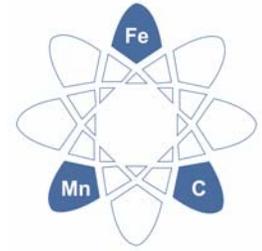


SFB 761 „Stahl *ab initio*“

Crystallographic Textures: Measurement, microstructure analysis, coupling to micro- mechanical mechanisms

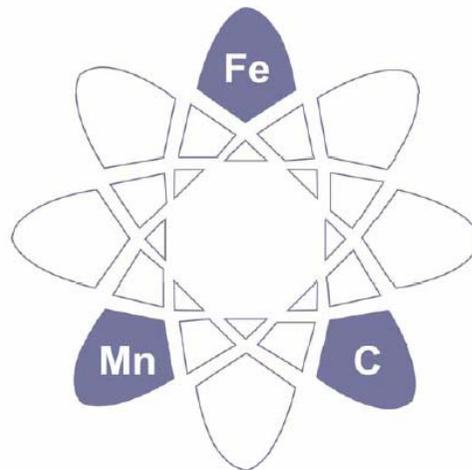
D. Raabe

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contact: d.raabe@mpie.de

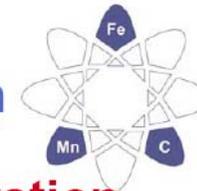
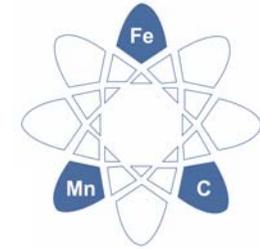


Lecture Series – Vorlesungsreihe im SFB 761

SFB 761 „Stahl *ab initio*“

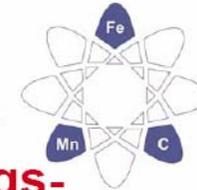
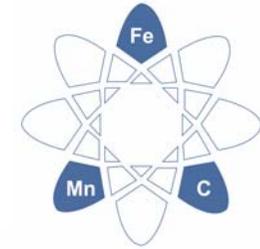


Quantenmechanisch geführtes Design
neuer Eisenbasis-Werkstoffe



Motivation und Entwicklungsprinzipien ändern sich

Stahlgruppe	Jahr	Entwicklungsprinzip	Motivation
nichtrostende Stähle	1912	empirisch V2A	chemische Industrie
mikrolegierte Stähle	1965	verfahrensgetrieben TM-Walzen, TEM	Erdöl- / Erdgas- industrie
Mehrphasenstähle	1990	phänomenologisch Gefügedesign, analytische Modelle	Automobil- industrie
Fe-Mn-C-Legierung	2007	<i>ab initio</i> Scale Hopping erkenntnisgetrieben	Leichtbau Sicherheit Energieeffizienz



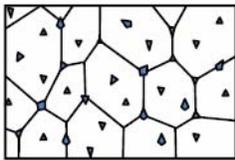
Fe-Mn-C-Legierungen sind thermodynamisch geprägt

Stahlgruppe

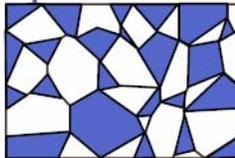
Parameter

Verformungs- mechanismen

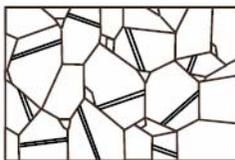
mikrolegierte Stähle



Mehrphasenstähle



Fe-Mn-C-Legierung



- Korngröße
- Kornform
- Ausscheidungen

+

- lokale chemische Zusammensetzung

+

- Stapelfehlerenergie
- Thermodynamik
- Phasenstabilität

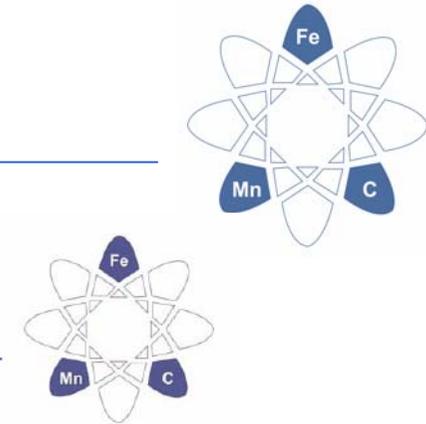
- homogene Versetzungsgleitung

+

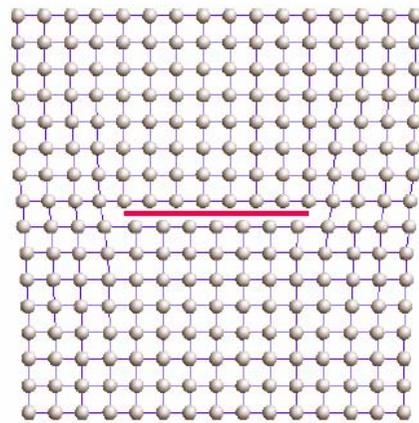
- inhomogene Versetzungsgleitung

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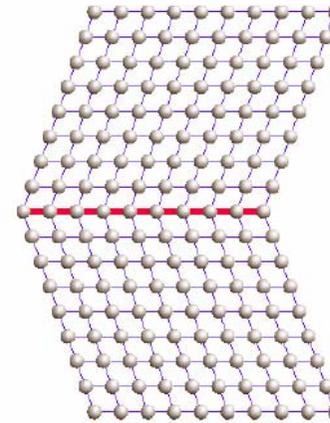
- TRIP -Effekt
- TWIP-Effekt



Kontrollgröße: Stapelfehlerenergie



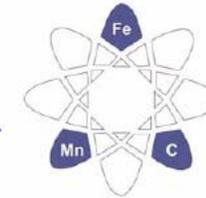
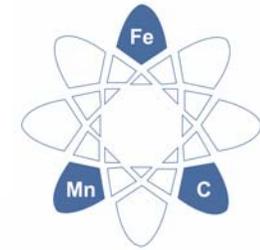
Partialversetzungen



Zwilling

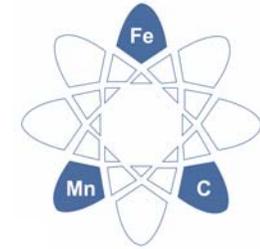
Stapelfehler

Die Stapelfehlerenergie in J/m^2 ist ein Maß für die Häufigkeit von Stapelfehlern in einem Metallgitter. Eine Veränderung der SFE kann zur Steuerung der Verformungsmechanismen genutzt werden.



Besonderheiten der Fe-Mn-C-Legierungen

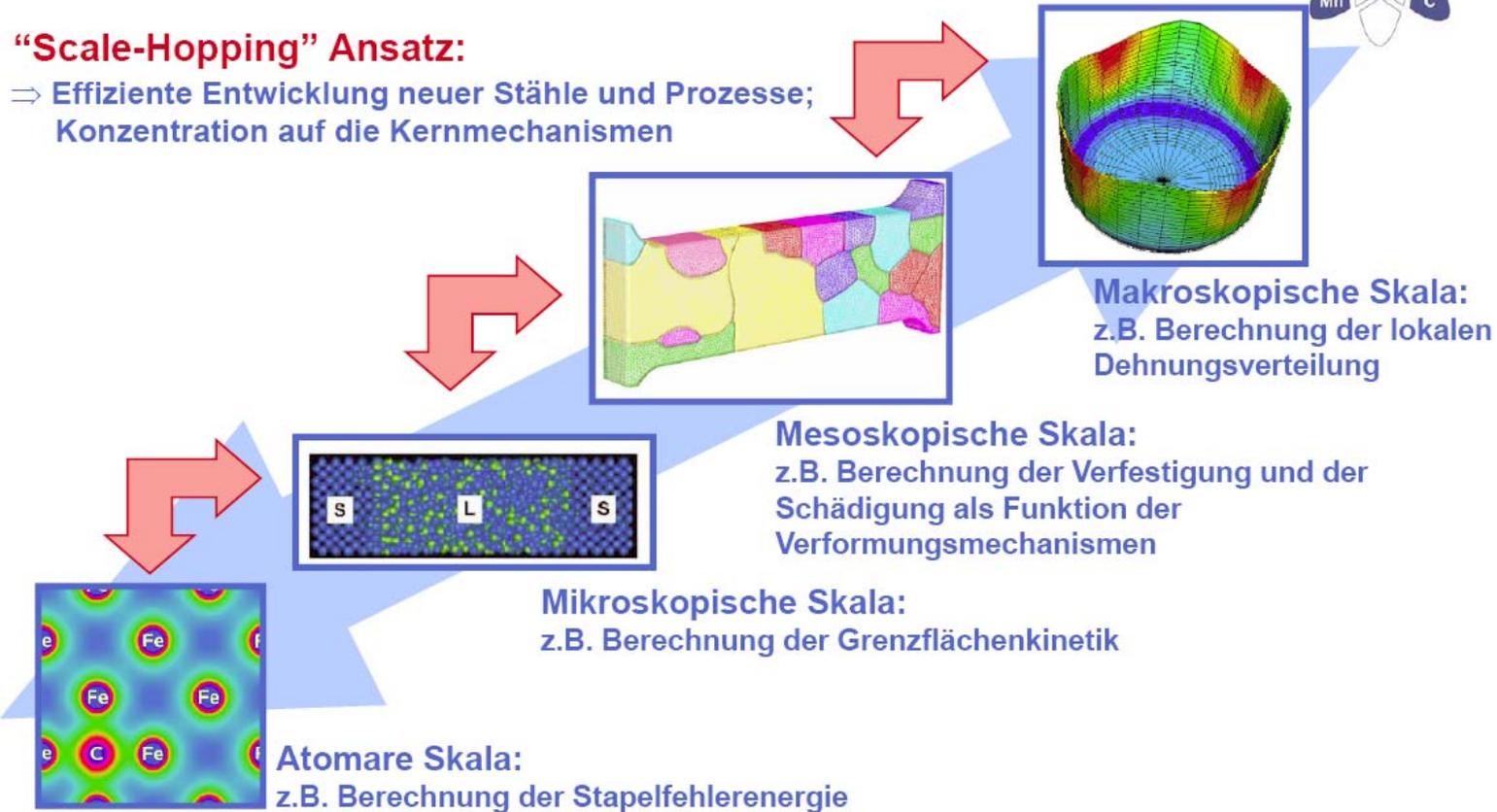
- Fe-Mn-C-Legierungen stellen nach den krz Fe-C-Stählen und den kfz Fe-Cr-Ni-Stählen potenziell eine **neue Matrix** für Eisen-Basis-Werkstoffe dar.
- Fe-Mn-C-Legierungen sind für die geplante neue **methodische Vorgehensweise** besonders geeignet.
- In einer Legierungsgruppe stehen alle bisher genutzten **Verformungsmechanismen** zur Verfügung.
- Wegen der großen Bedeutung der Stapelfehlerenergie ist dieses Legierungskonzept besonders geeignet für eine **thermodynamische Modellierung**.

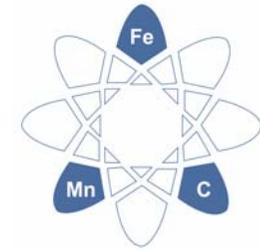


Modellierungsansätze auf unterschiedlichen Ebenen werden gezielt eingesetzt

“Scale-Hopping” Ansatz:

⇒ Effiziente Entwicklung neuer Stähle und Prozesse;
Konzentration auf die Kernmechanismen





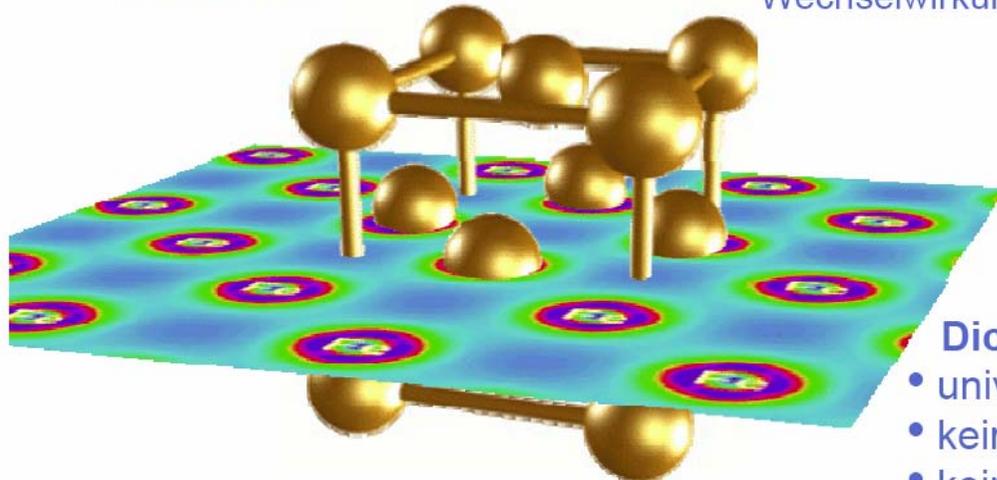
Die Dichtefunktionaltheorie ermöglicht numerisch beherrschbare *ab initio* Ansätze



Schrödinger-Gleichung: $H\Psi = E\Psi$ für Atom-Elektron-Vielteilchensystem

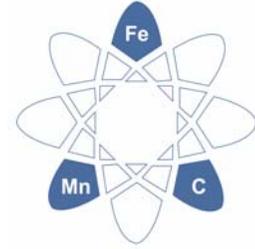
- Vielteilchenwellenfunktion
- Gesamtenergie
- Hamilton-Operator mit Wechselwirkungstermen

Kristalle



Dichtefunktionaltheorie

- universeller Ansatz
- keine empirischen Annahmen
- keine Anpassung an Experimente



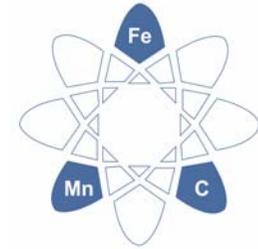
Crystallographic Textures: Measurement, microstructure analysis, coupling to micro- mechanical mechanisms

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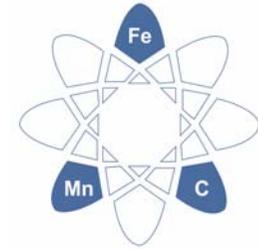


Basics



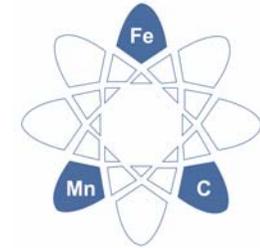
- **Textur:** Volumengewichtete Gesamtheit aller Kristallorientierungen in einer Probe. Bevorzugte Texturen entstehen durch Verformung (Walzen), Glühen, bei der Erstarrung oder durch elektrolytische Abscheidung. Die Textur lässt sich näherungsweise durch ideale Lagen kennzeichnen. Man versteht darunter die Orientierung der meisten Kristalle in bezug auf charakteristische Richtungen des Werkstückes. Charakteristische Richtungen sind die Walzebene (WE) und die Walzrichtung (WR). Bei Blechen wird die Angabe verwendet: $(hkl) [uvw]$. (hkl) ist die parallel zur Walzebene liegende Gitterebene, $[uvw]$ ist die in Walzrichtung liegende Gitterrichtung.
- **OVF:** Orientierungsverteilungsfunktion, 3D Textur, quantitativ
- **Polfigur:** 2D Projektion der Orientierungsverteilungsfunktion, qualitativ
- **Isotropie:** Richtungsunabhängigkeit (*Tropos (gr.): Richtung*)
- **Anisotropie:** Richtungsabhängigkeit (Gefügezeitigkeit, Textur, etc.) Da in einer Elementarzelle die Eigenschaften richtungsabhängig sind, sind sie es auch in einem Korn. Ein Metallstück besteht aber aus vielen Körnern, die in der Regel alle unterschiedliche Richtungen annehmen.
- **R-Wert:** Verhältnis von Breiten- zu Dickenabnahme an einer Stelle des Fließortes

Basics



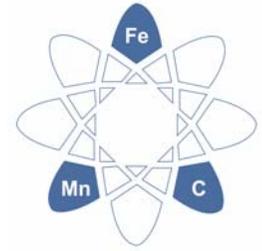
- **Makrotexturen / statistische Texturen:** Die Makrotextur eines Polykristalles ist die statistische Beschreibung des Gefügeparameters der Orientierungsverteilung der Kristallite und wird durch die OVF quantifiziert. Die zugrundeliegenden Polfigurdaten werden dabei meist über Röntgen- oder Neutronenstreuexperimente ermittelt. Die Makrotextur gibt somit den Volumenbruchteil, aber nicht den Ort innerhalb eines Kristalles, die Nachbarschaft oder die Art der Korngrenzen einer bestimmten Orientierung an.
- **Mikrotexturen / Einzelorientierungsmessung:** Die Mikrotextur eines Polykristalles ist die lokale Beschreibung des Gefügeparameters der räumlich aufgelösten Orientierungsverteilung der Kristallite und wird entweder durch Orientierungsgefügekarten aus OIM-Daten oder ergänzend auch durch die OVF quantifiziert. Die zugrundeliegenden Daten werden dabei meist über Beugung in der Elektronenmikroskopie ermittelt. Die Mikrotextur gibt somit den Volumenbruchteil UND den Ort innerhalb eines Kristalles inklusive der Nachbarschaft und der Art der Korngrenzen einer bestimmten Orientierung an.

