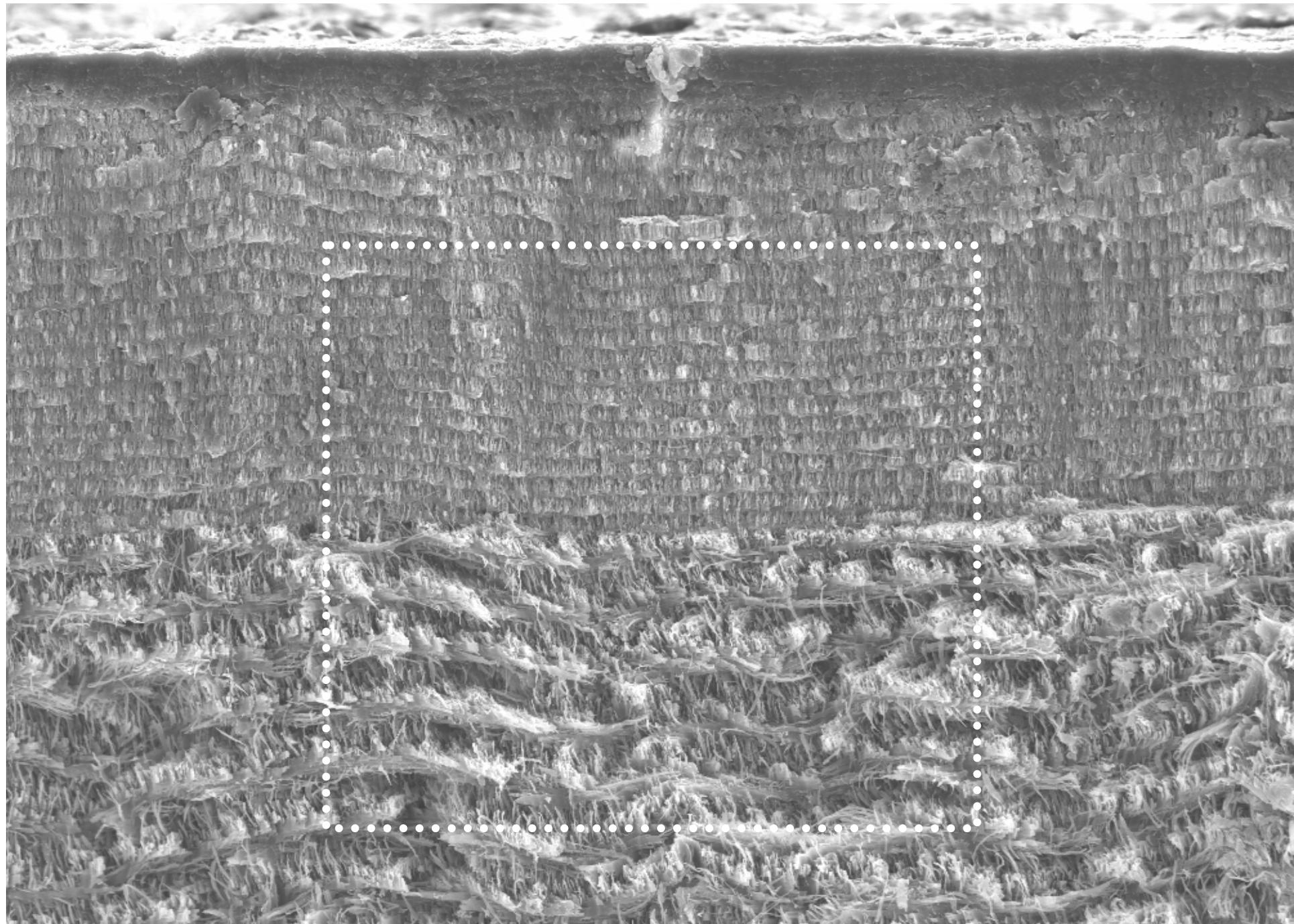
# Structure Hierarchy (*Homarus americanus*)