Basics



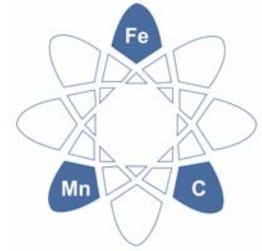
- **Texturmodifizierende Technologien:** Der wichtigste Parameter zur Beschreibung der Anisotropie polykristalliner Werkstoffe ist die Textur. Eine Textur, bei der die Kristalle einer Phase bestimmte Vorzugsorientierungen innehaben, bewirkt durch die über die Gitterstruktur der Kristallite bedingte Anisotropie physikalischer Eigenschaften eine solche auch für das polykristalline Material. Die maximal mögliche Anisotropie ist dabei erreicht, wenn alle Kristallite gleich orientiert sind. Im Falle einer regellosen Textur, wobei alle Orientierungen gleich häufig vorhanden sind, ist das Verhalten des polykristallinen Materials isotrop (man sagt quasi isotrop), obwohl seine Bausteine (Kristallite) selbst ein anisotropes Verhalten zeigen. Die Eigenschaften des Vielkristalls sind, wie die des Einkristalls, richtungsabhängig falls keine regellose Textur vorliegt. Dies verdeutlichen die im Zugversuch bestimmten Größen der Streckgrenze, Zugfestigkeit und Bruchdehnung an Streifen, die in verschiedenen Winkeln relativ zur Walzrichtung entnommen wurden.
- **Textureinstellung:** Durch gezielte Erzeugung bestimmter Texturen können die anisotropen Eigenschaften eines Werkstoffes innerhalb der oben erwähnten Grenzen variiert, und so den jeweils vorliegenden Einsatzbedingungen angepaßt werden. Den drei Prozessen plastische Deformation, Erholung und Rekristallisation kommt dabei die größte technische Bedeutung zu. Die Fähigkeit der kristallinen Phasen, sich plastisch verformen zu können, beruht vor allem auf der Entstehung und Bewegung von Versetzungen und der Zwillingsbildung. Dagegen wird während der Rekristallisation, die z.B. durch thermische Behandlung, die Dichte der Versetzungen reduziert. Thermodynamisch bedingte Phasenübergänge innerhalb einer Legierung oder eines Minerals verursachen sogenannte Transformationstexturen, die durch feste Orientierungsbeziehungen zwischen Ausgangs- und Endkristallen beschrieben werden können.

Overview



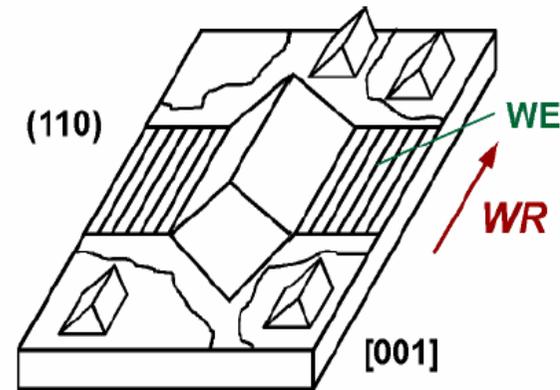
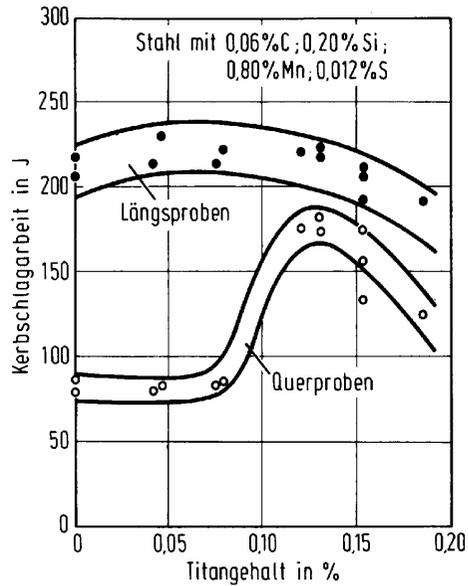
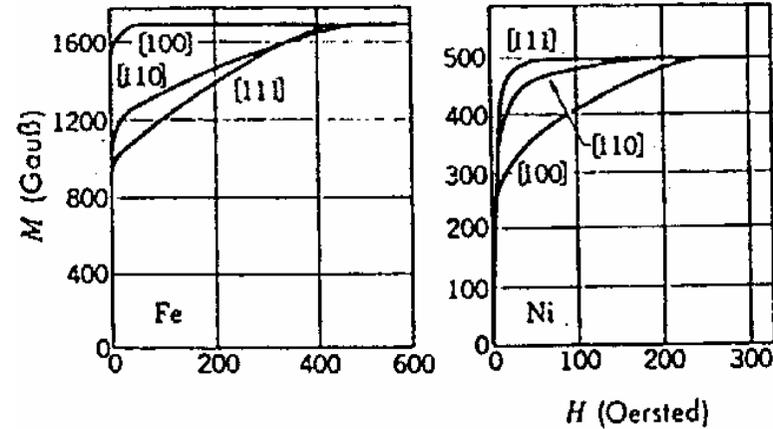
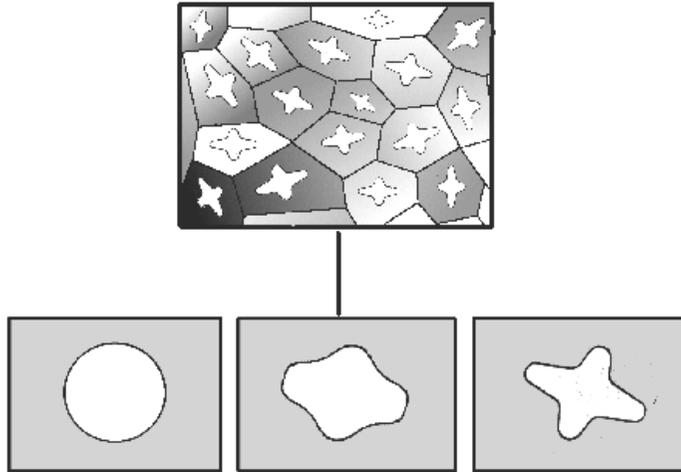
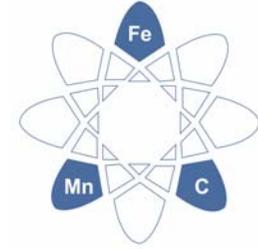
- **Anisotropy**
- **Presentation**
- **Measurement**
- **Textures and Mechanics**
- **Examples of Texture Research**

Overview

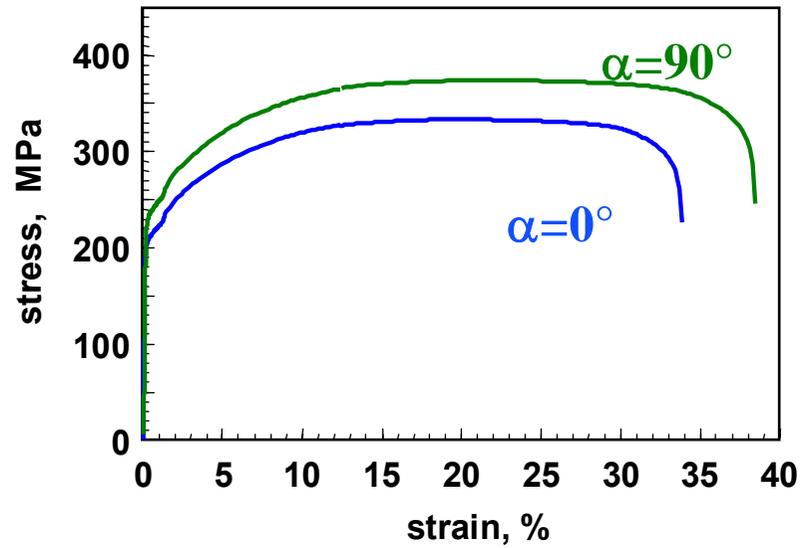
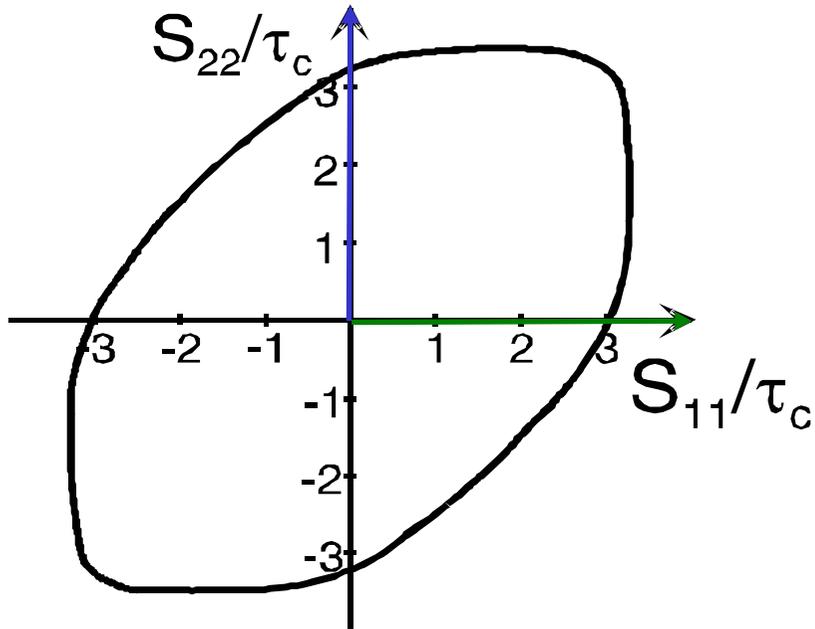
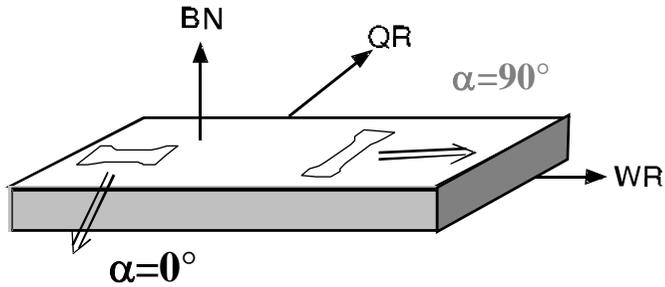
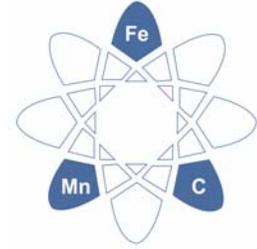


- **Anisotropy**
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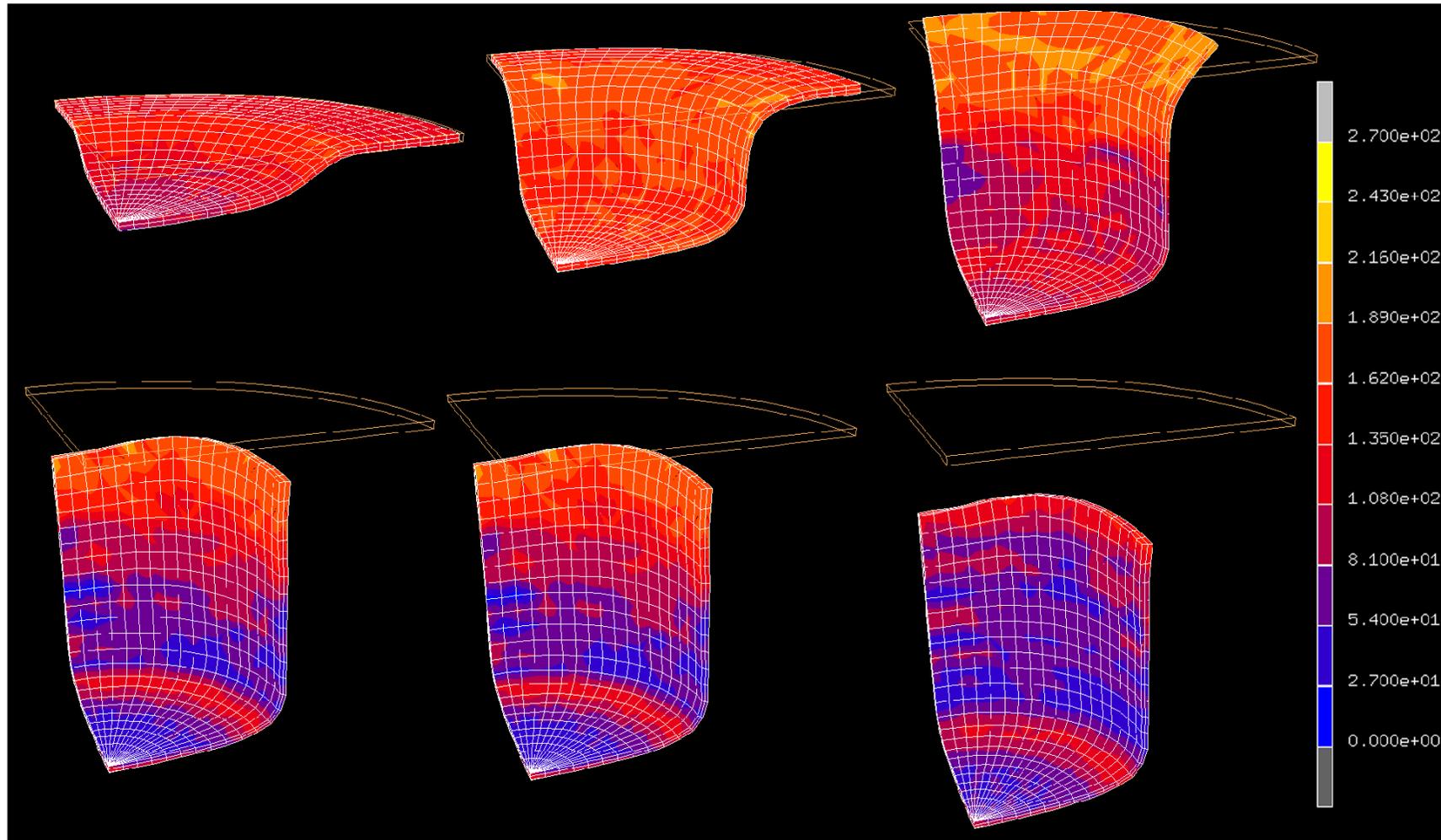
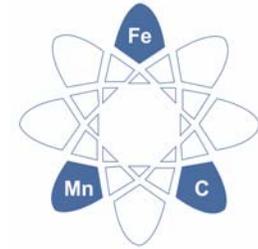
Anisotropy