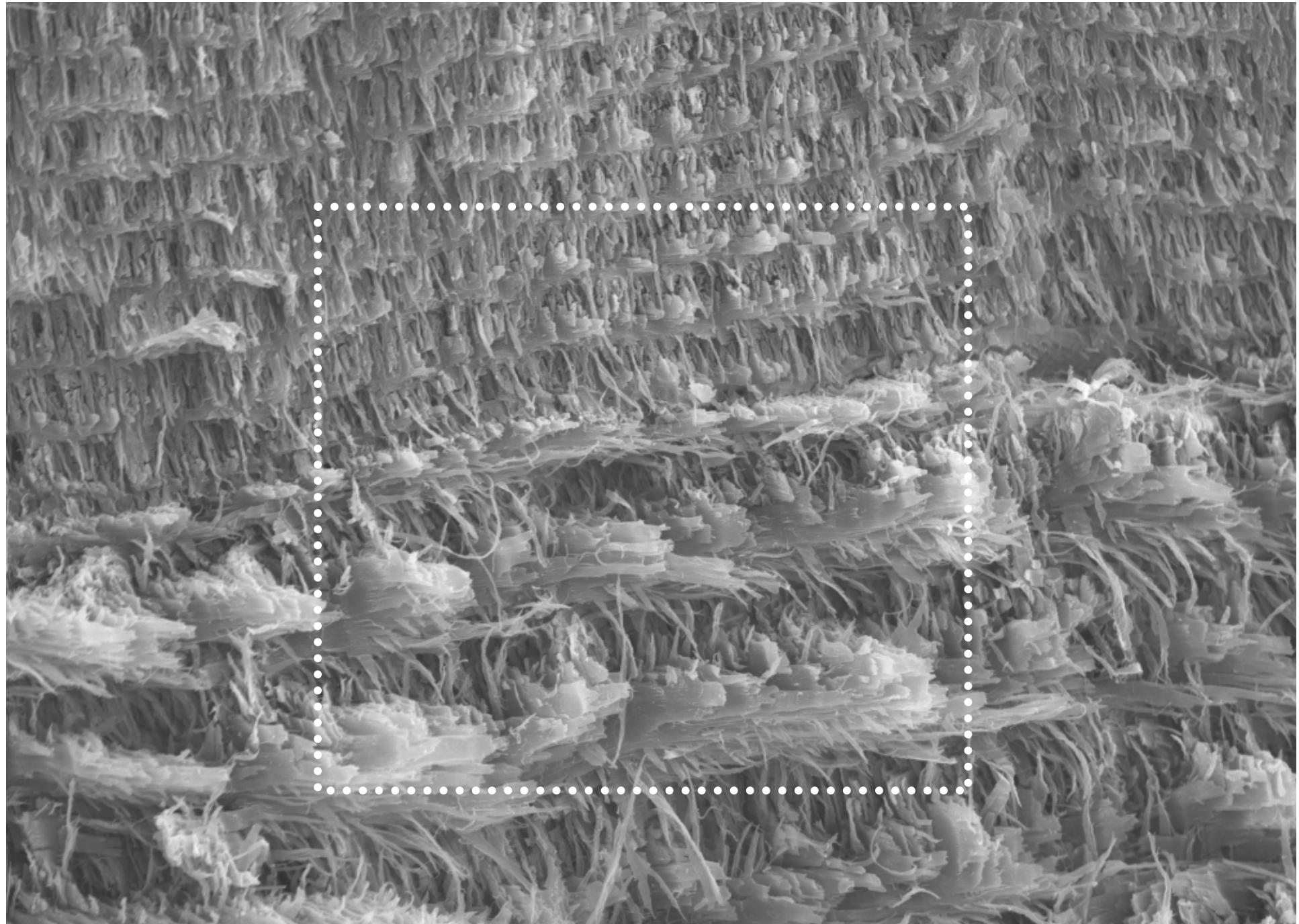




— 200  $\mu\text{m}$  —

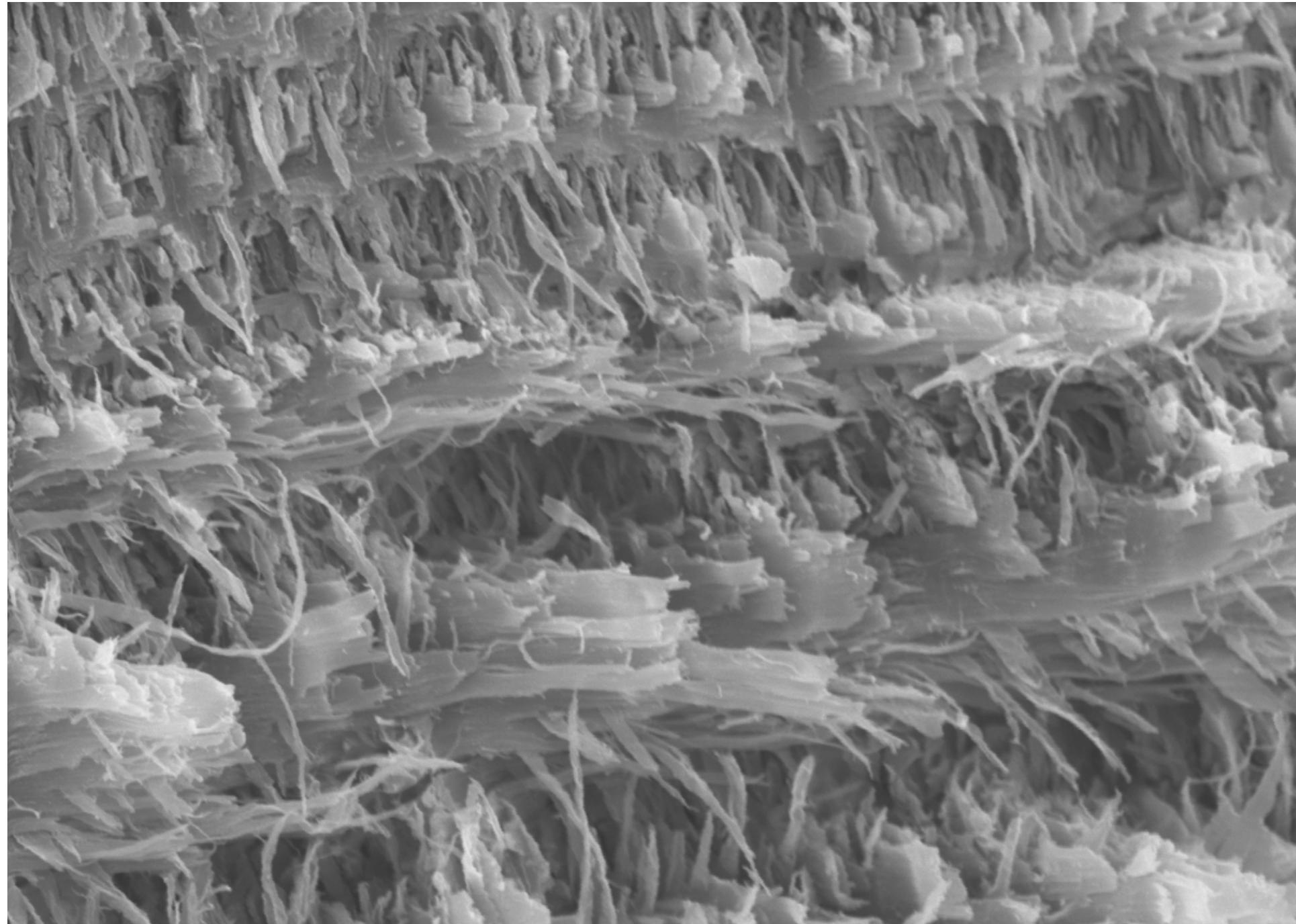


— 100 µm —

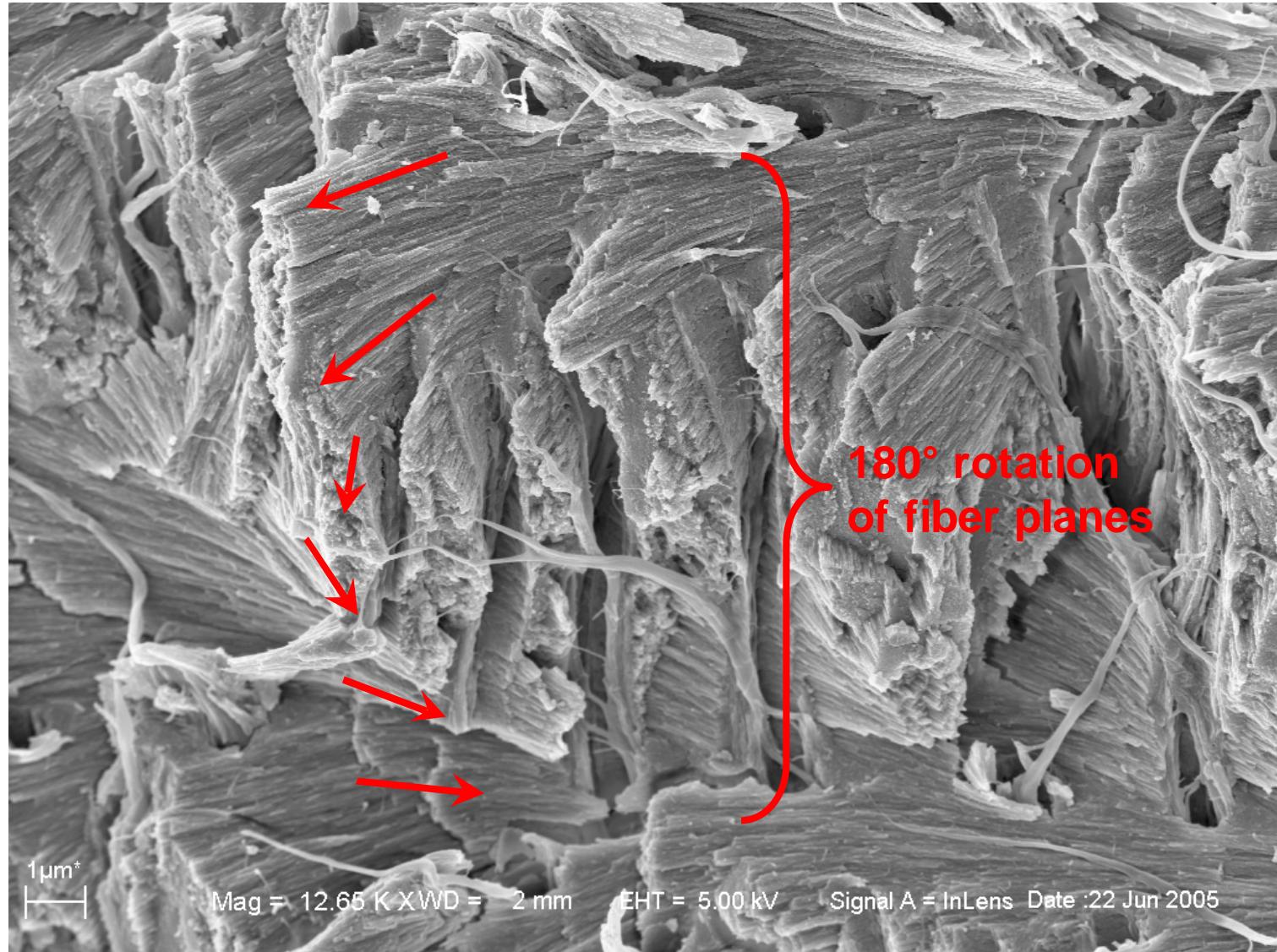


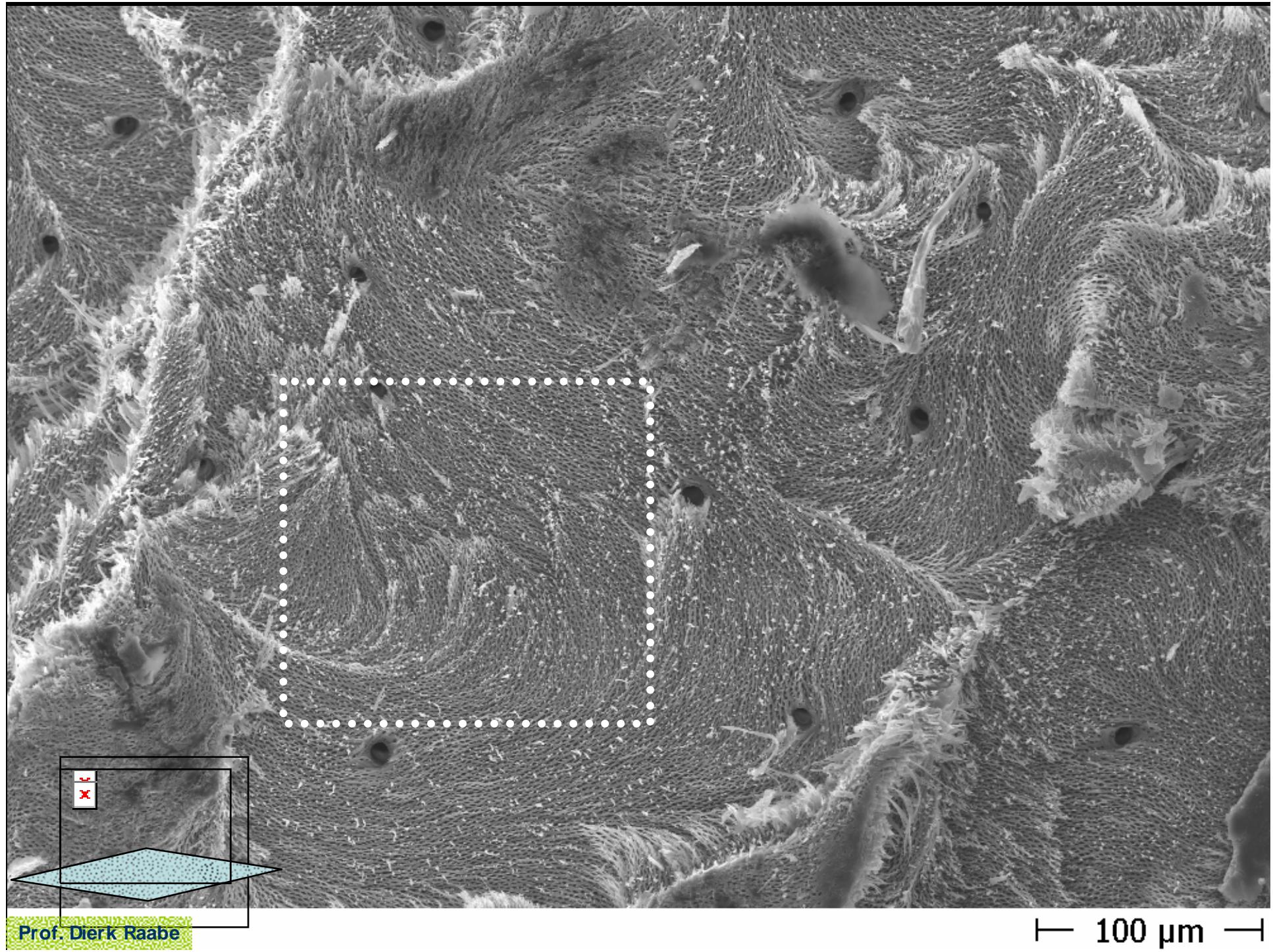
Prof. Dierk Raabe

— 30 µm —



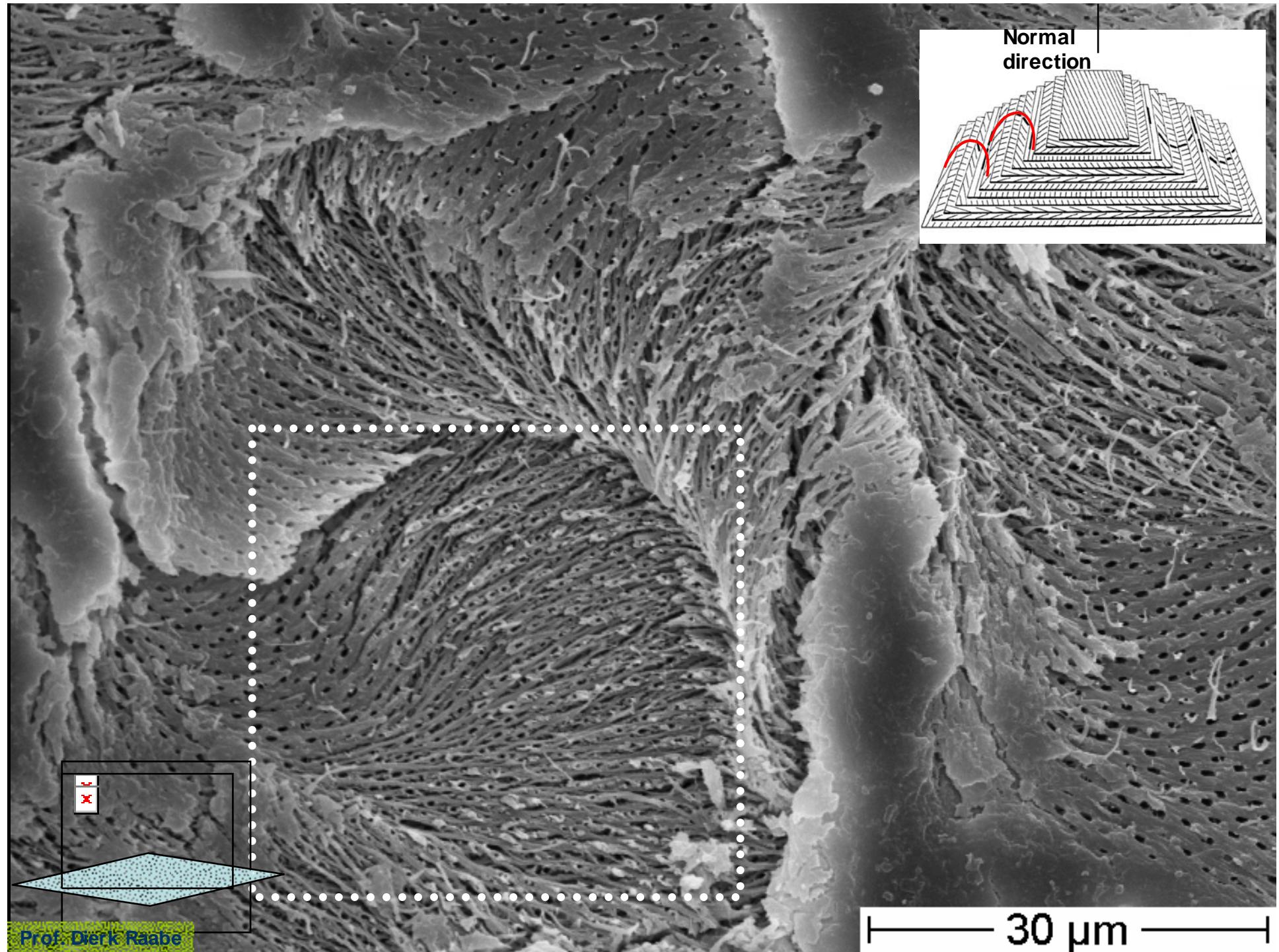
# SEM: Lobster endocuticle, untreated

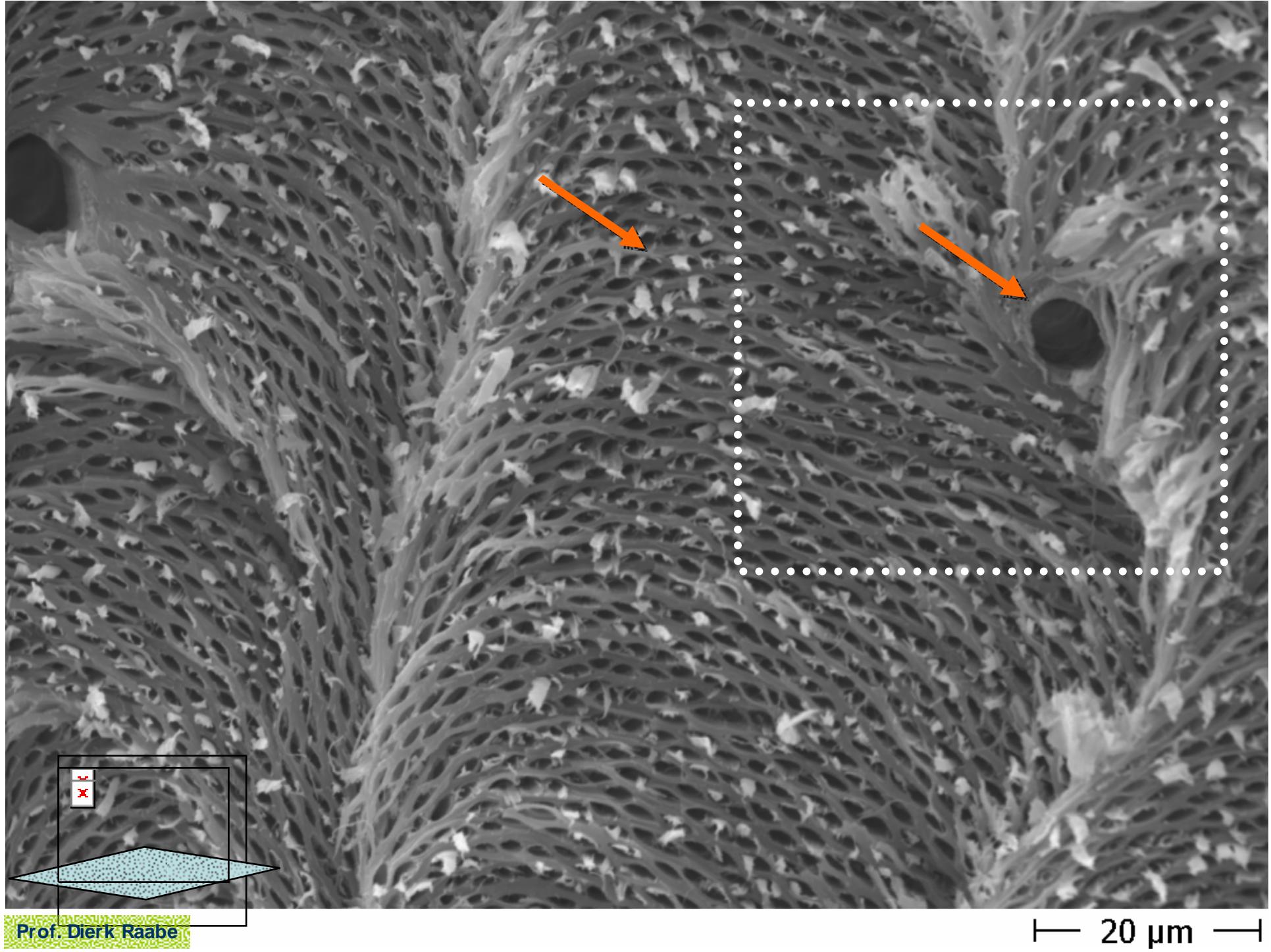




— 100  $\mu\text{m}$  —

Prof. Dierk Raabe

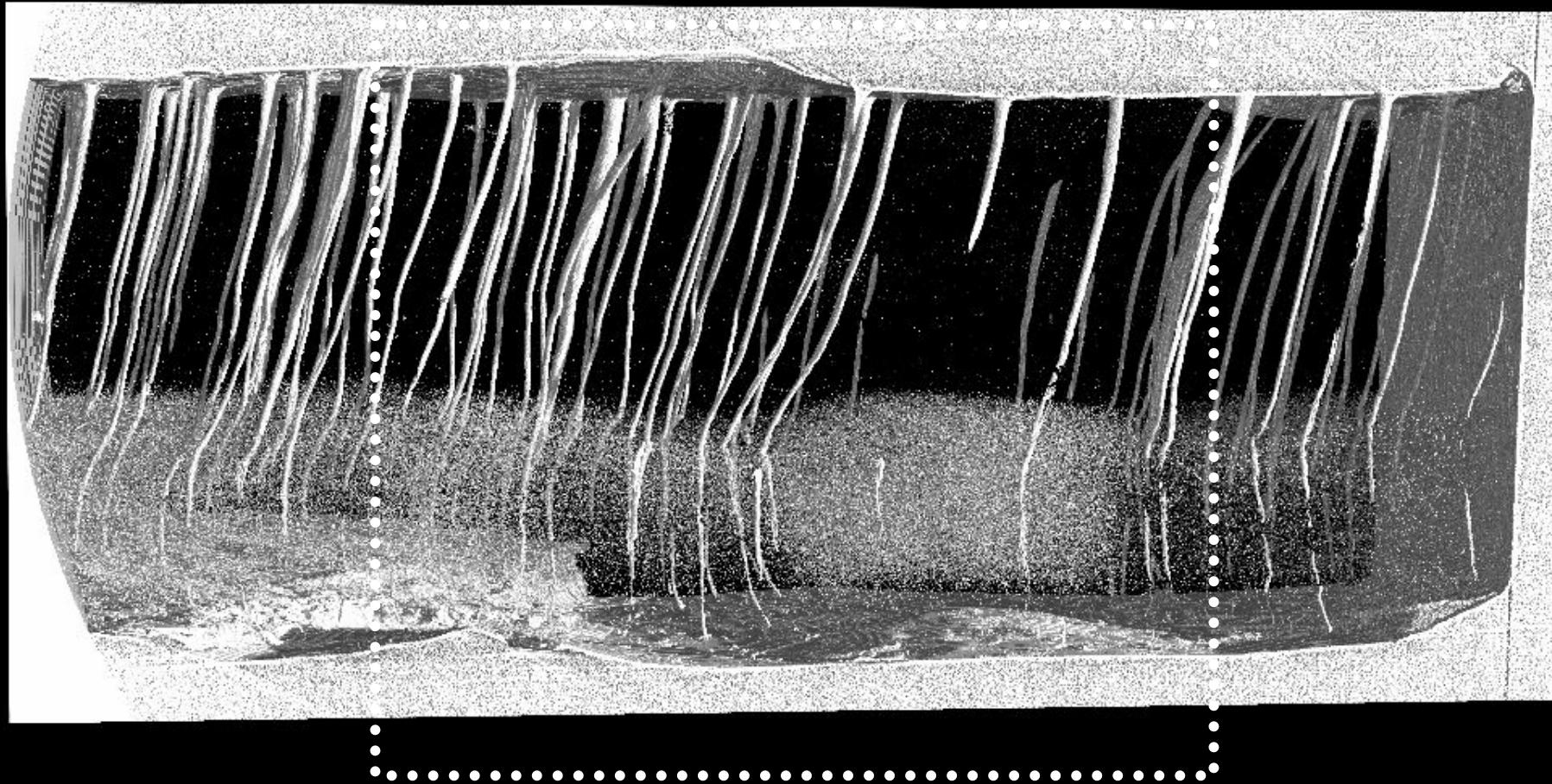




Prof. Dierk Raabe

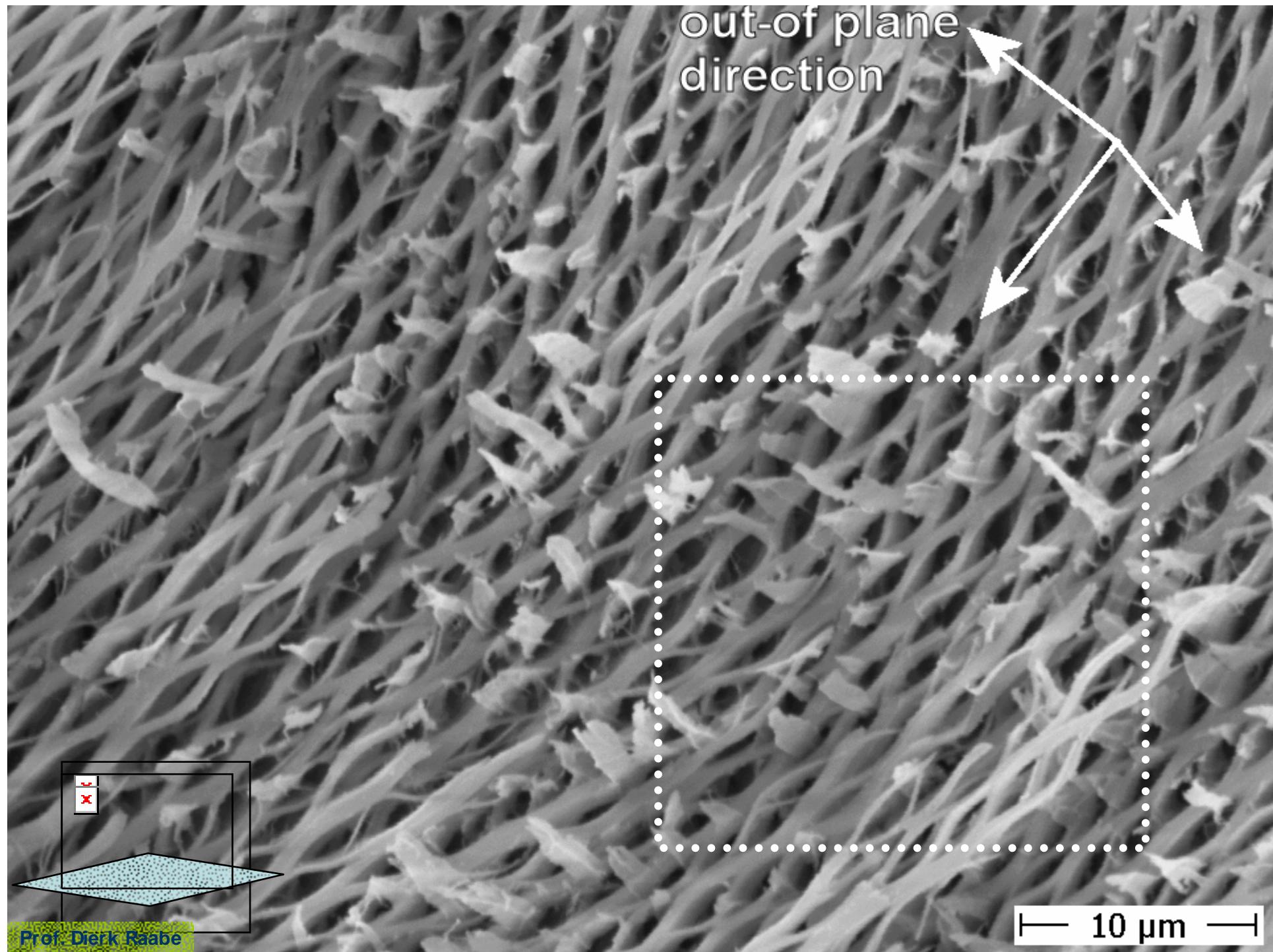
— 20  $\mu\text{m}$  —

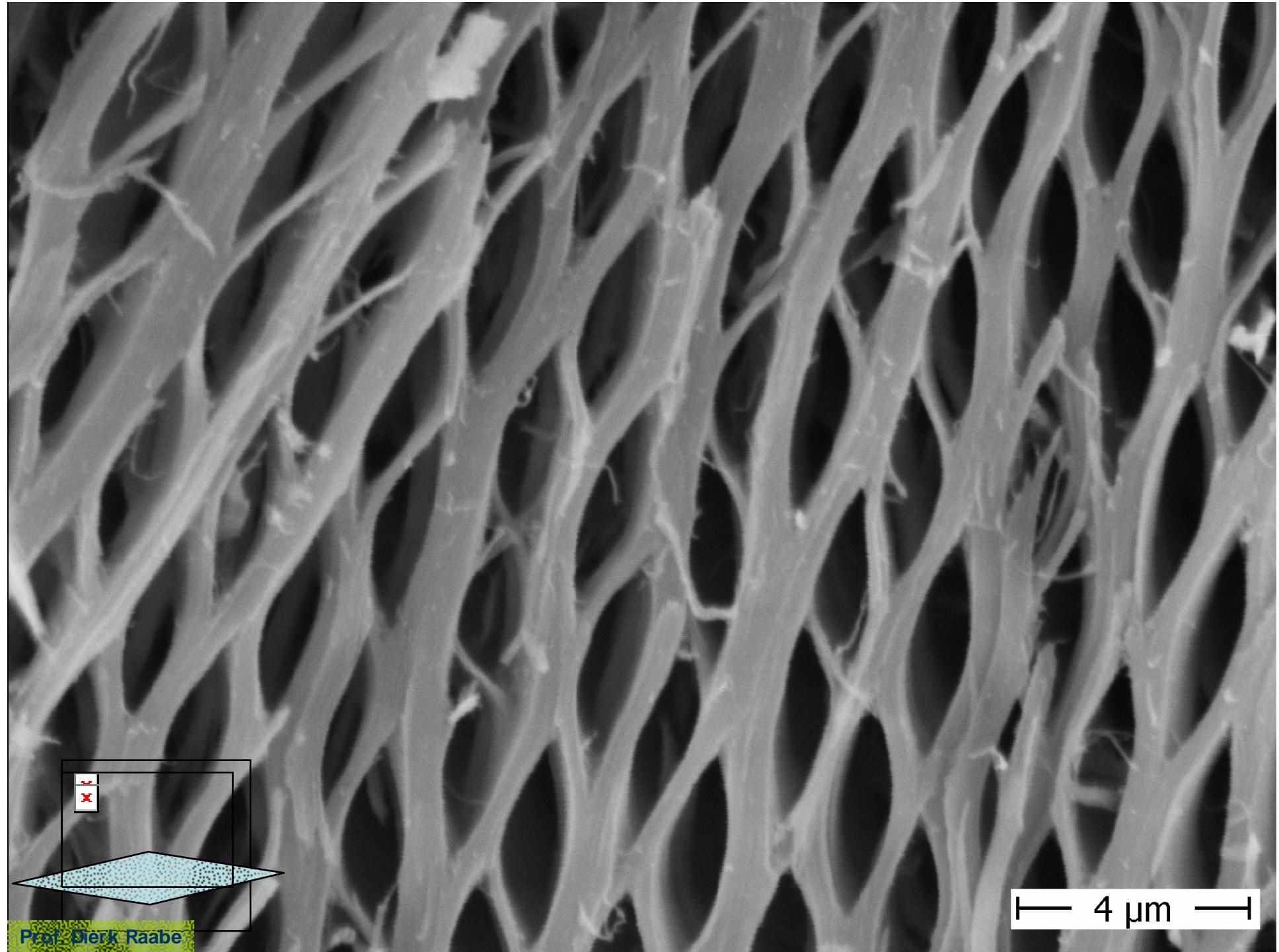
# X-ray tomography, cuticle, horseshoe crab