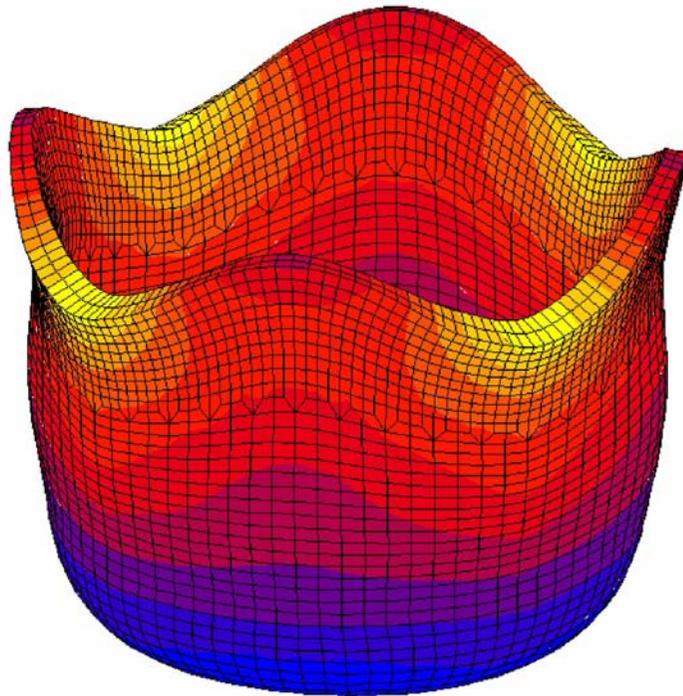
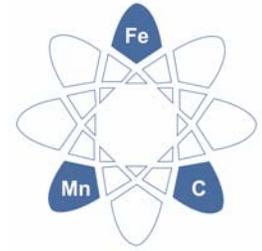
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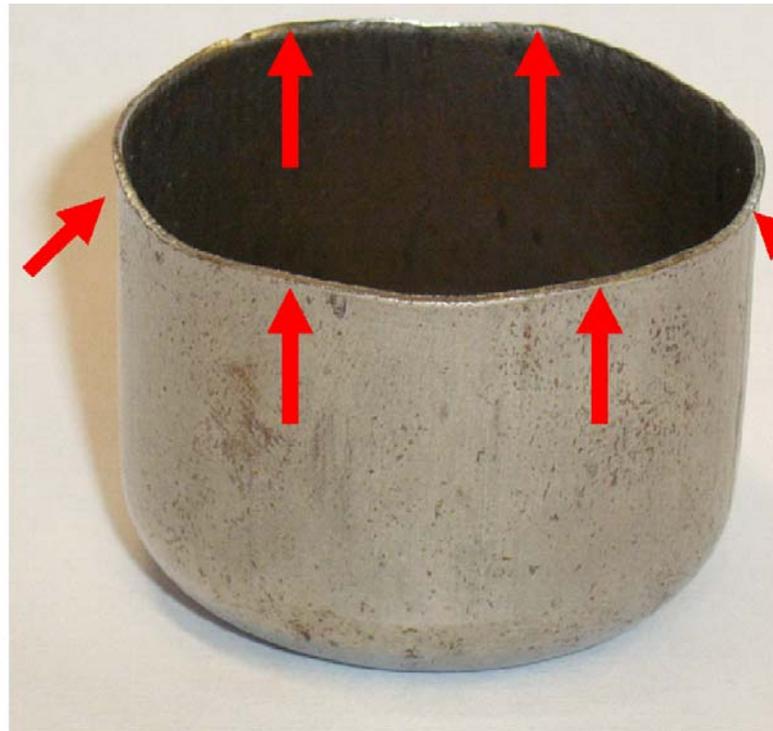
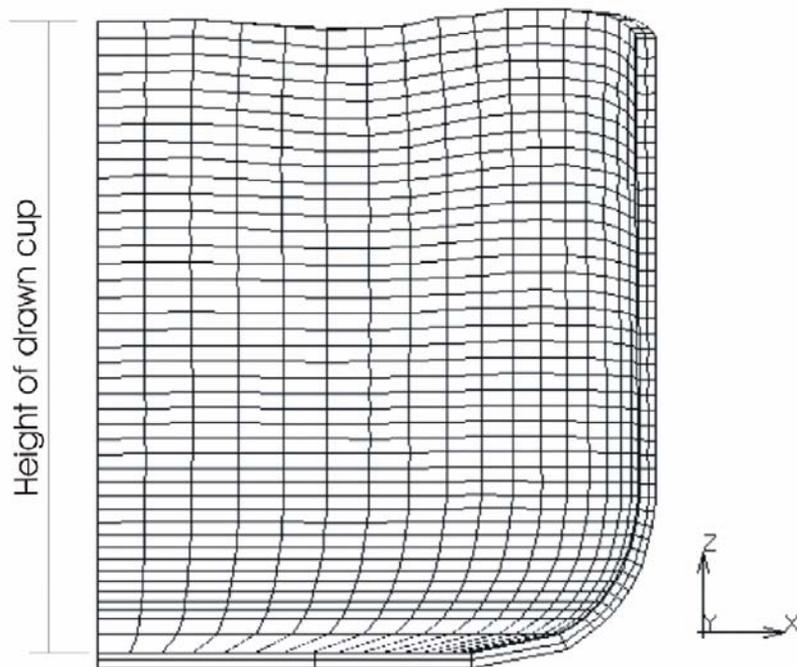
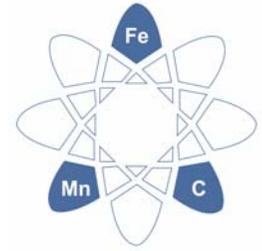
Anisotropy



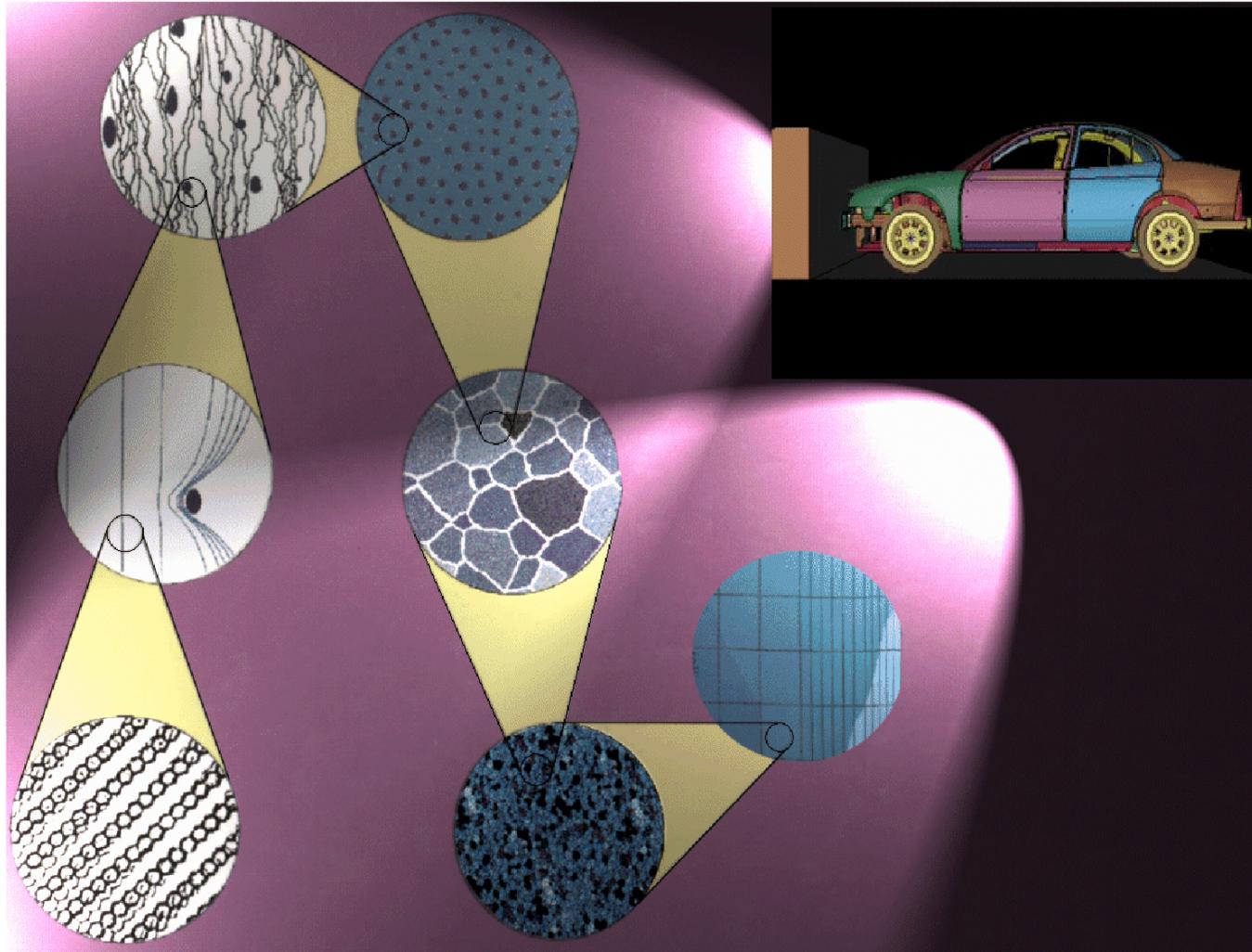
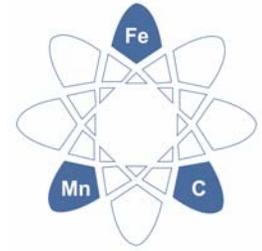
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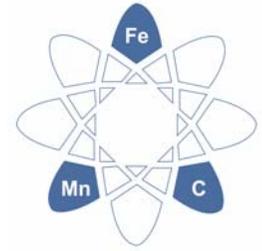
Anisotropy



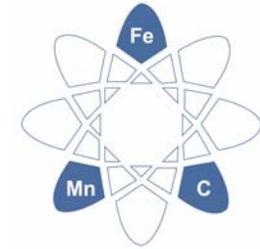
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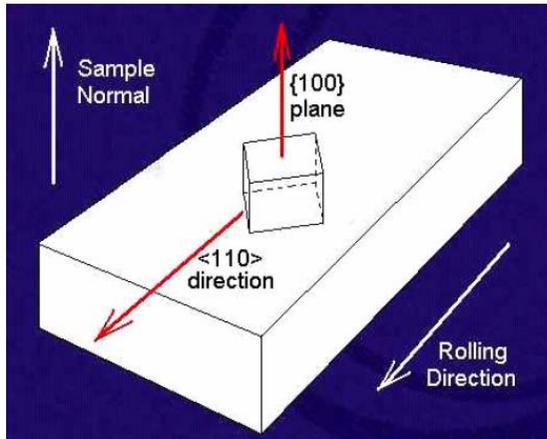
Overview



- Anisotropy
- **Presentation**
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Texture presentation



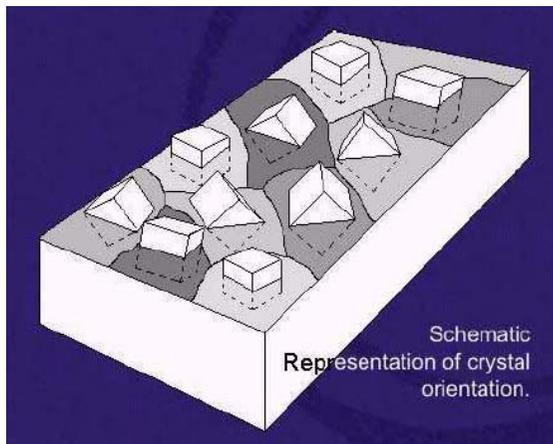
quantify orientations

Miller indices $\{hkl\}\langle uvw \rangle$

Euler angles $\varphi_1, \phi, \varphi_2$

Rodrigues vectors

Quaternions



texture: orientation distribution of crystals

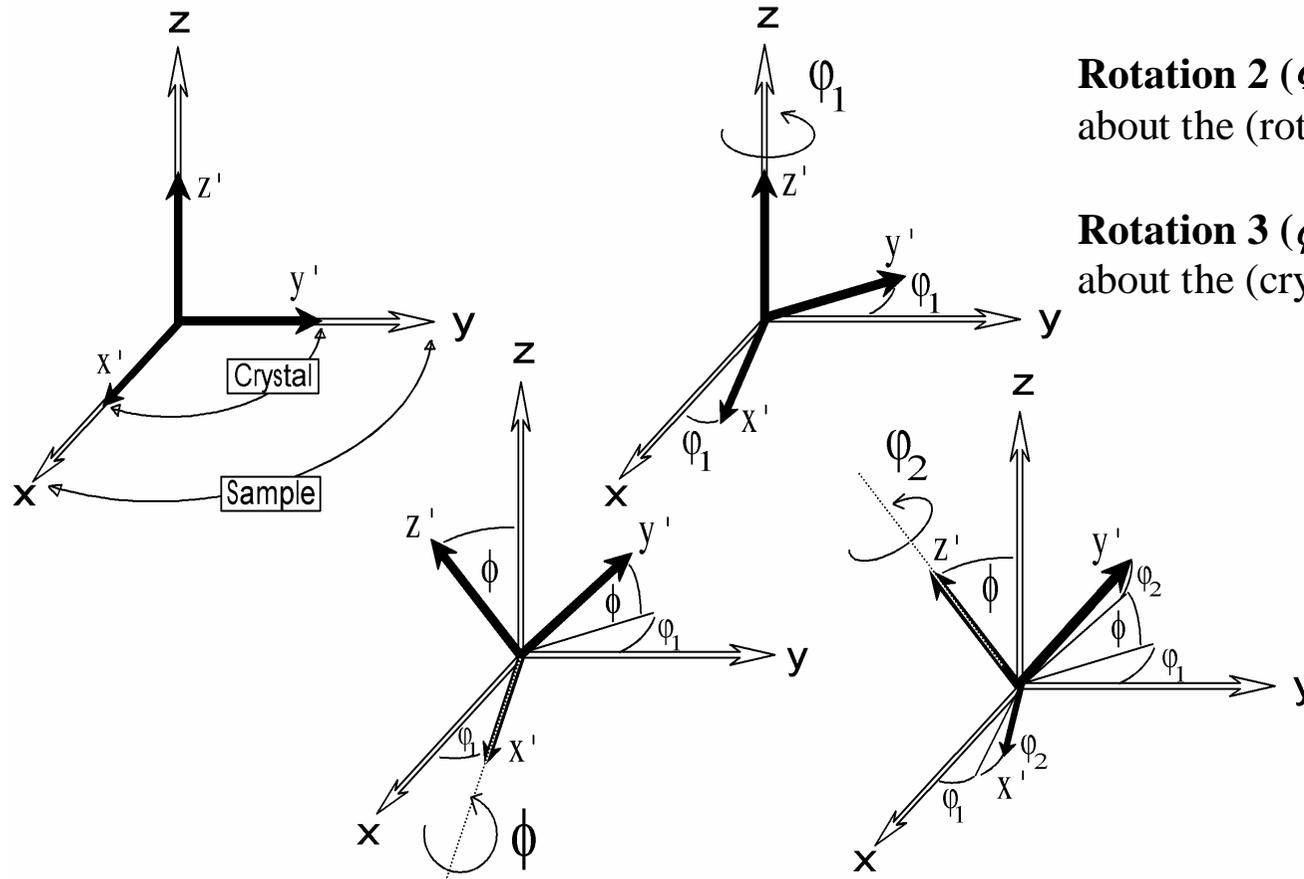
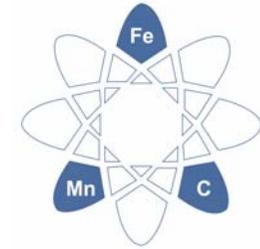
note:

crystallographic texture

topological texture (of fibers or interfaces)

surface texture (surface topography)

Texture presentation

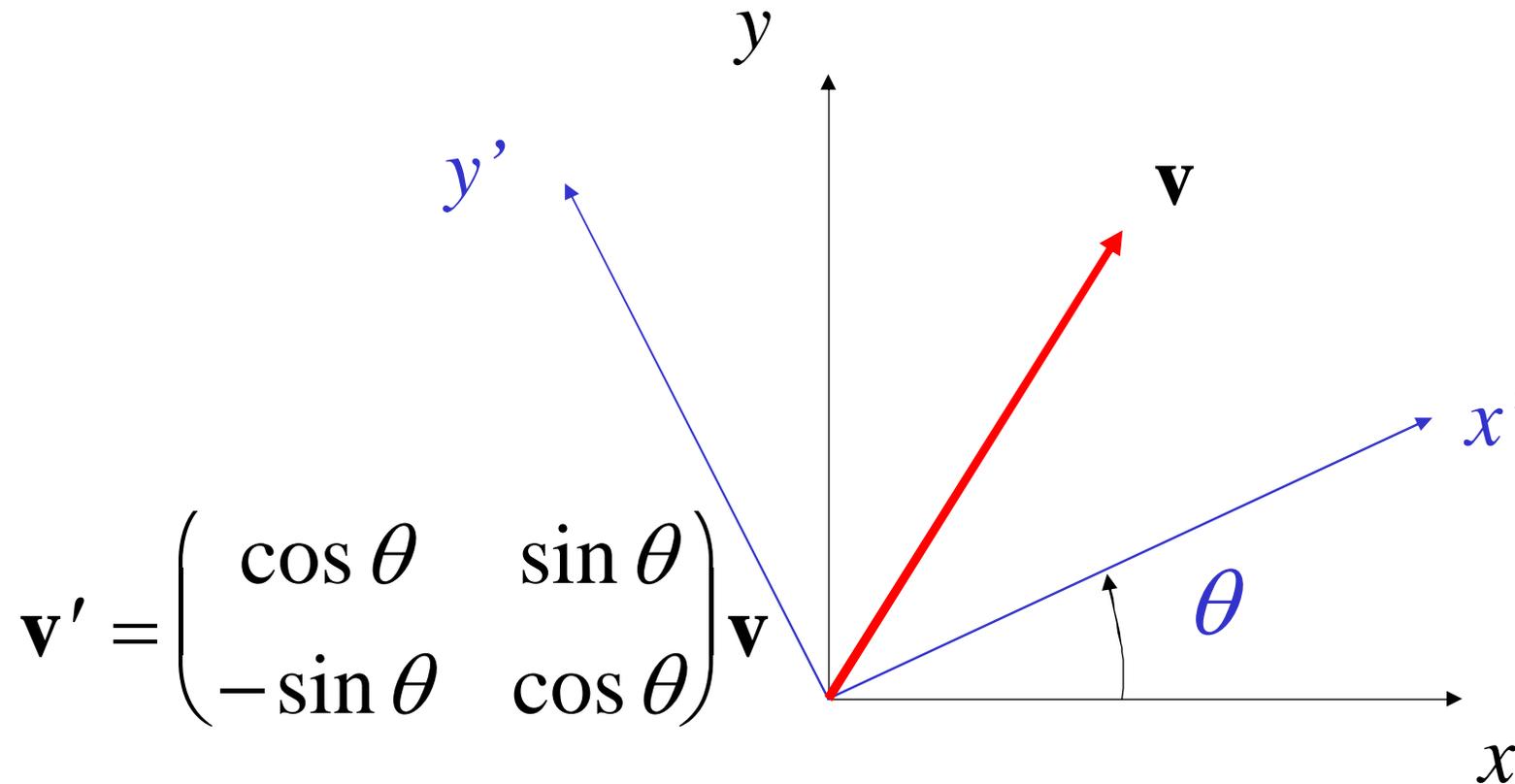
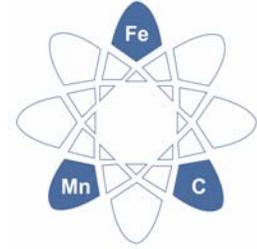


Rotation 1 (ϕ_1): rotate axes (anticlockwise) about the (sample) 3 [ND] axis; Z_1 .