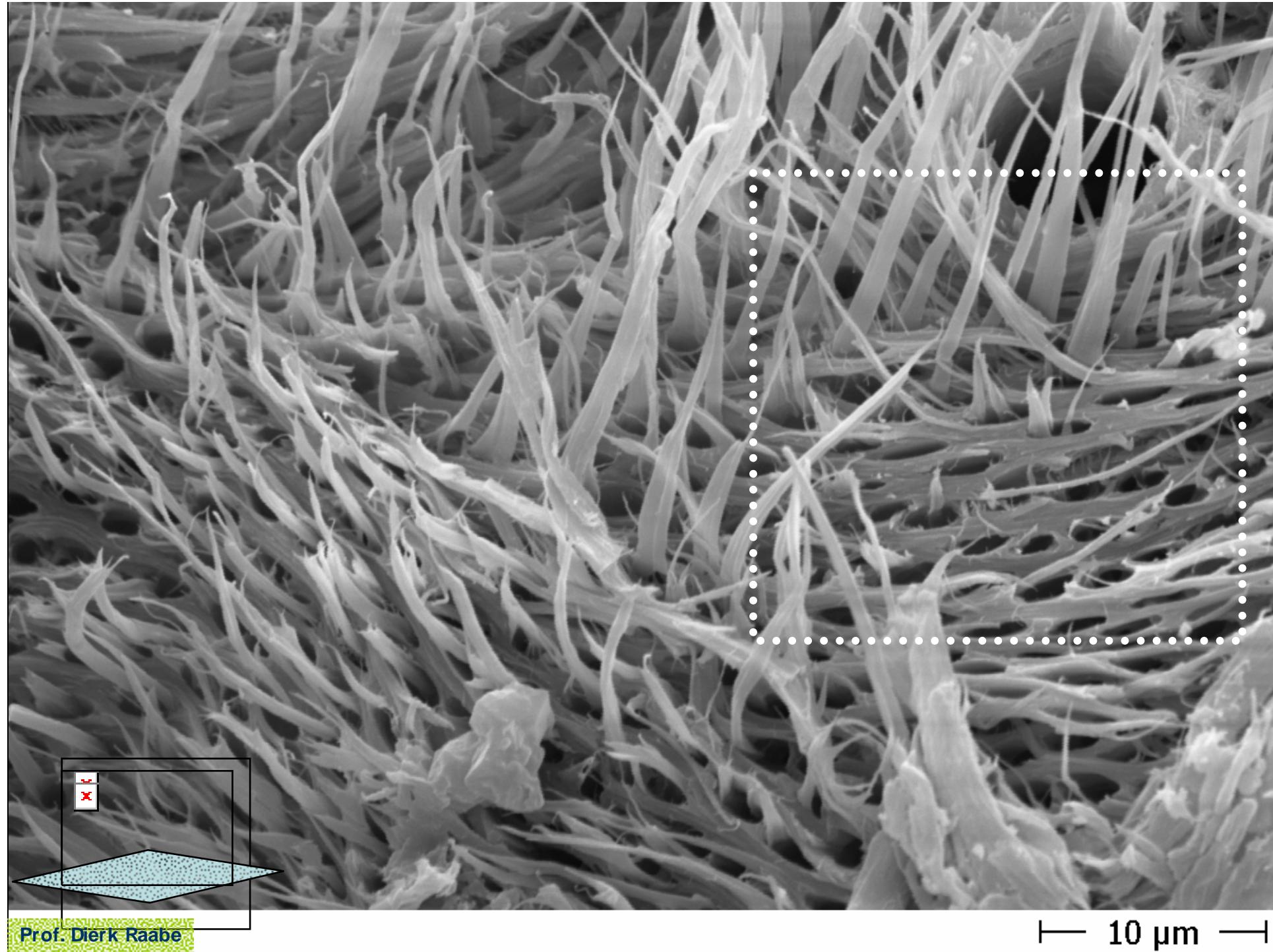


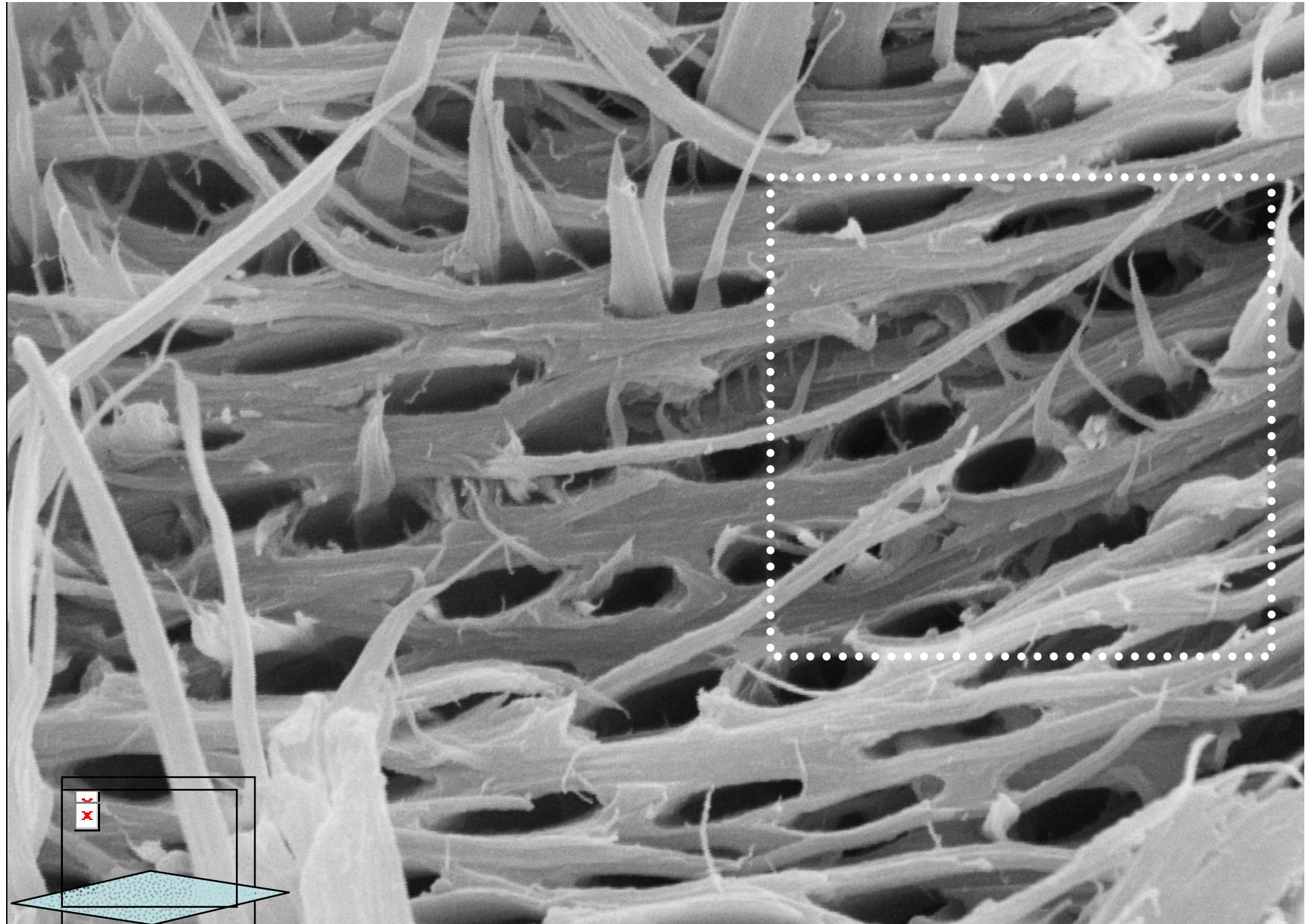
measurements at : HMI Berlin

Prof. Dierk Raabe



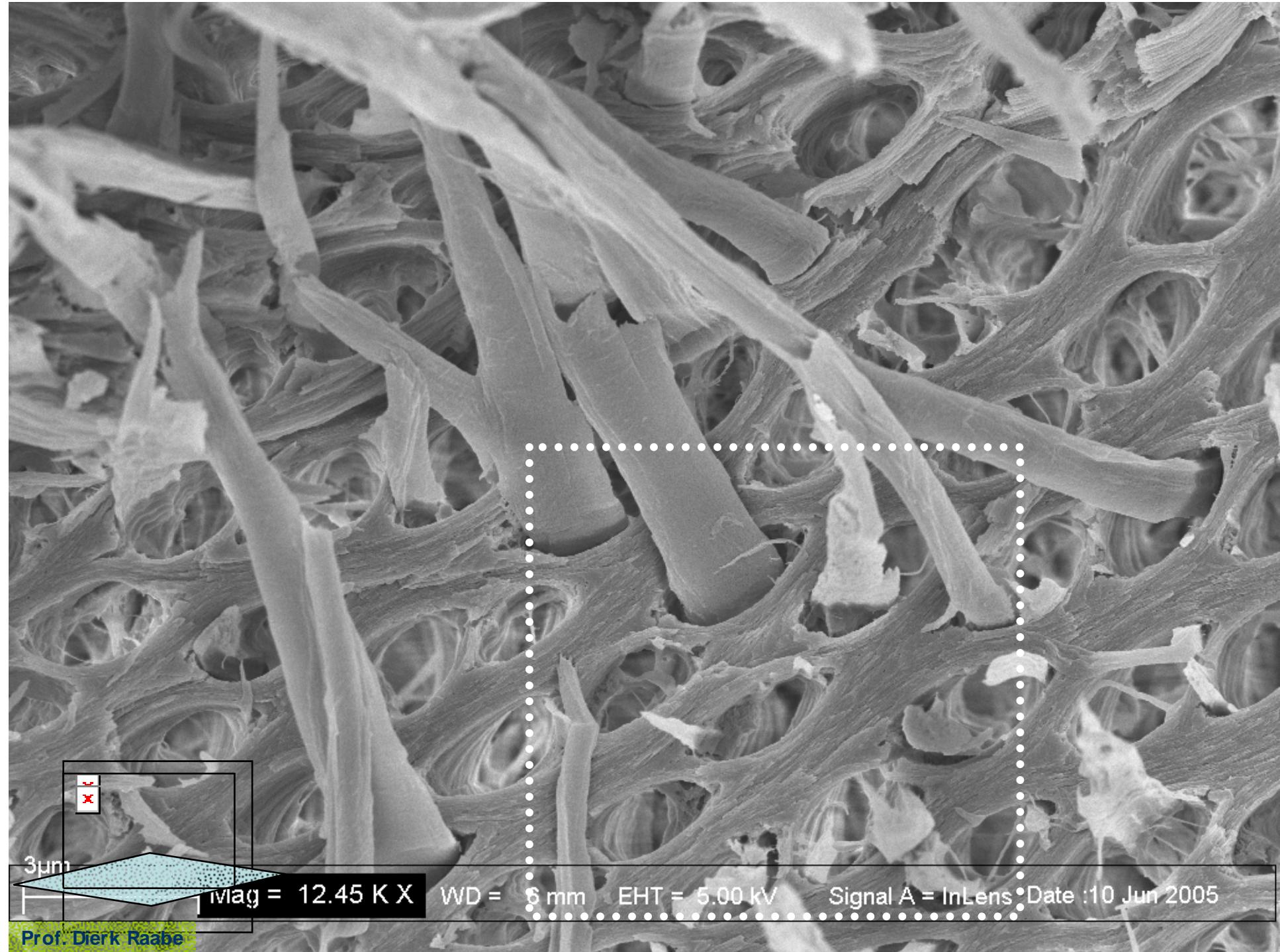


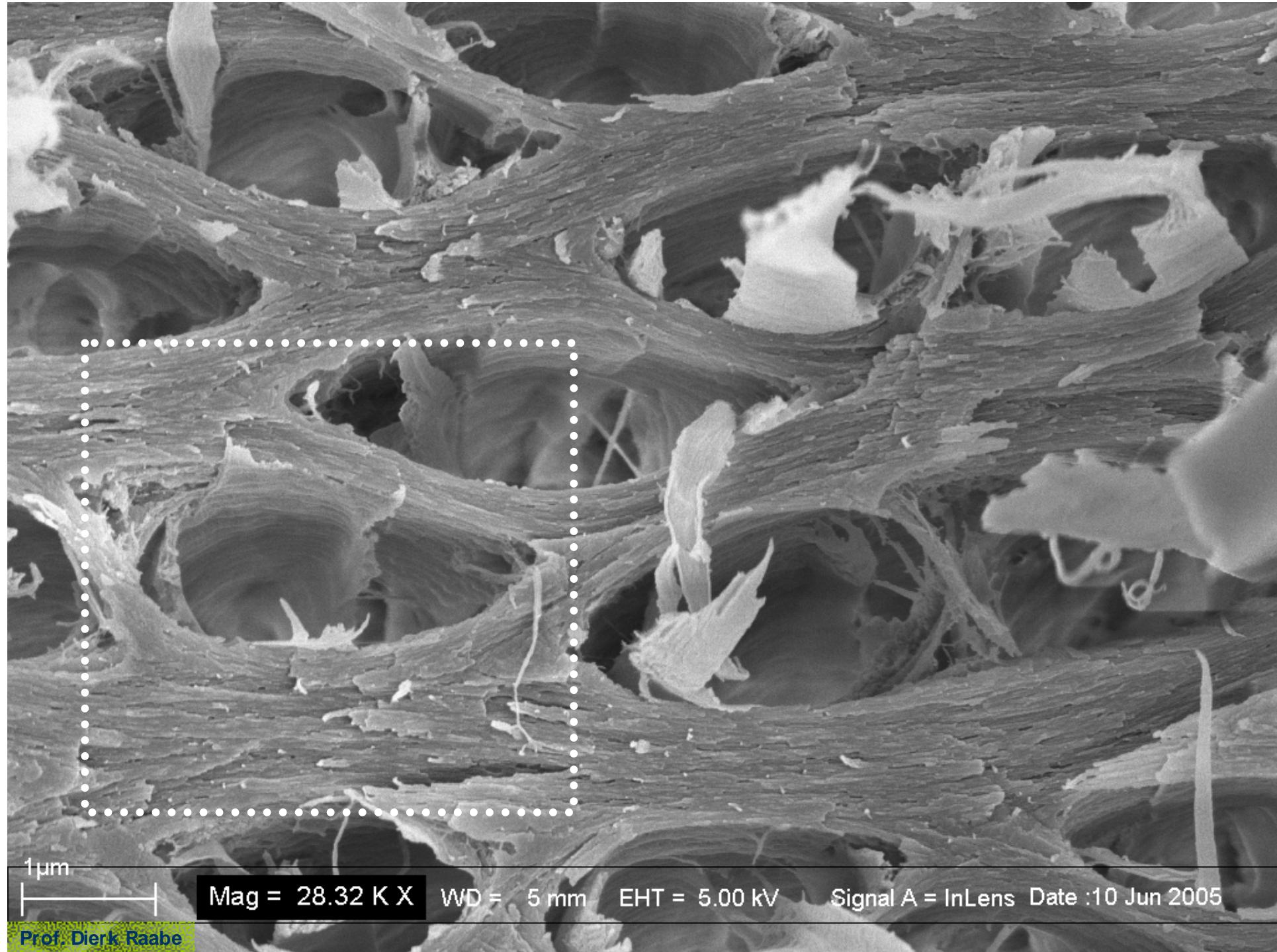




Prof. Dierk Raabe

— 4  $\mu\text{m}$  —

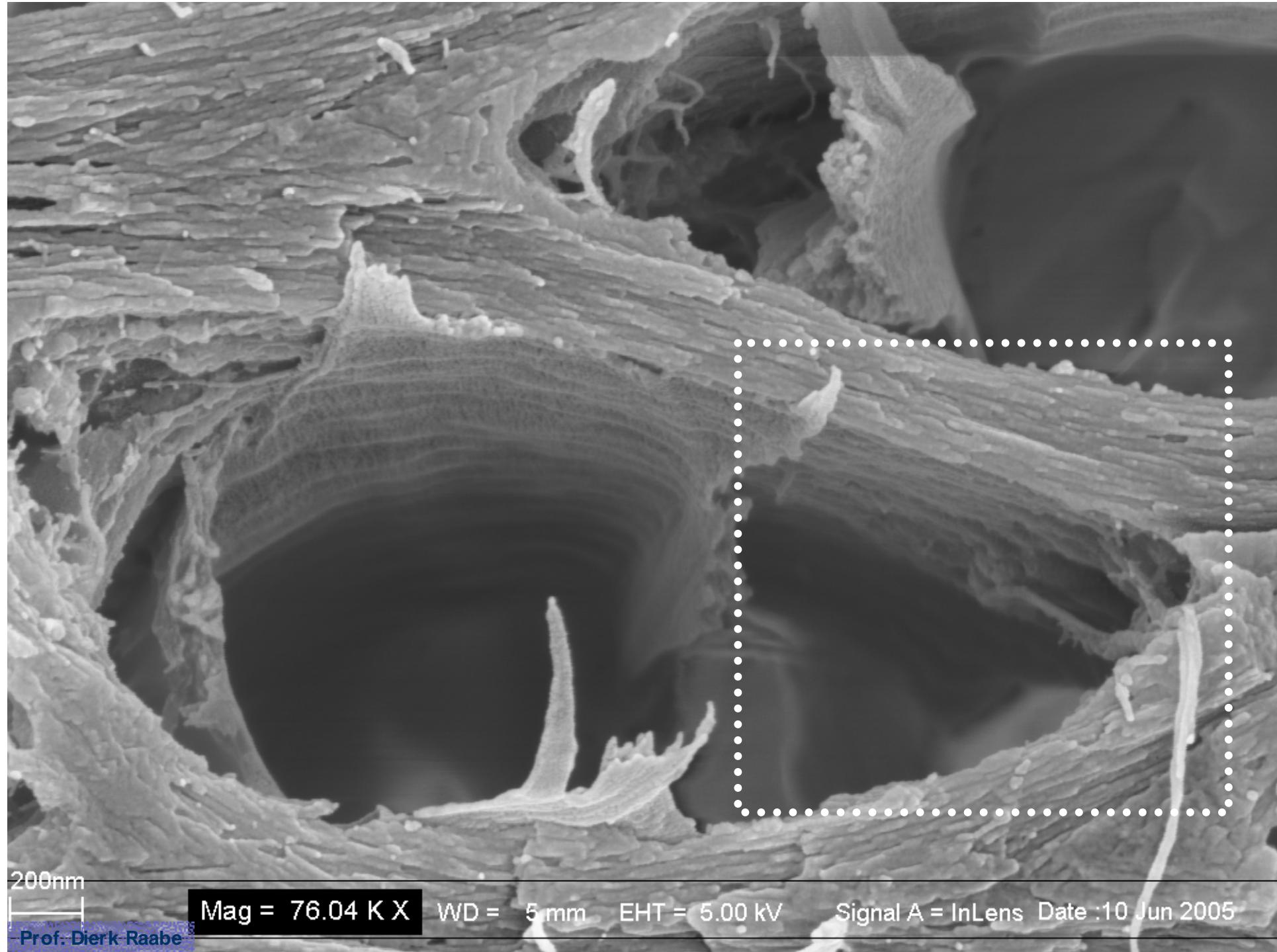




1μm



Mag = 28.32 K X WD = 5 mm EHT = 5.00 kV Signal A = InLens Date :10 Jun 2005



200nm

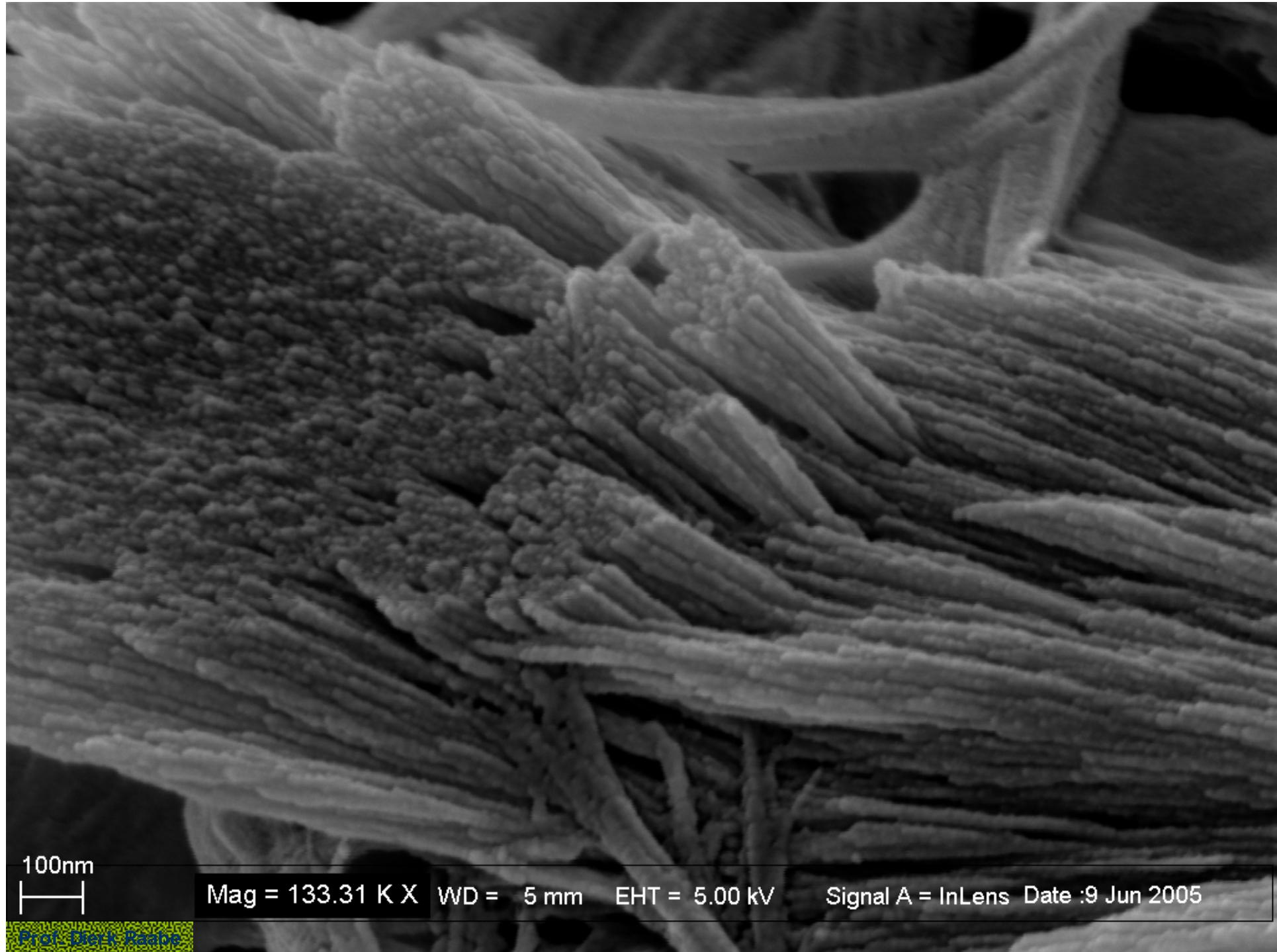


Mag = 76.04 K X

WD = 5 mm EHT = 5.00 kV

Signal A = InLens Date :10 Jun 2005

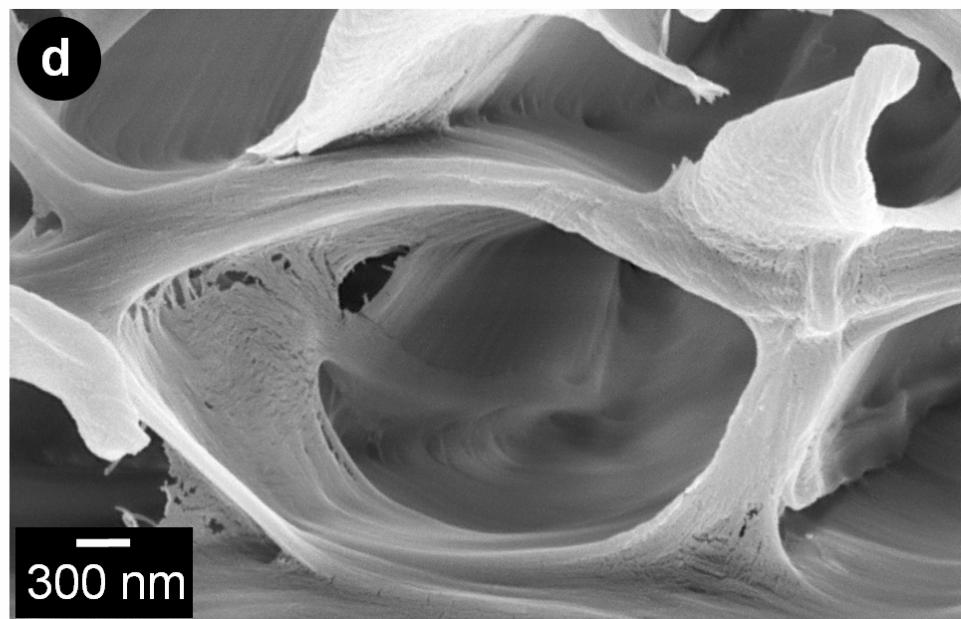
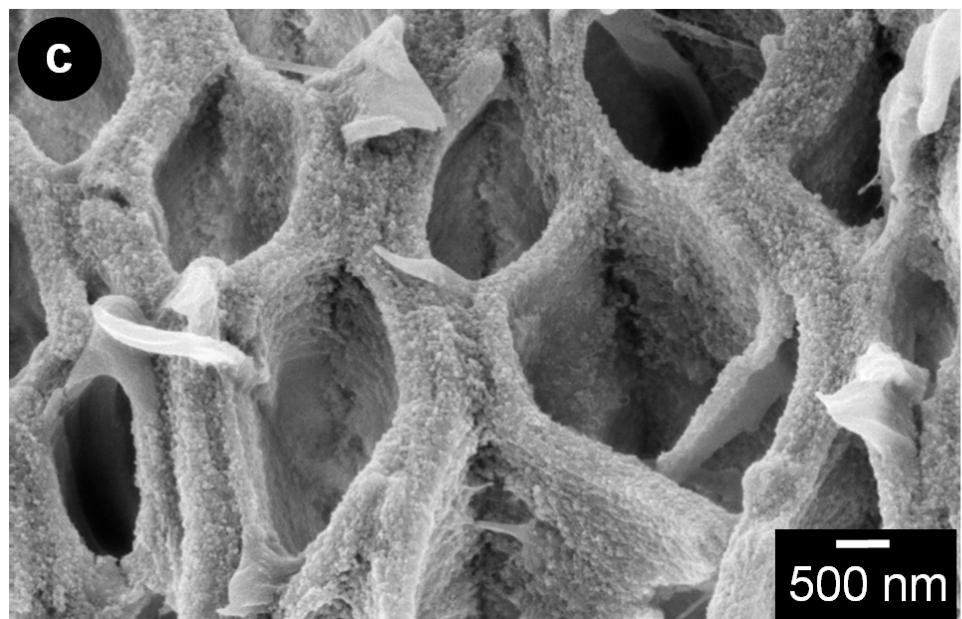
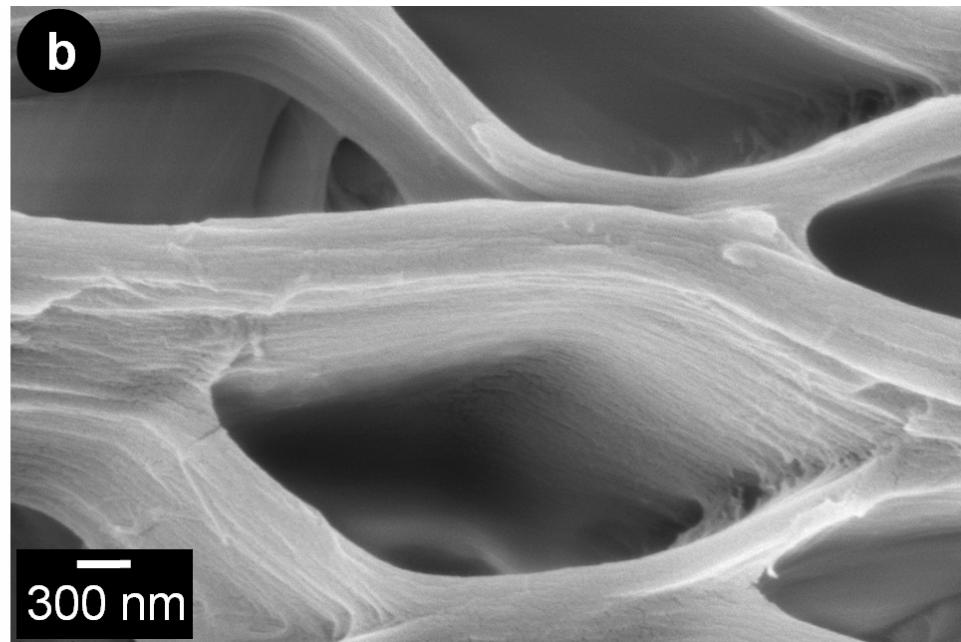
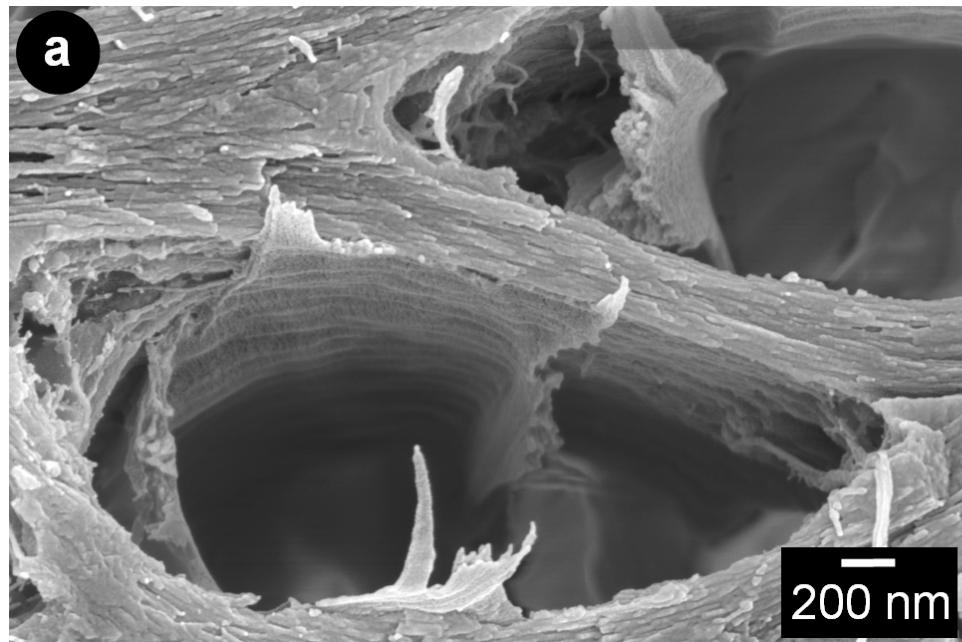
Prof. Dierk Raabe