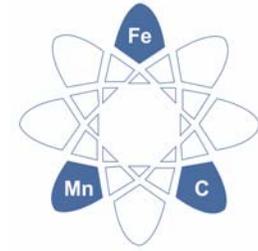
Rotation 2 (Φ): rotate axes (anticlockwise) about the (rotated) 1 axis [100] axis; X .

Rotation 3 (ϕ_2): rotate axes (anticlockwise) about the (crystal) 3 [001] axis; Z_2 .

Texture presentation



Texture presentation



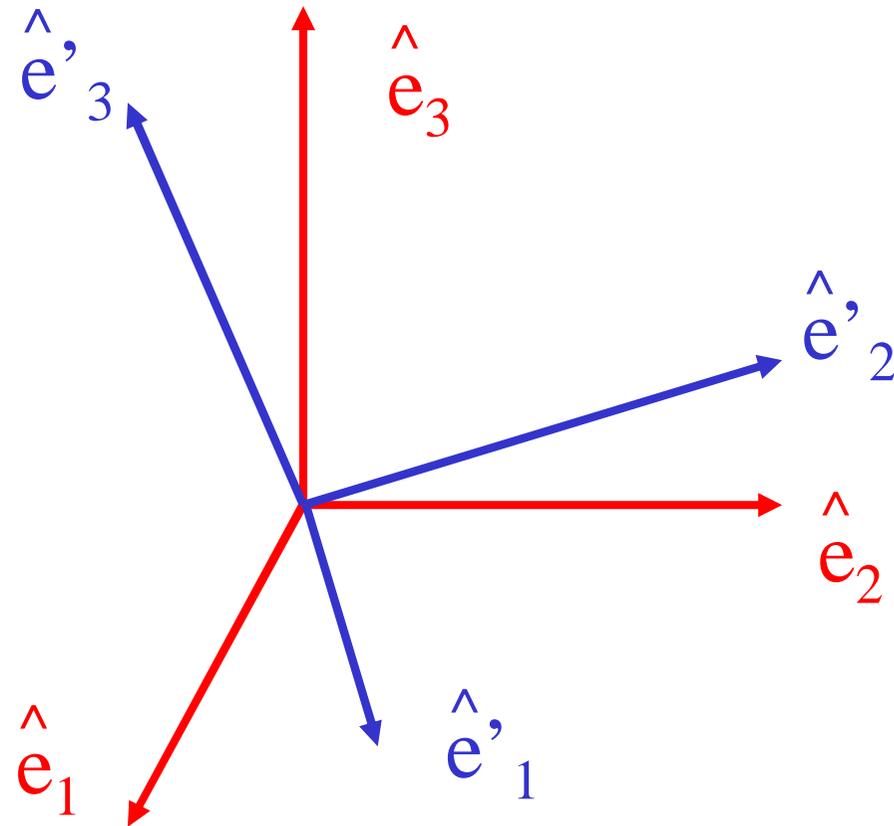
Definition of an Axis Transformation:

e = old axes; e' = new axes

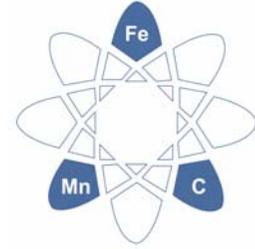
Sample to **Crystal** (primed)

$$a_{ij} = \hat{e}'_i \otimes \hat{e}_j$$

$$= \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$



Texture presentation

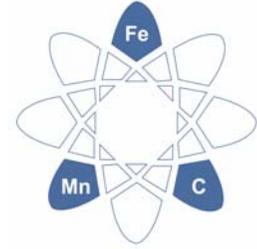


$$Z_1 = \begin{pmatrix} \cos \phi_1 & \sin \phi_1 & 0 \\ -\sin \phi_1 & \cos \phi_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, X = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \Phi & \sin \Phi \\ 0 & -\sin \Phi & \cos \Phi \end{pmatrix},$$

$$Z_2 = \begin{pmatrix} \cos \phi_2 & \sin \phi_2 & 0 \\ -\sin \phi_2 & \cos \phi_2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$A = Z_2 X Z_1$$

Texture presentation



$$\mathbf{A} = \mathbf{Z}_2 \mathbf{X} \mathbf{Z}_1 =$$

[uvw]

$$\cos \varphi_1 \cos \varphi_2$$

$$-\sin \varphi_1 \sin \varphi_2 \cos \Phi$$

$$-\cos \varphi_1 \sin \varphi_2$$

$$-\sin \varphi_1 \cos \varphi_2 \cos \Phi$$

$$\sin \varphi_1 \sin \Phi$$

$$\sin \varphi_1 \cos \varphi_2$$

$$+\cos \varphi_1 \sin \varphi_2 \cos \Phi$$

$$-\sin \varphi_1 \sin \varphi_2$$

$$+\cos \varphi_1 \cos \varphi_2 \cos \Phi$$

$$-\cos \varphi_1 \sin \Phi$$

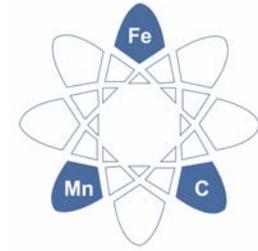
(hkl)

$$\sin \varphi_2 \sin \Phi$$

$$\cos \varphi_2 \sin \Phi$$

$$\cos \Phi$$

Texture presentation

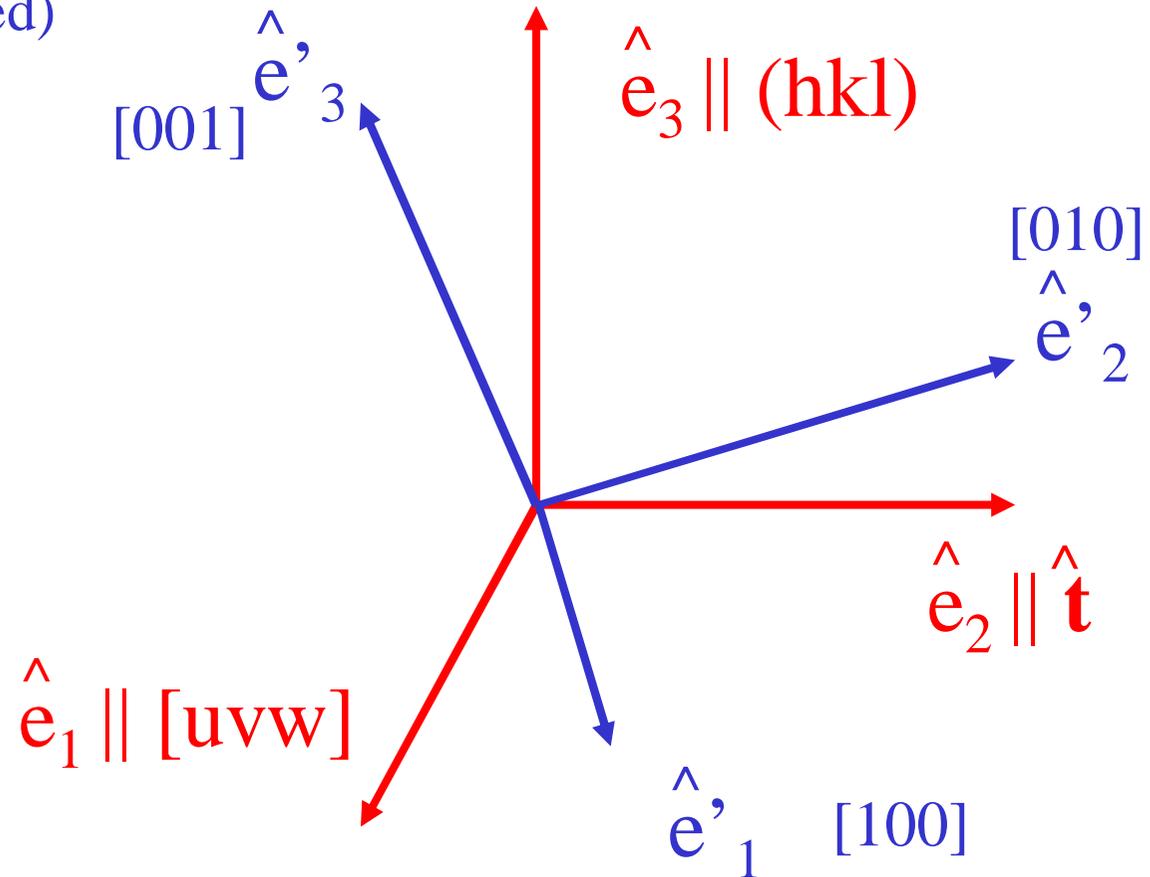


Geometry of $\{hkl\}\langle uvw \rangle$

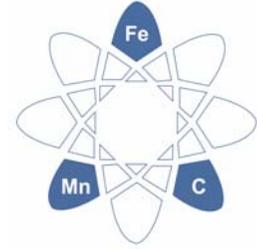
Sample to Crystal (primed)

Miller index notation of texture component specifies direction cosines of xtal directions \parallel to sample axes.

$$\mathbf{t} = \mathbf{hkl} \times \mathbf{uvw}$$



Texture presentation



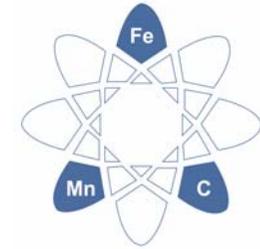
$$\hat{\mathbf{n}} = \frac{(h, k, l)}{\sqrt{h^2 + k^2 + l^2}}$$

$$\hat{\mathbf{b}} = \frac{(u, v, w)}{\sqrt{u^2 + v^2 + w^2}}$$

$$\hat{\mathbf{t}} = \frac{\hat{\mathbf{n}} \times \hat{\mathbf{b}}}{|\hat{\mathbf{n}} \times \hat{\mathbf{b}}|}$$

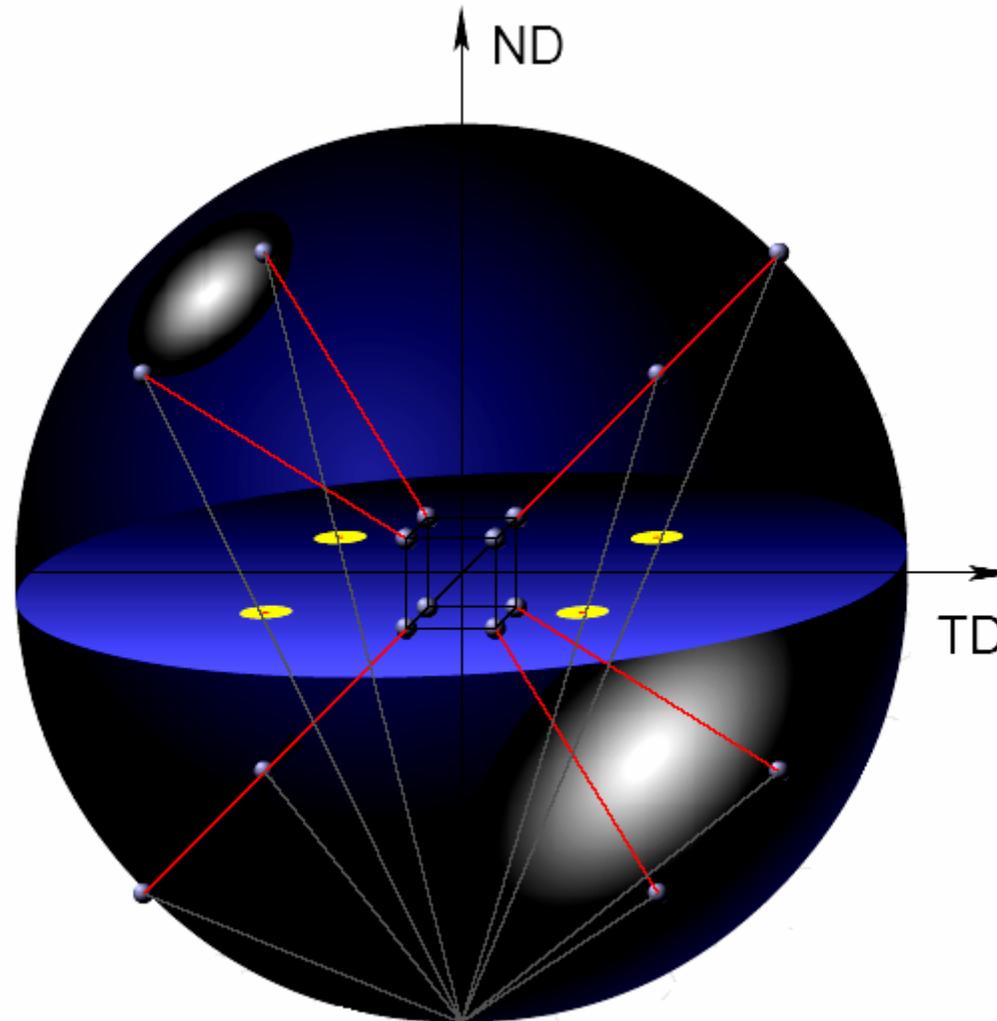
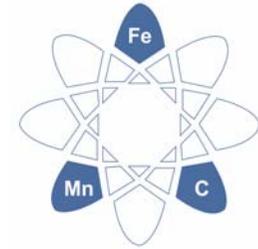
$$a_{ij} = \text{Crystal} \begin{matrix} \text{Sample} \\ \left(\begin{array}{ccc} b_1 & t_1 & n_1 \\ b_2 & t_2 & n_2 \\ b_3 & t_3 & n_3 \end{array} \right) \end{matrix}$$

Texture presentation

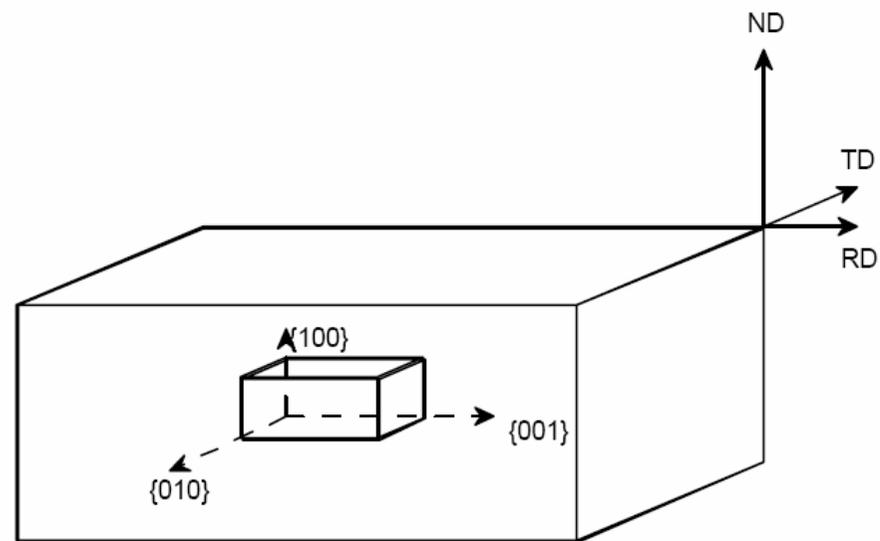
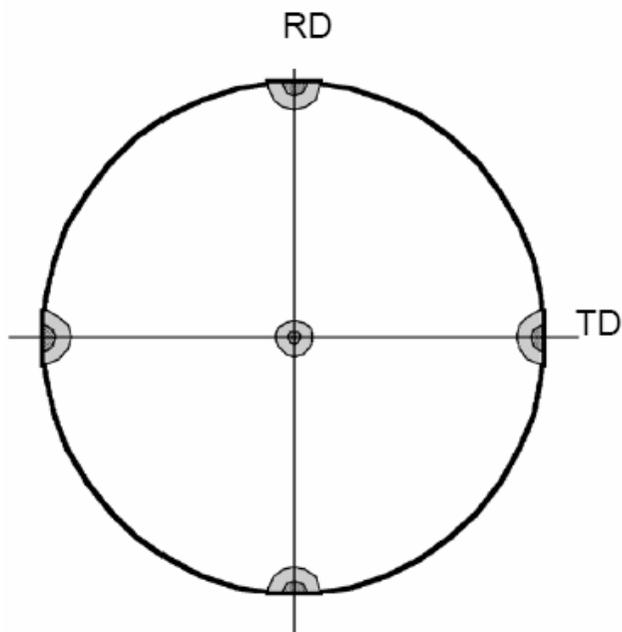
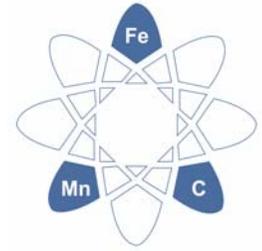


$$a_{ij} = \text{Crystal} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \begin{matrix} \text{Sample} \\ t_1 \\ t_2 \\ t_3 \end{matrix} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix} \begin{pmatrix} \cos \varphi_1 \cos \varphi_2 & \sin \varphi_1 \cos \varphi_2 & \sin \varphi_2 \sin \Phi \\ -\sin \varphi_1 \sin \varphi_2 \cos \Phi & +\cos \varphi_1 \sin \varphi_2 \cos \Phi & \cos \varphi_2 \sin \Phi \\ -\cos \varphi_1 \sin \varphi_2 & -\sin \varphi_1 \sin \varphi_2 & \cos \varphi_2 \sin \Phi \\ -\sin \varphi_1 \cos \varphi_2 \cos \Phi & +\cos \varphi_1 \cos \varphi_2 \cos \Phi & \cos \Phi \\ \sin \varphi_1 \sin \Phi & -\cos \varphi_1 \sin \Phi & \end{pmatrix}$$