100nm

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

Prof. Dietk Raabe



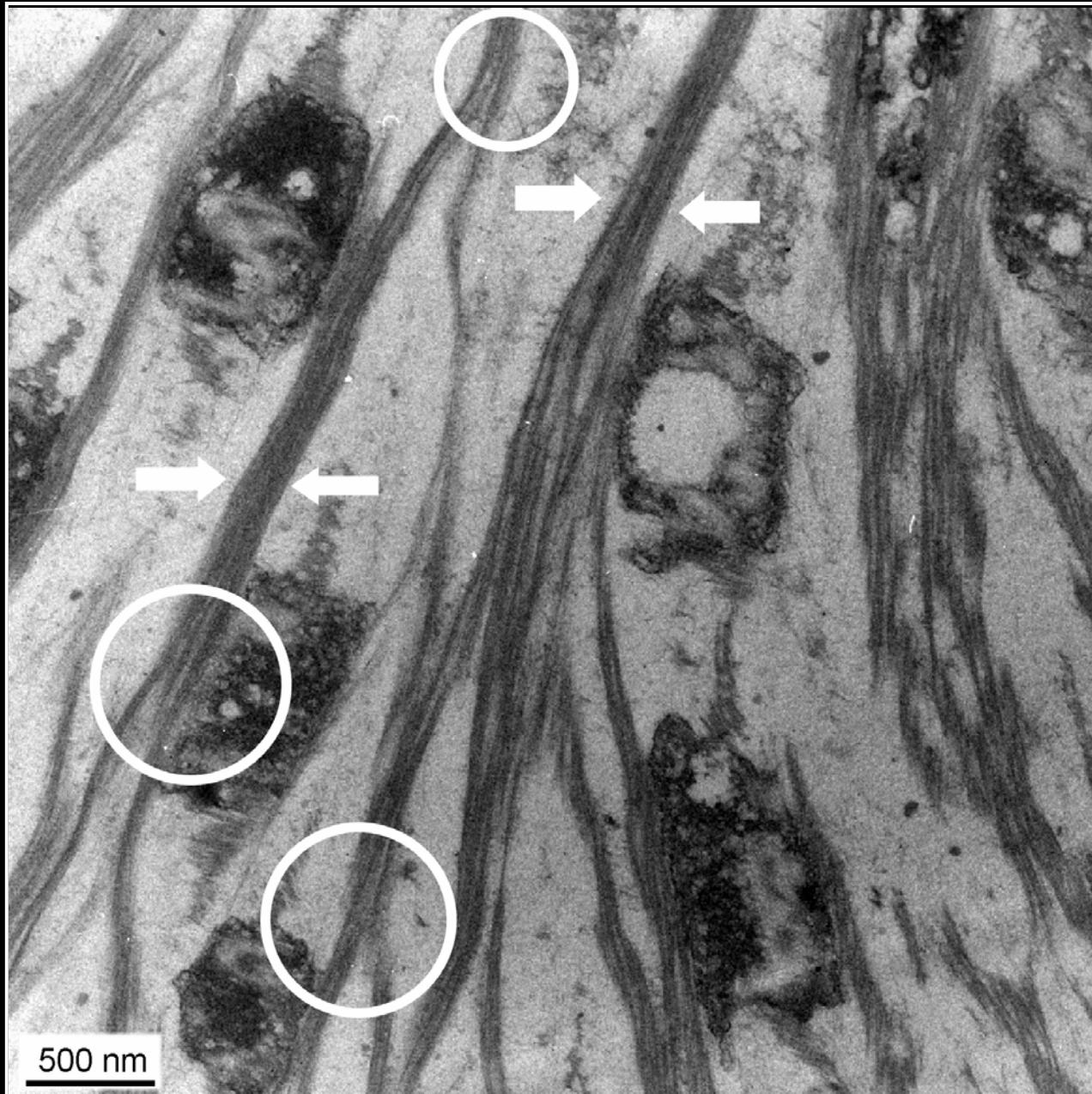
(a) Untreated cuticle, (b) decalcified cuticle (EDTA, 0.15M), (c) deproteinized cuticle (NaOH, 1M) and (d) decalcified and deproteinized cuticle (EDTA, 0.15M + NaOH, 1M).

# TEM, lobster

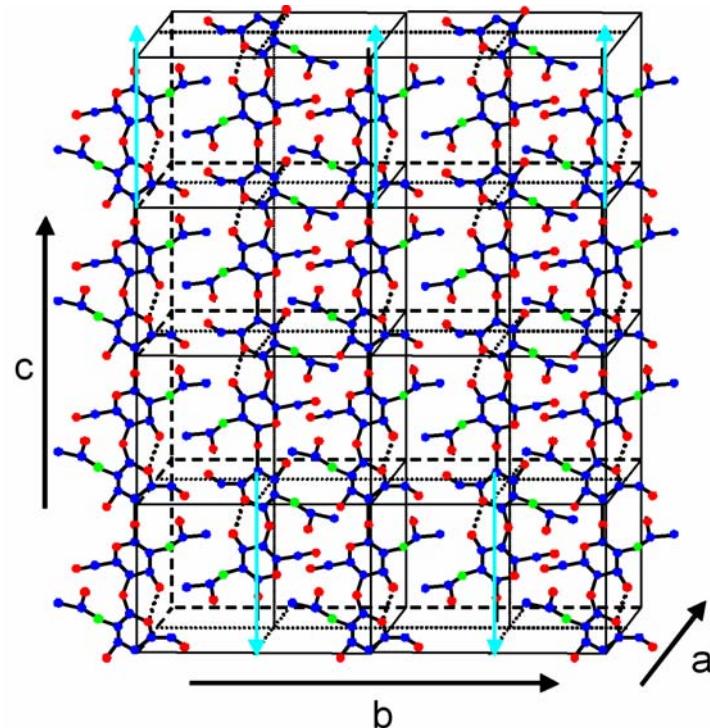


chitin fibril  
bundles

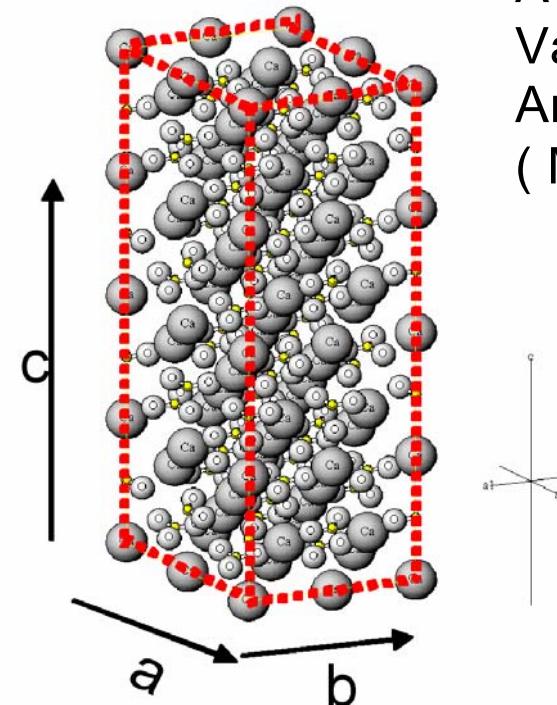
branching



# Phases and crystallography in crustaceans



- Density: 1,41 gm/cm<sup>3</sup>
- Lin. absorbtion coef : 3700  $\mu m^{-1}$  (@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



CC (calcite)  
ACC  
Vaterite  
Aragonite  
( Mg ! )

- Density: 2,71 gm/cm<sup>3</sup>
- Lin. Absorbtion Coef. : 200  $\mu m^{-1}$  (@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