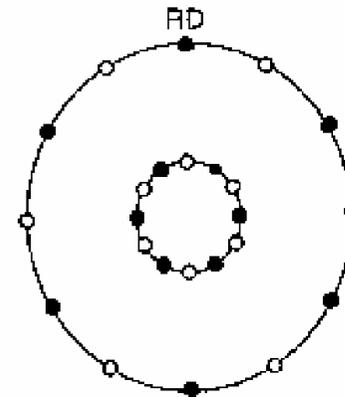
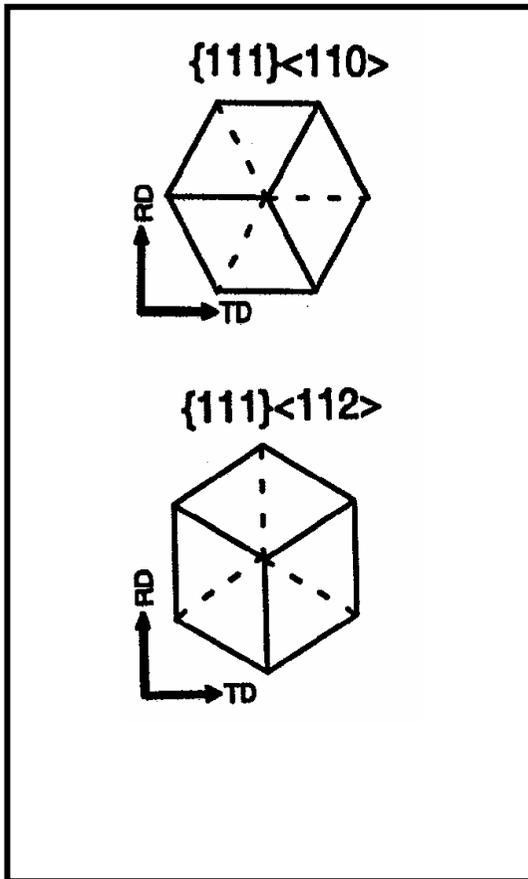
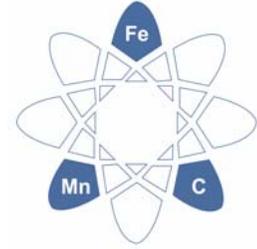
Texture presentation



Texture presentation



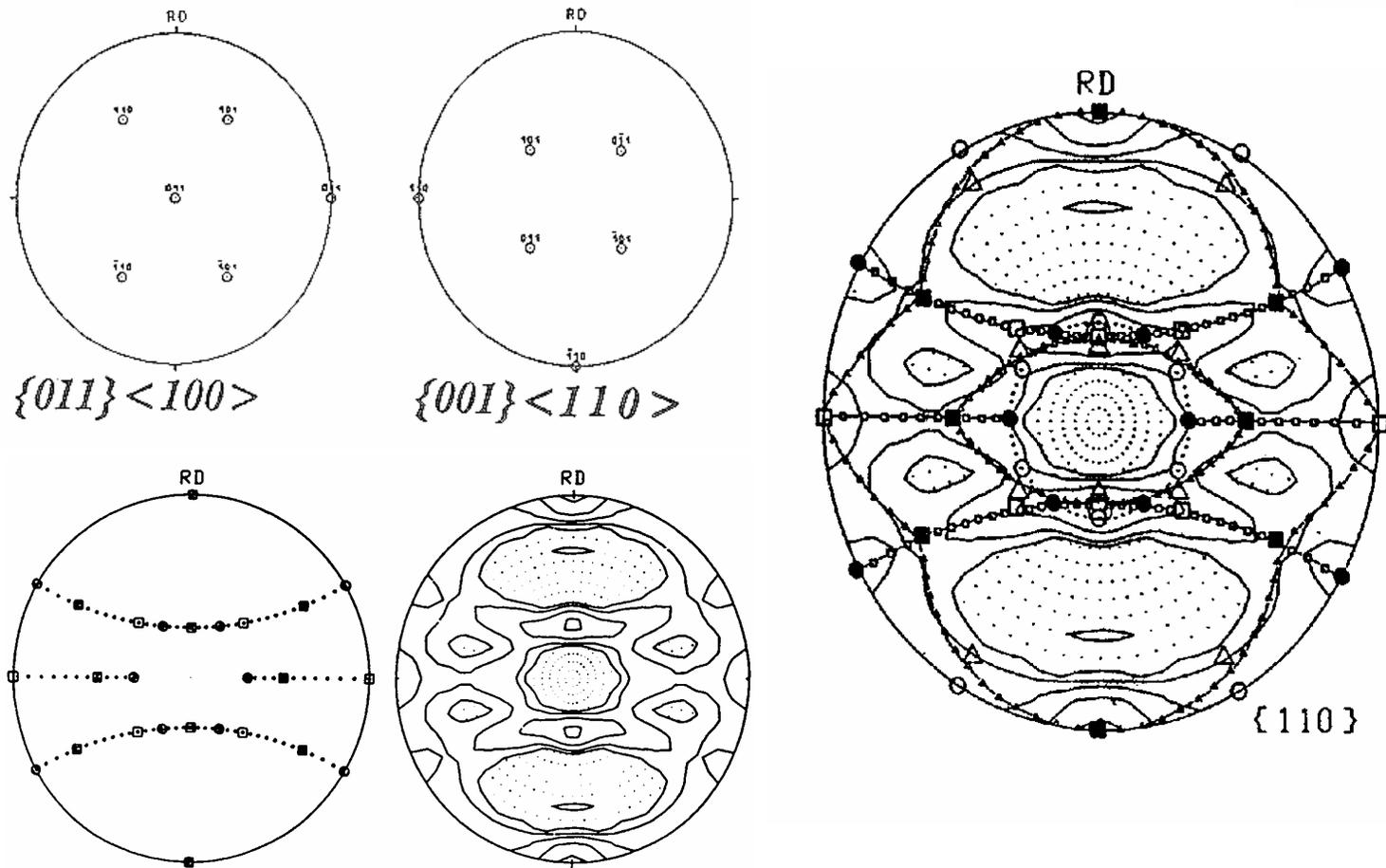
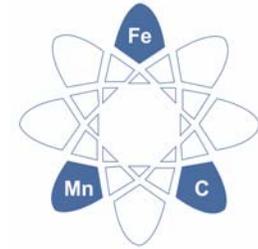
Texture presentation

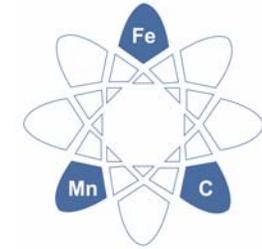


γ -Faser mit $\langle 111 \rangle \parallel$ ND

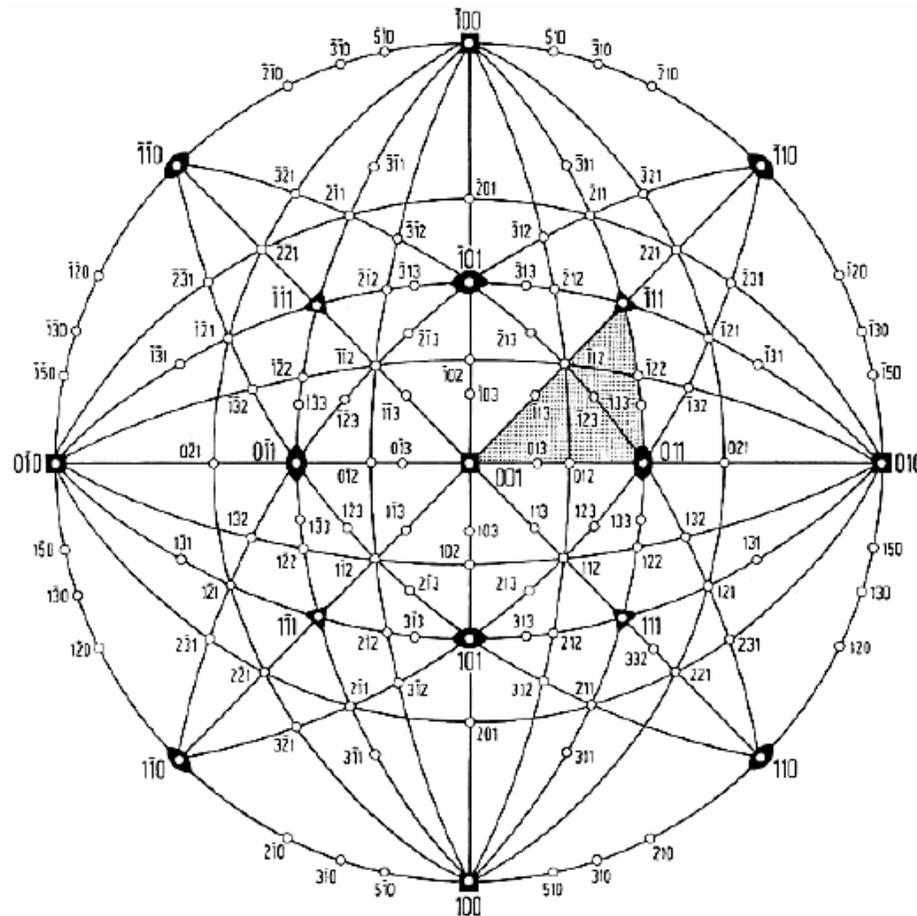
- $\{111\}\langle 112 \rangle$
- $\{111\}\langle 110 \rangle$

Texture presentation



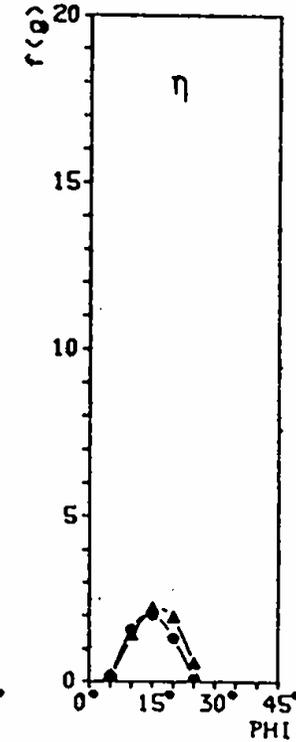
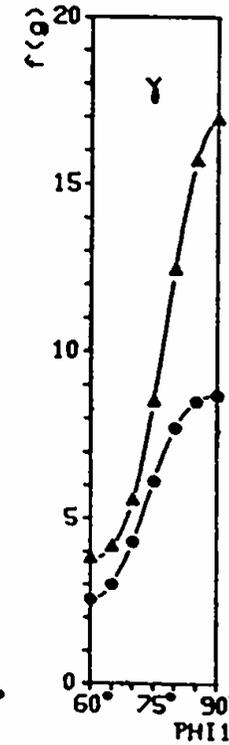
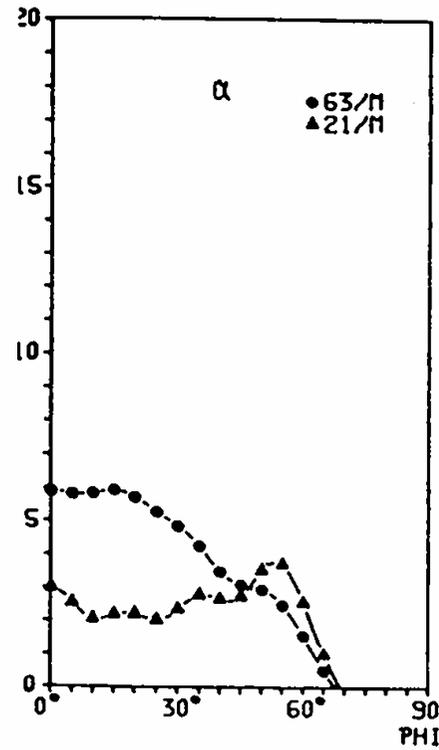
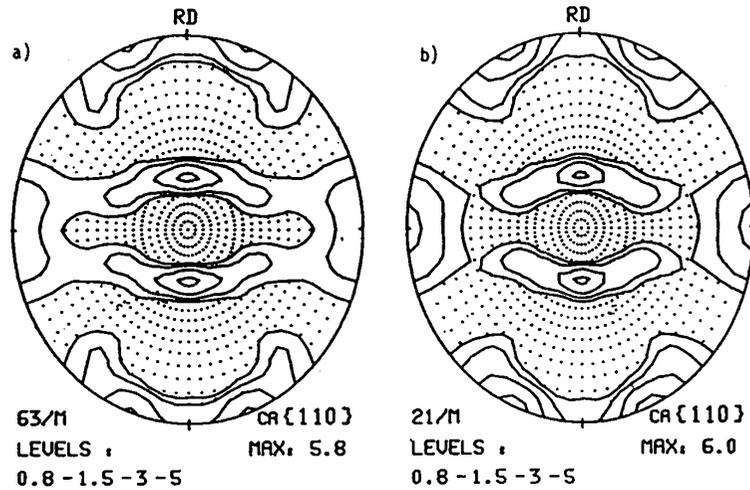
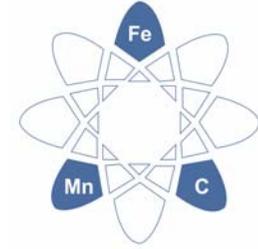


Texture presentation



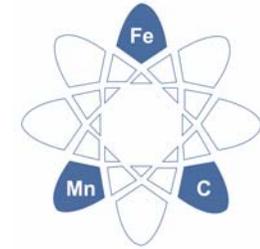
Es existieren 24 kristallographisch identische Dreiecke mit den Ecken $\langle 001 \rangle$, $\langle 011 \rangle$ und $\langle 111 \rangle$. Da alle Dreiecke identisch sind, reicht es aus, nur das sogenannte Standard-Dreieck $[001]$, $[011]$ und $[-111]$ zu betrachten. Zusammen mit dem Wulff'schen Netz können nun Winkel zwischen Kristallorientierungen graphisch bestimmt werden.

Texture presentation

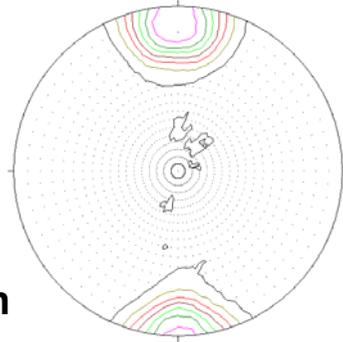


Texture presentation

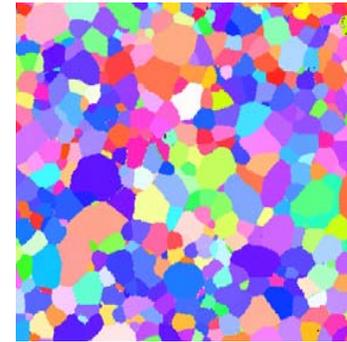
D. Raabe: Textures and Microstructures 23 (1995) 115–129
 „Examination of the iterative series-expansion method for quantitative texture analysis“



pole figures



inversion



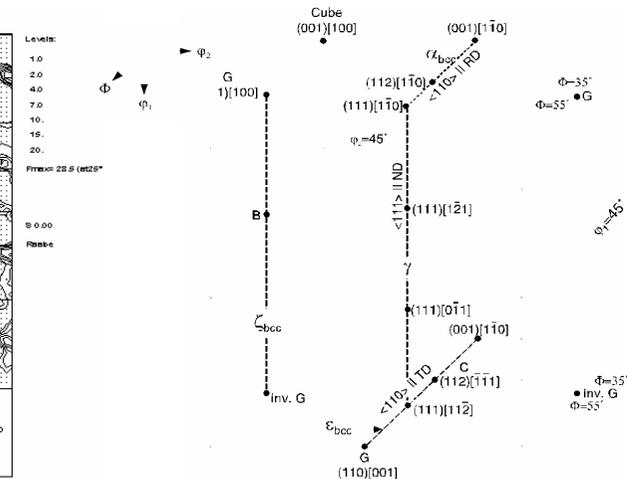
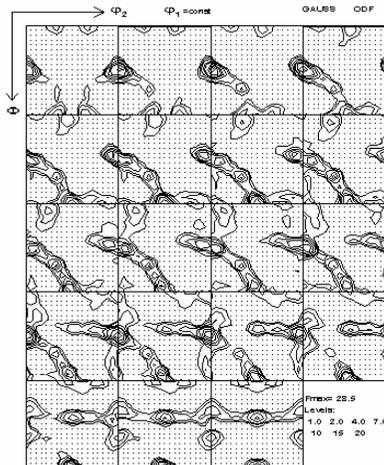
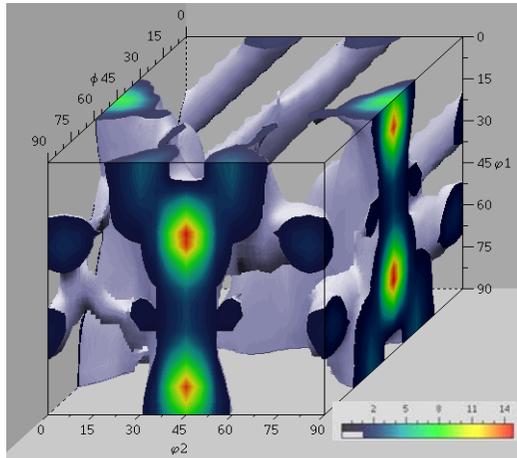
EBSD maps

binning

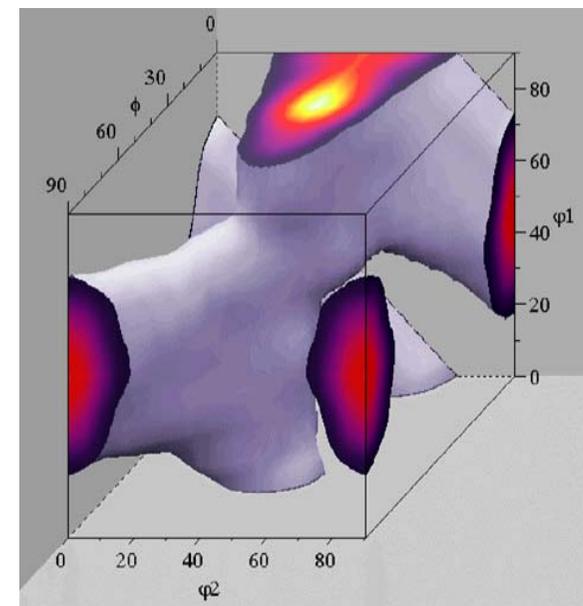
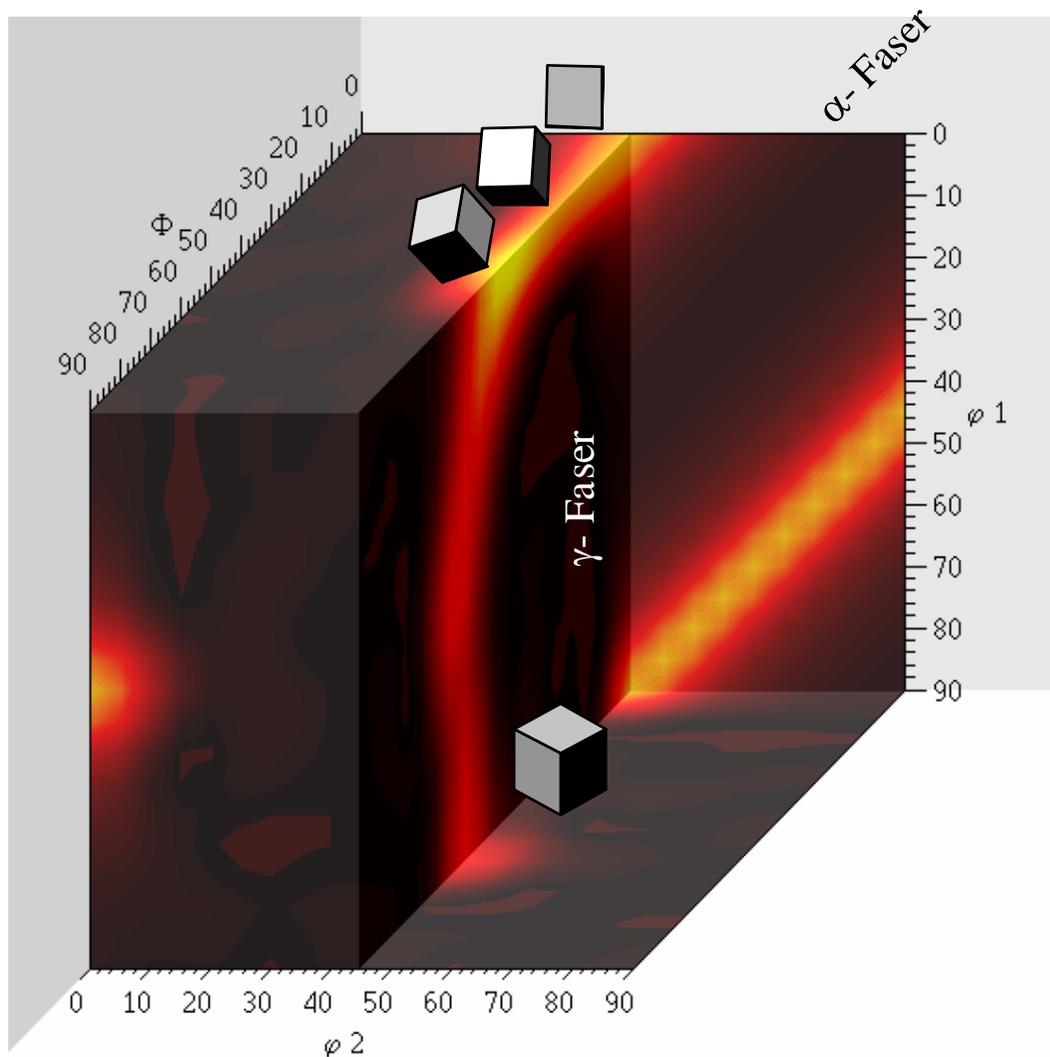
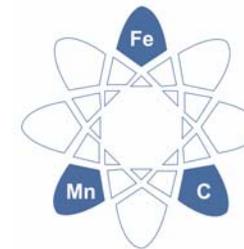
$$p(\alpha, \beta) = \int_{\gamma} f(\alpha, \beta, \gamma) d\gamma$$

$$f(\alpha, \beta, \gamma) = \sum_c I^c f^c(\alpha, \beta, \gamma)$$

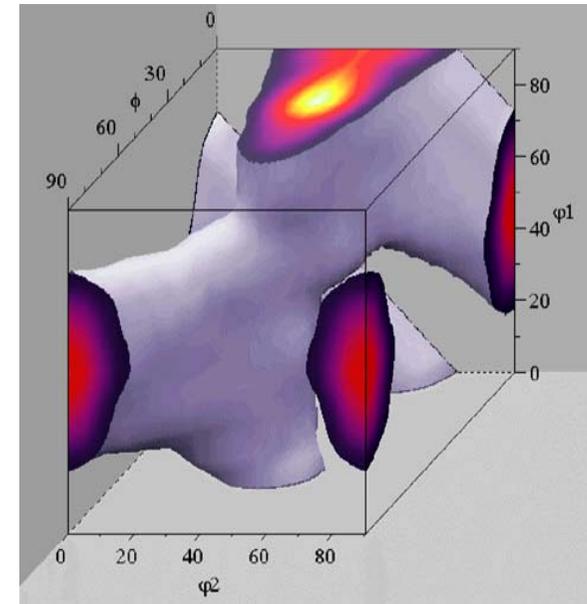
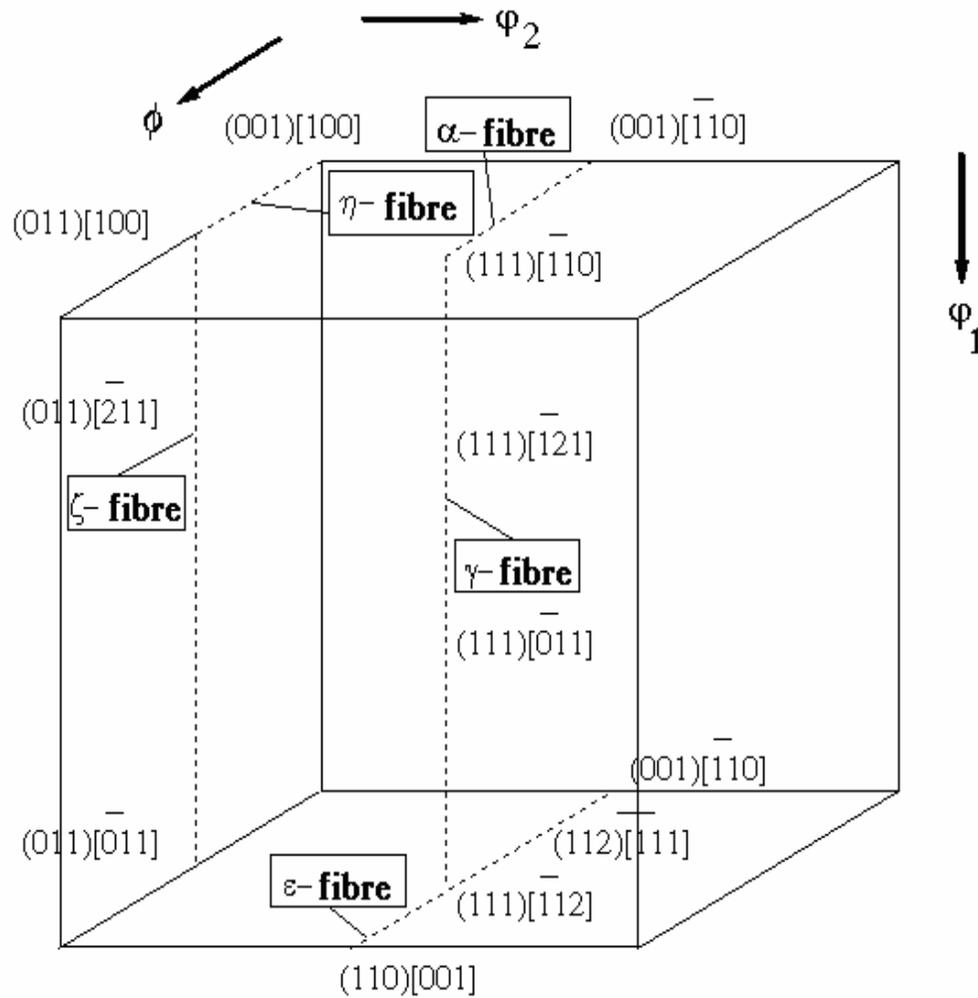
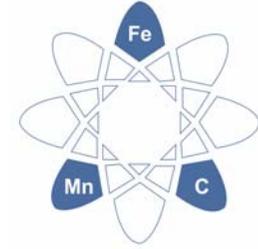
ODF, orientation distribution function



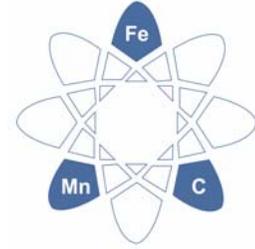
Texture presentation



Texture presentation



Texture presentation



Name of the Fibre	Fibre Axis	Orientations on the Fibre
α -fibre	$\langle 110 \rangle \parallel \text{RD}$	$\{001\}\langle 110 \rangle$ - $\{112\}\langle 110 \rangle$ and $\{111\}\langle 110 \rangle$
γ -fibre	$\langle 111 \rangle \parallel \text{ND}$	$\{111\}\langle 110 \rangle$ - $\{111\}\langle 112 \rangle$
η -fibre	$\langle 100 \rangle \parallel \text{RD}$	$\{001\}\langle 100 \rangle$ - $\{011\}\langle 100 \rangle$ (Goss)
ζ -fibre	$\langle 110 \rangle \parallel \text{ND}$	Goss, $\{110\}\langle 112 \rangle$ and $\{110\}\langle 110 \rangle$
ε -fibre	$\langle 110 \rangle \parallel \text{TD}$	$\{001\}\langle 110 \rangle$, $\{112\}\langle 111 \rangle$, $\{4\ 4\ 11\}\langle 11\ 11\ 8 \rangle$, $\{111\}\langle 112 \rangle$, $\{11\ 11\ 8\}\langle 4\ 4\ 11 \rangle$ and Goss
β -fibre	$\approx \langle 111 \rangle \parallel \text{ND}$	$\{111\}\langle 110 \rangle$, $\{557\}\langle 583 \rangle$ and $\{111\}\langle 112 \rangle$

M. Hölscher, D. Raabe, K. Lücke: Steel Research 62 (1991) 567–575

„Rolling and recrystallization textures of bcc steels“

C. Klinkenberg, D. Raabe, K. Lücke: Steel Research 63 (1992) 227–276

„Influence of volume fraction and dispersion rate of grain boundary cementite on the cold rolling textures of low carbon steels“

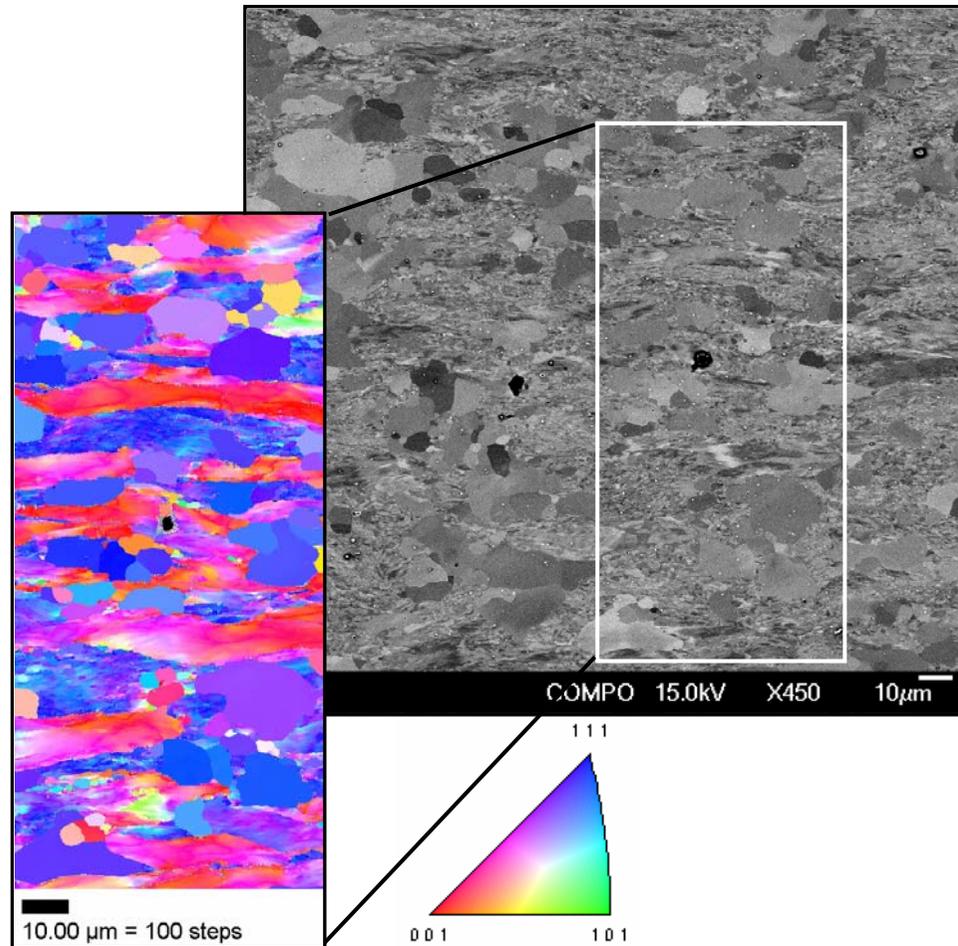
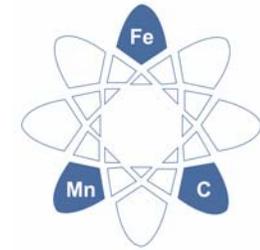
D. Raabe, C. Klinkenberg, K. Lücke: Steel Research 64 (1993) 262–266