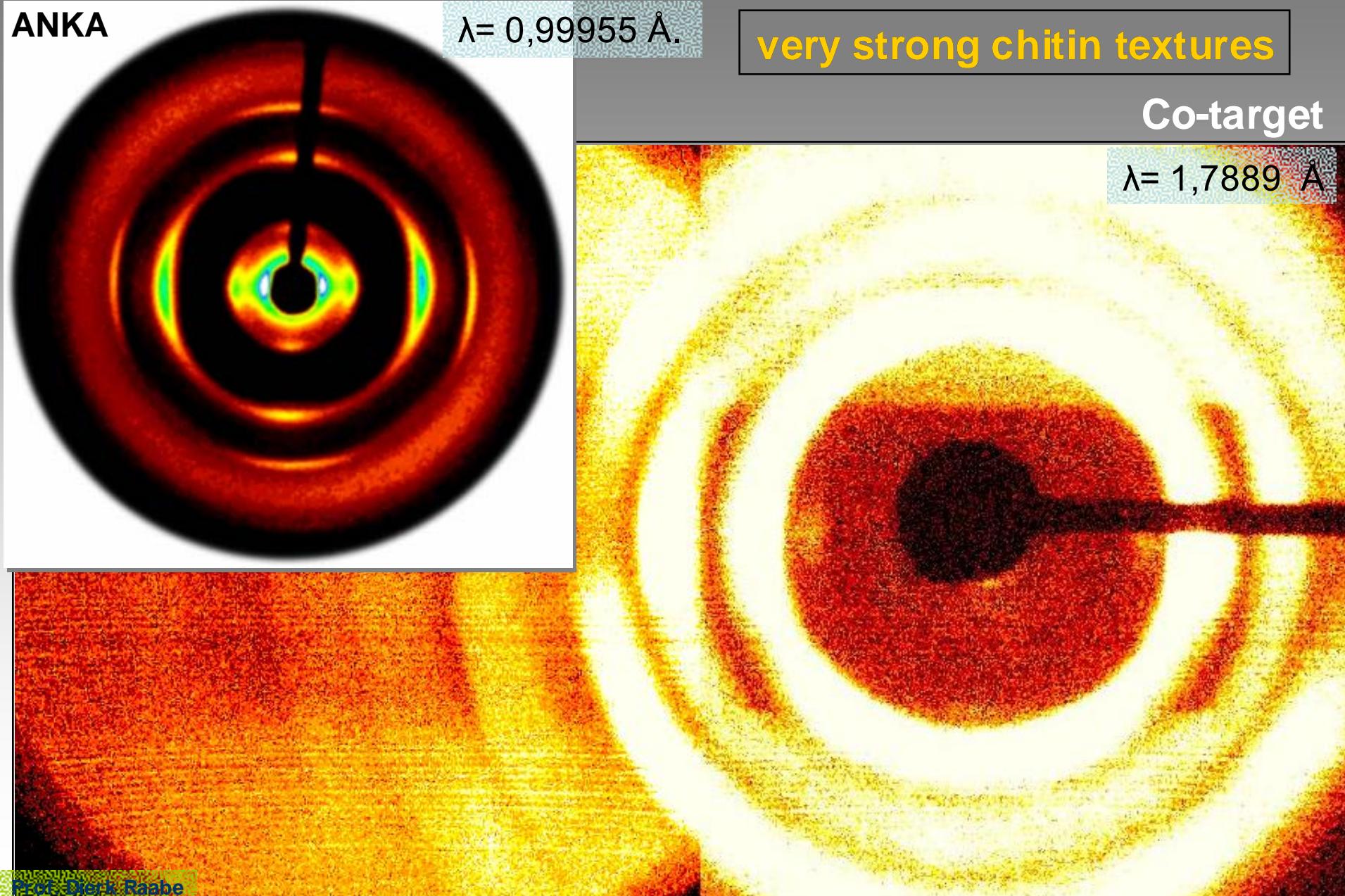
ANKA

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

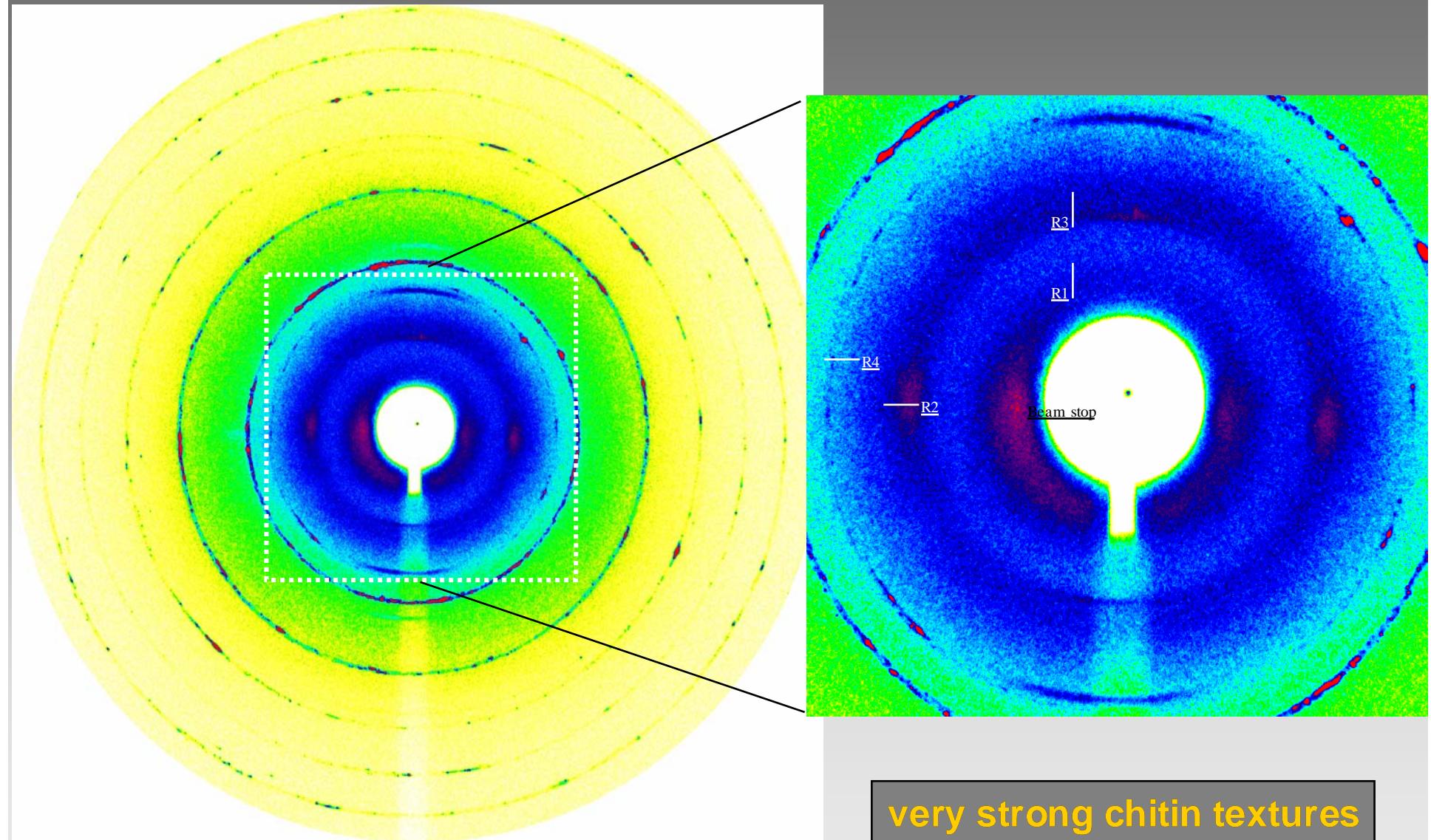
very strong chitin textures

Co-target

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

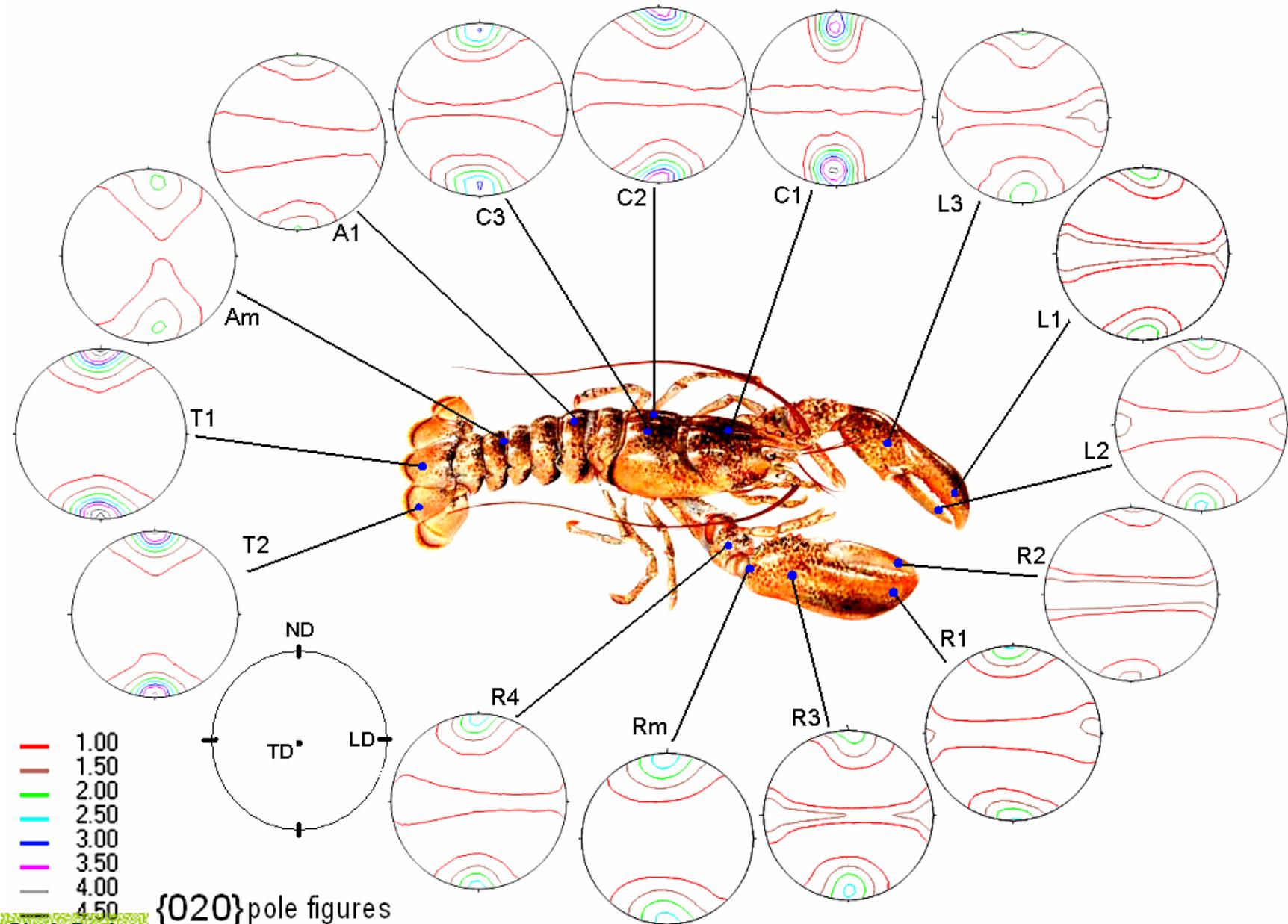


# Synchrotron x-ray, wide angle, lobster

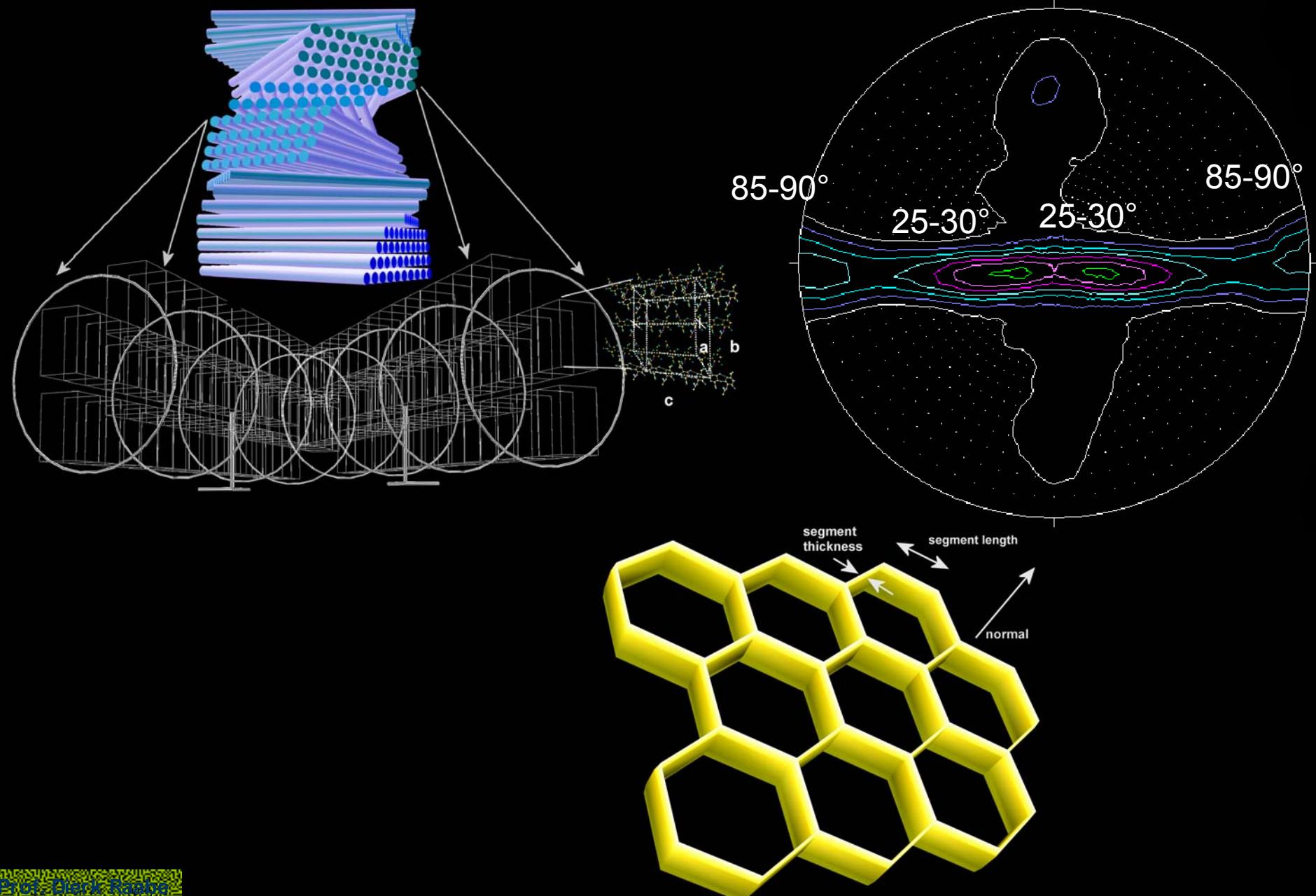


very strong chitin textures  
clusters of calcite ?