„Texture development during intercritical annealing of low carbon steel“

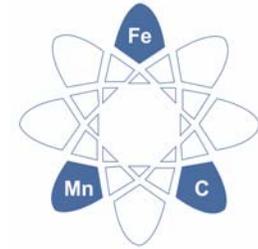
M. Hölscher, D. Raabe, K. Lücke: Acta metall. 42 (1994) 879–886

„Relationship between rolling textures and shear textures in f.c.c. and b.c.c. metals“

Texture presentation



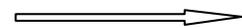
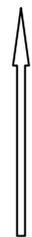
Texture presentation



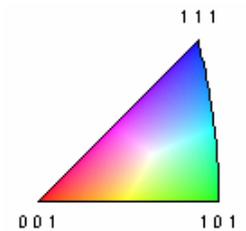
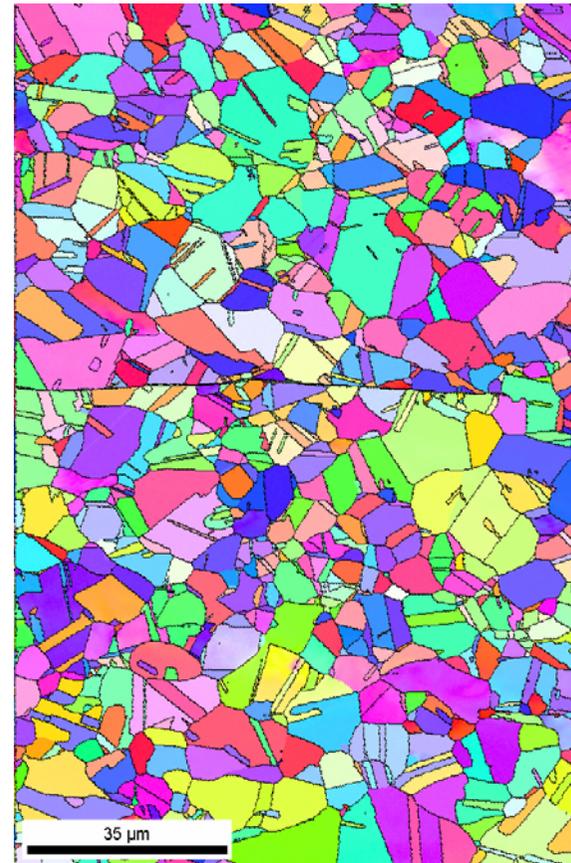
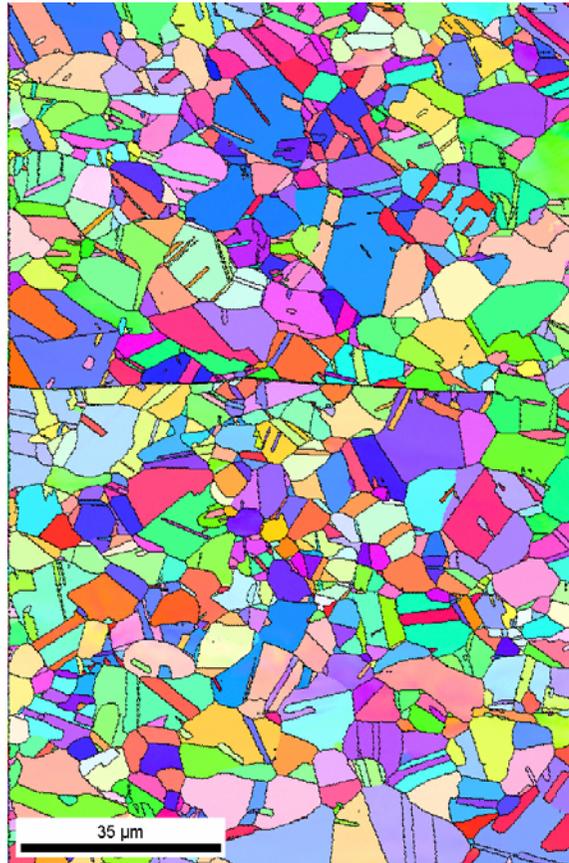
ND

RD

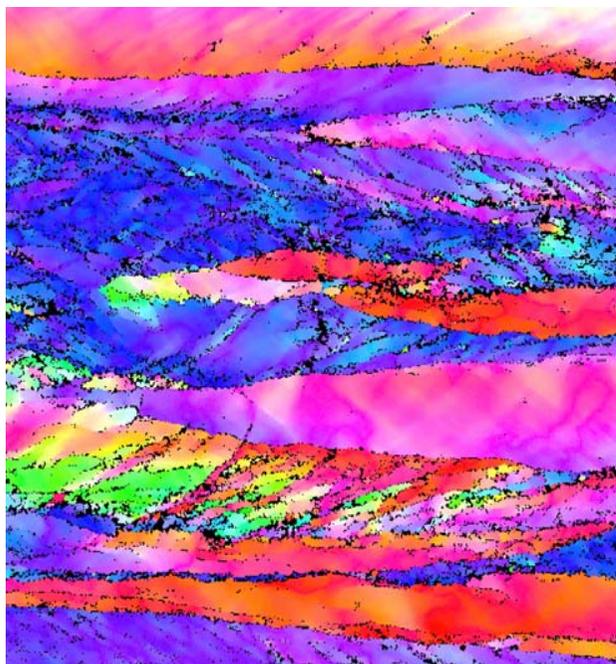
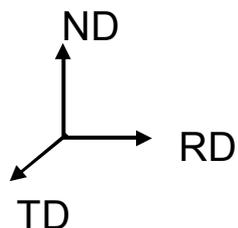
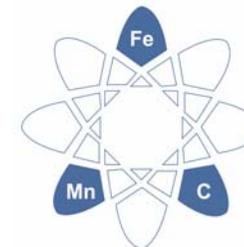
ND



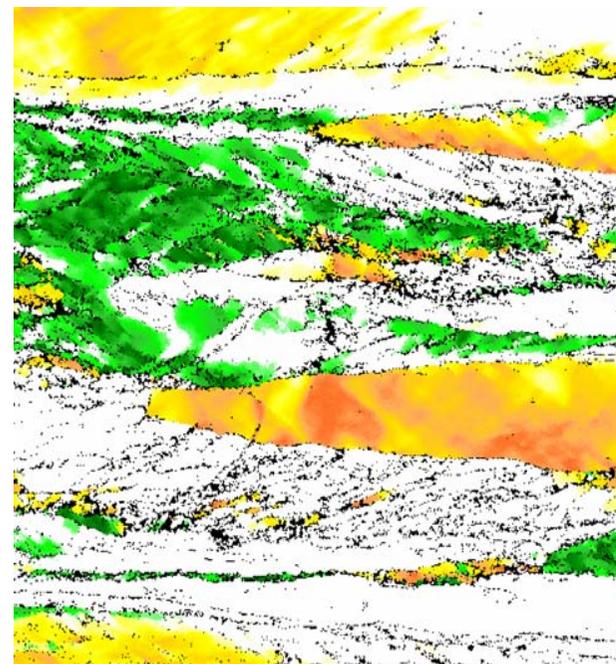
RD



Texture presentation

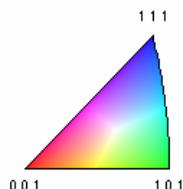


9.00 μm = 90 steps IPF [001]

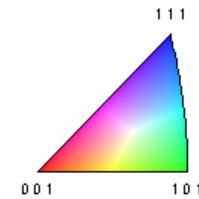
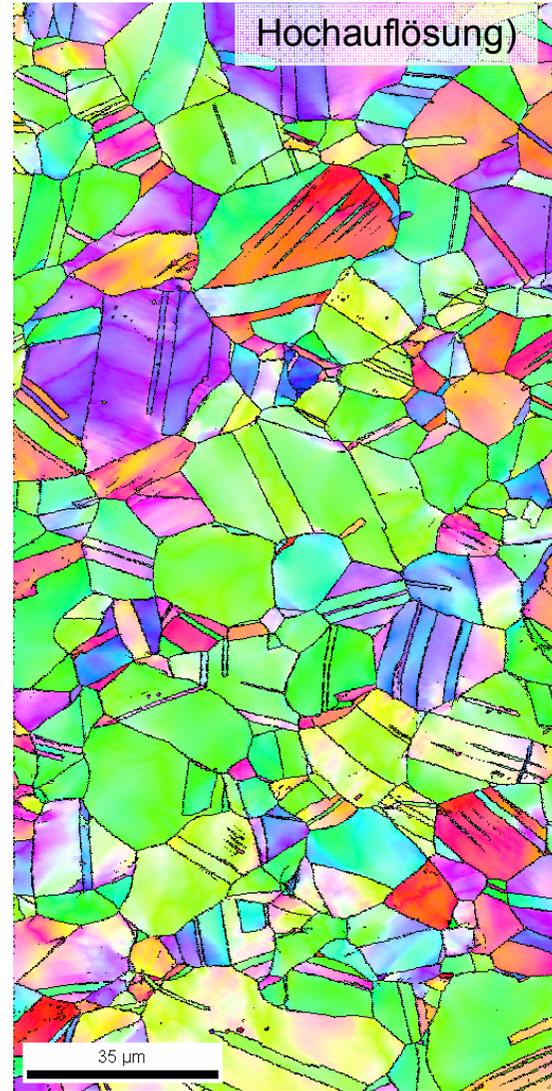
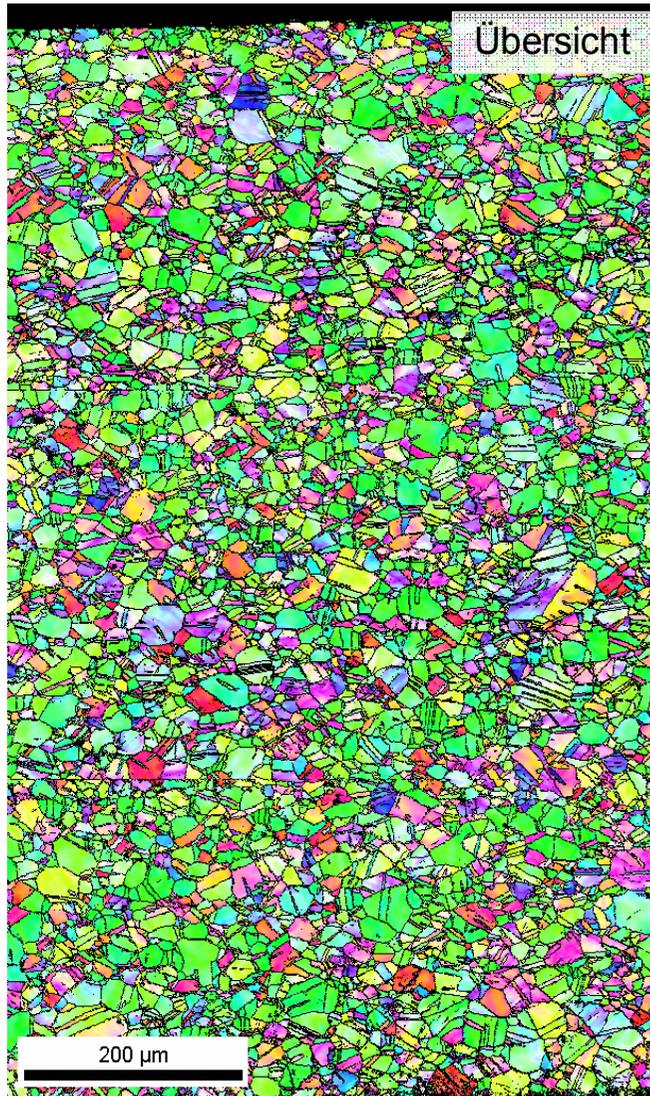
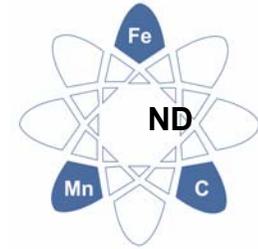


9.00 μm = 90 steps Direction

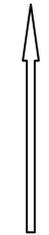
Direction	Min	Max	Total Fraction	Partition Fraction
$\langle 110 \rangle [100]$	0°	10°	0.276	0.276
$\langle 111 \rangle [001]$	0°	10°	0.183	0.183