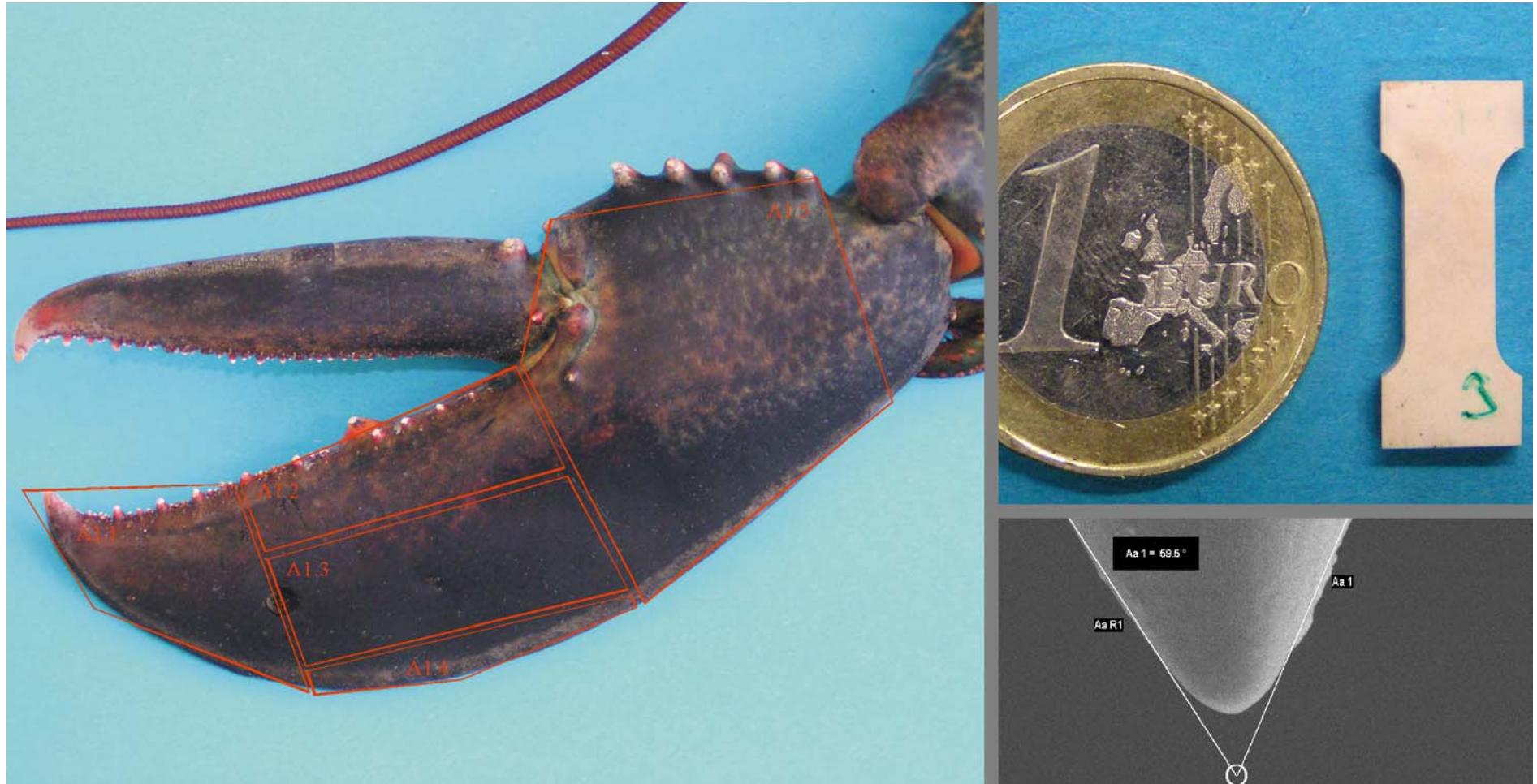
# Smart design, local coordinate system



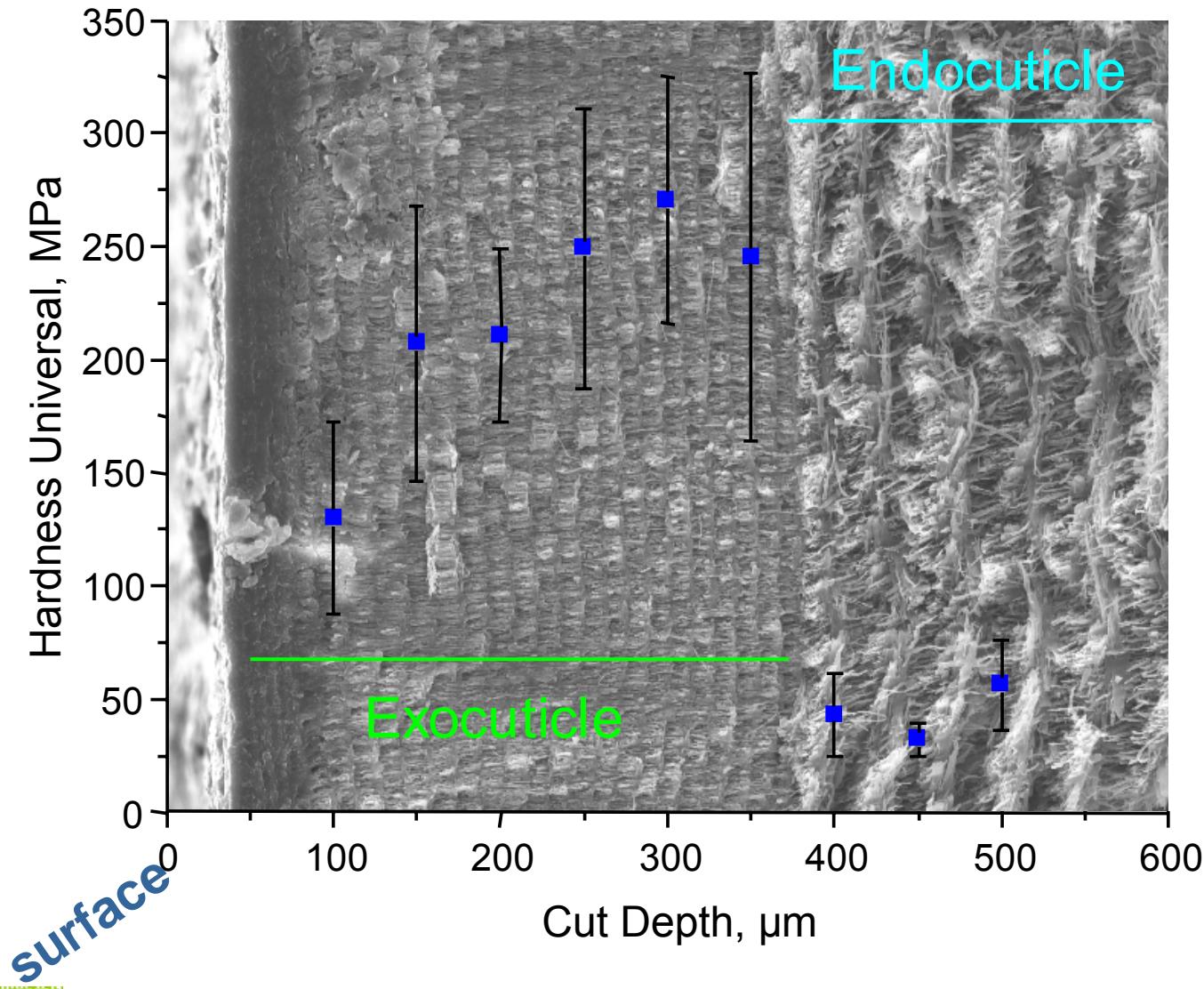
# Structure and texture of chitin



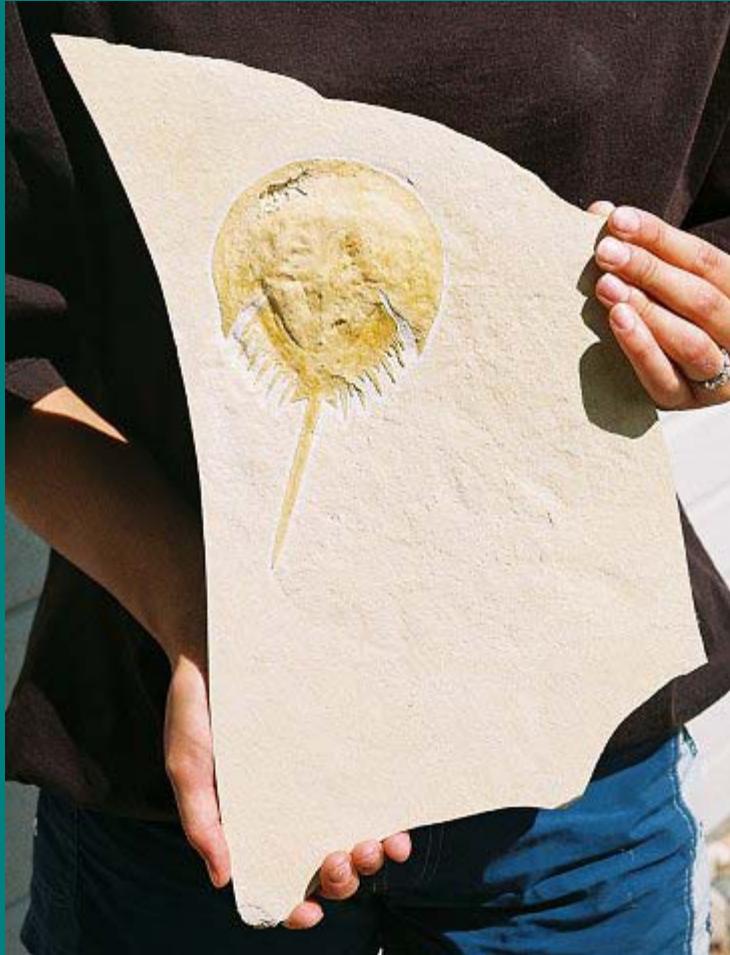
# Tensile testing, Indentation



# Hardness



# 400 Mio. years nanocomposites

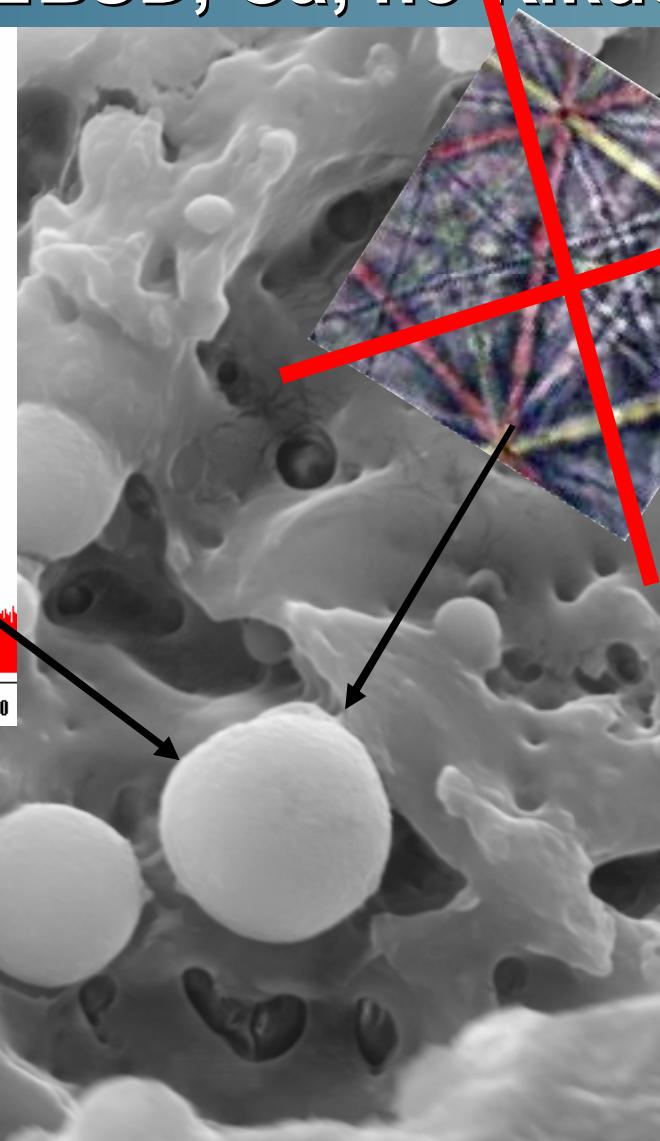
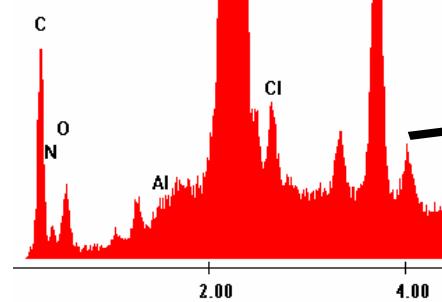
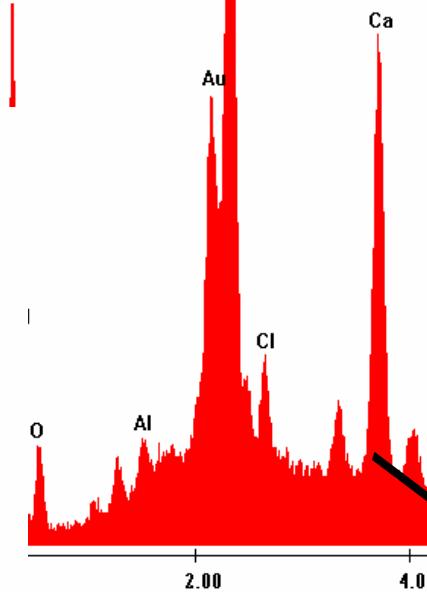


# Horseshoe crab, FIB+EBSD, Ca, no Kikuchi

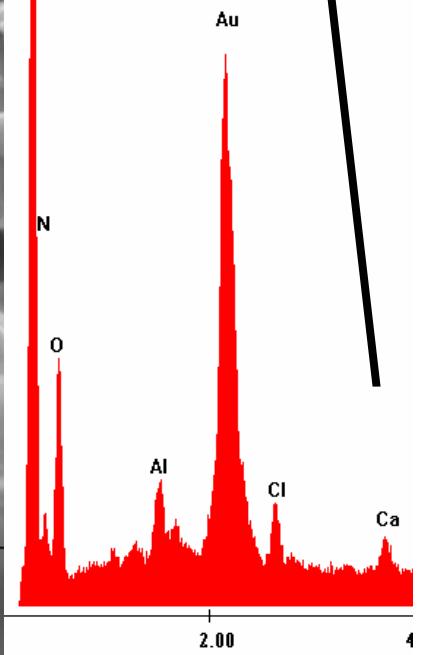


particle

particle



matrix



3µm

EHT = 15.00 kV

Mag = 8.61 K X

WD = 10 mm

Signal A = SE2

Date  
Time

!! 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