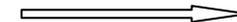
Texture presentation

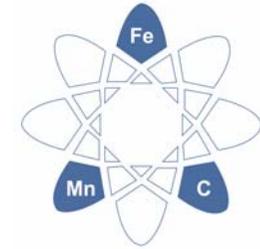


Blechnormale



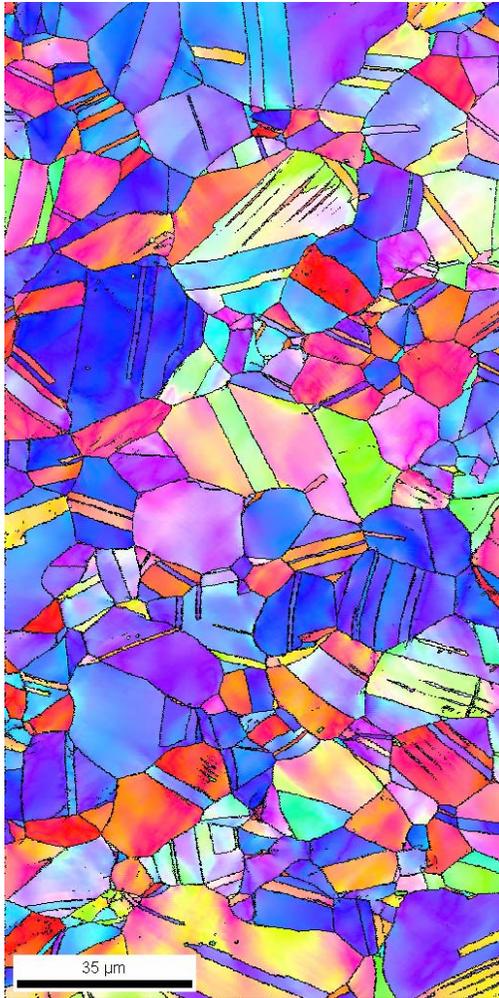
Walzrichtung



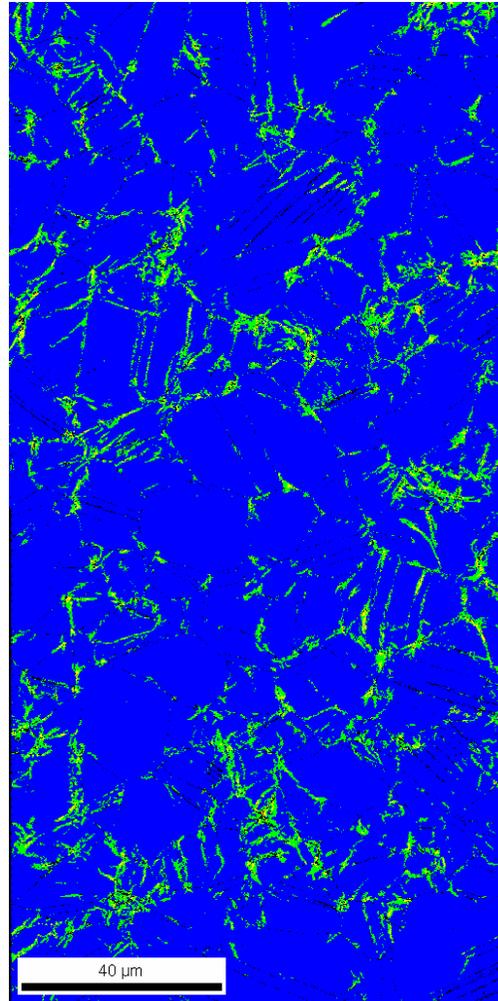


Texture presentation

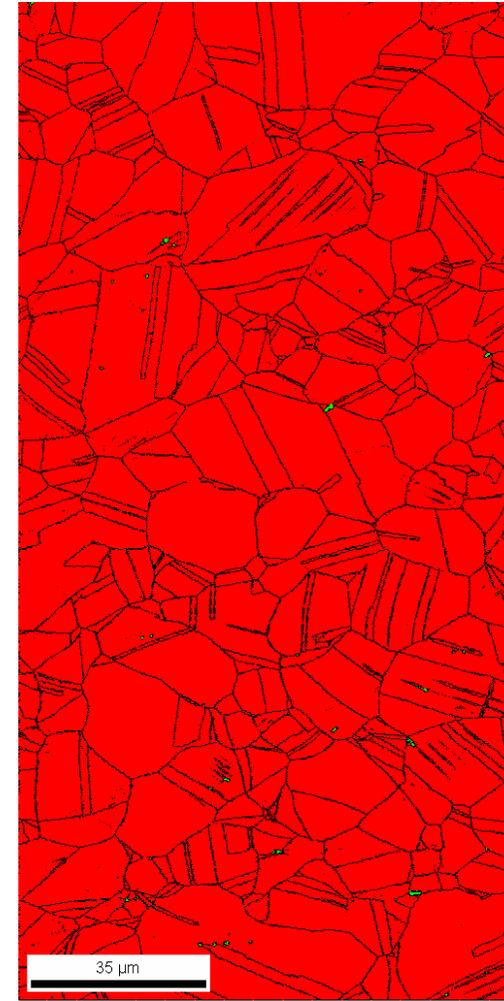
Millerindizes uvw

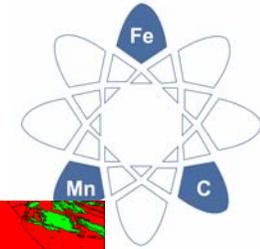


Mittlere lokale Misorientierung



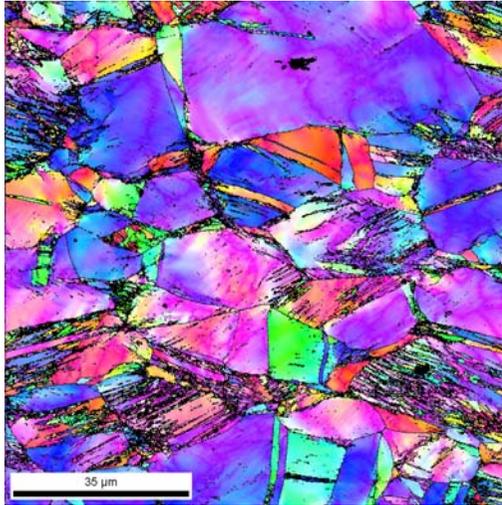
Phasenanteile



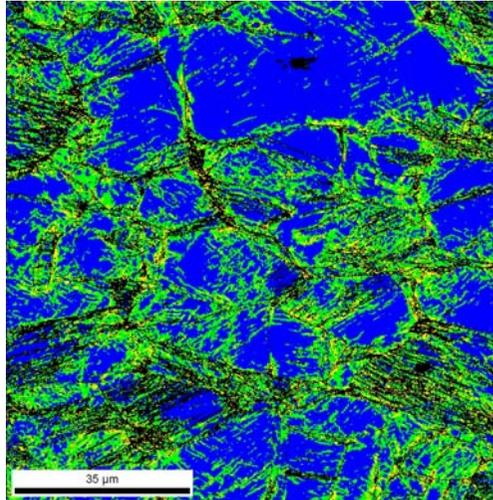


Texture presentation

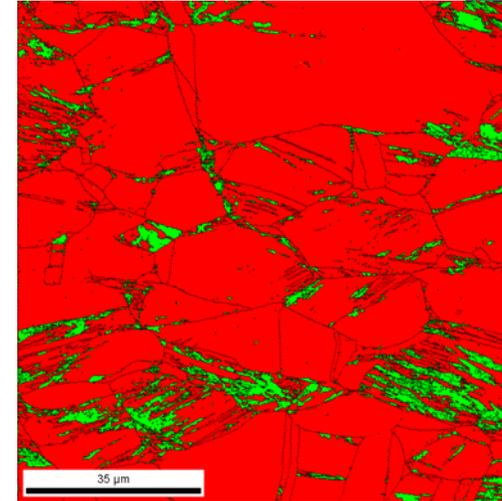
Millerindizes uww



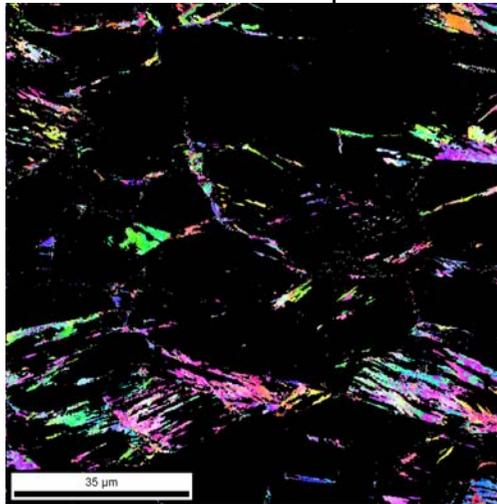
Mittlere lokale Misorientierung (KAM1)



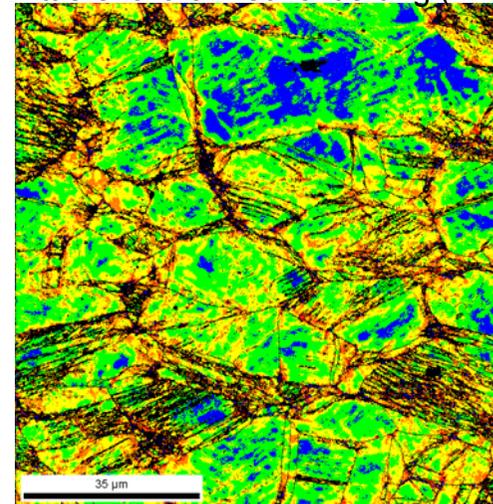
Phasenanteile



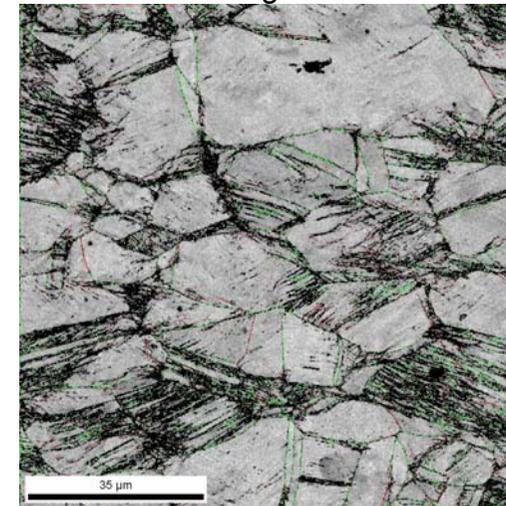
Textur Ferritphase



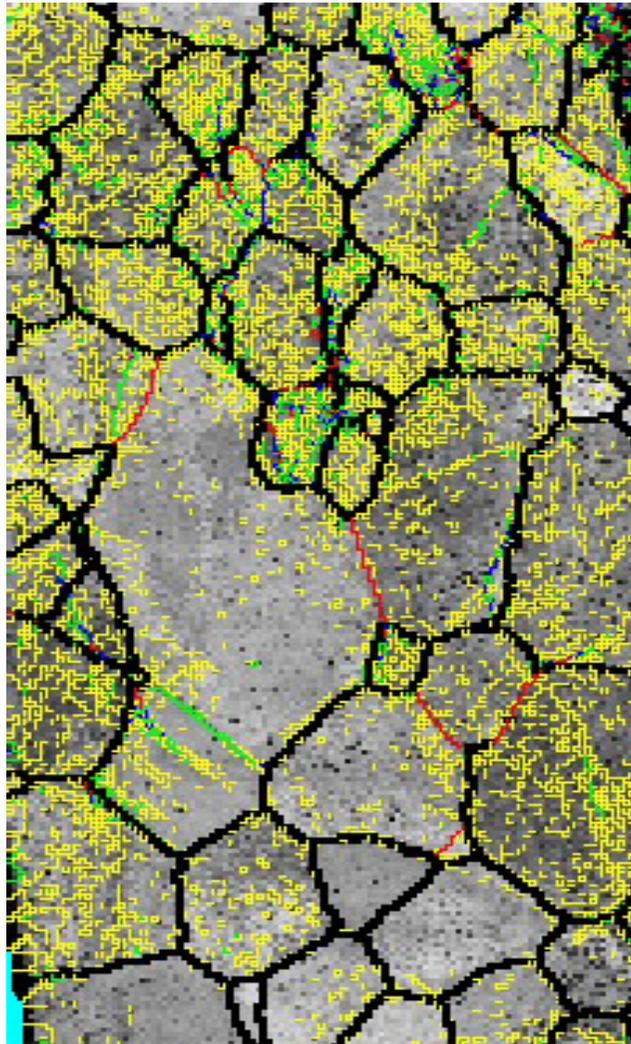
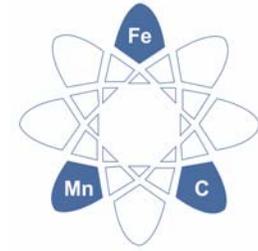
Mittlere lokale Misorientierung (KAM3)



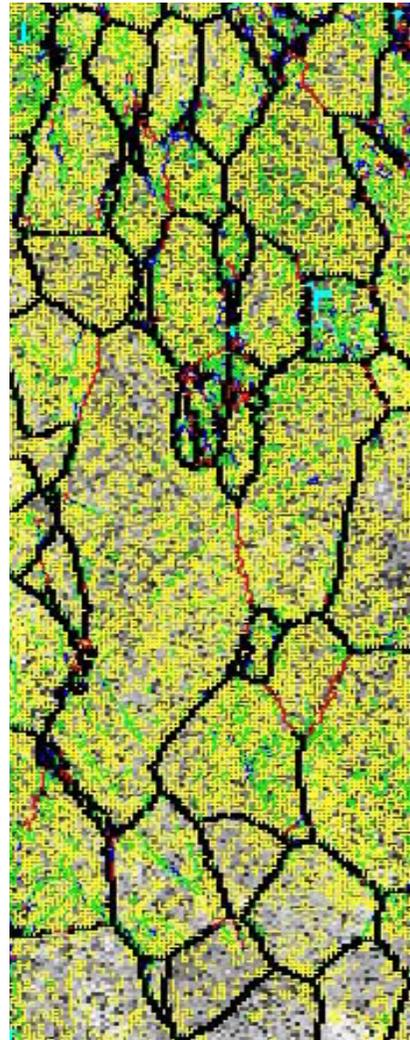
Korngrenzen



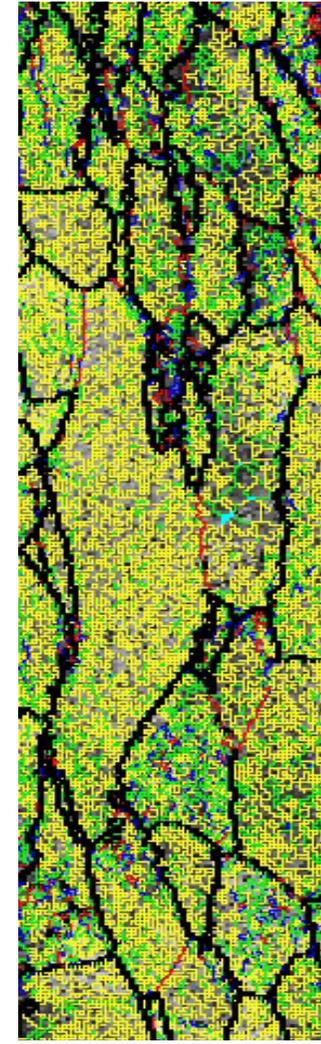
Texture presentation



8%

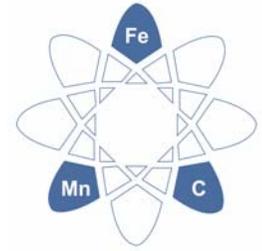


23%



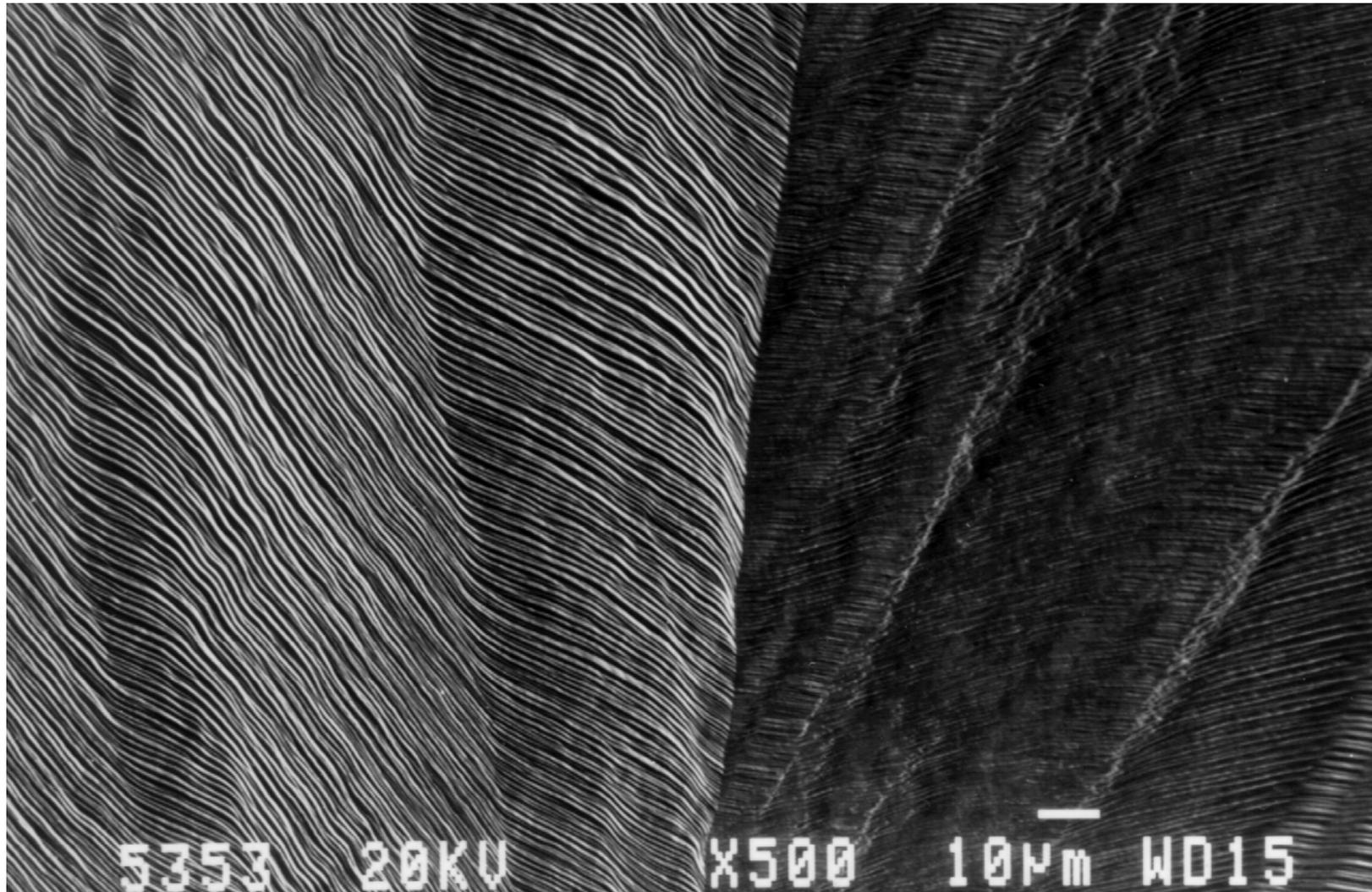
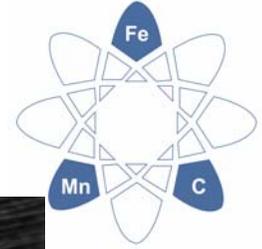
35%

Overview

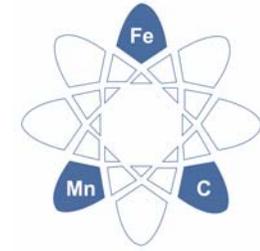


- Anisotropy
- Presentation
- **Measurement**
- Textures and Mechanics
- Examples of Texture Research

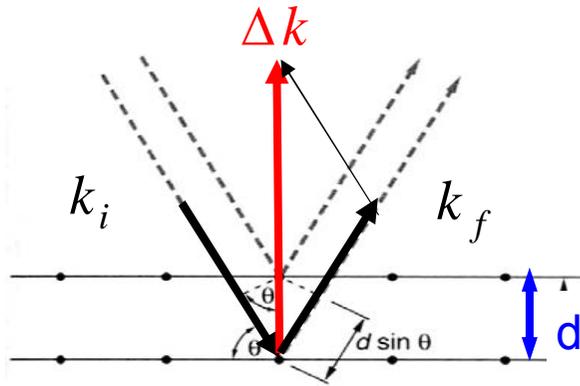
Texture measurement



Texture measurement

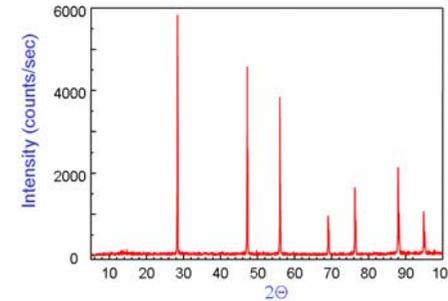


Bragg diffraction



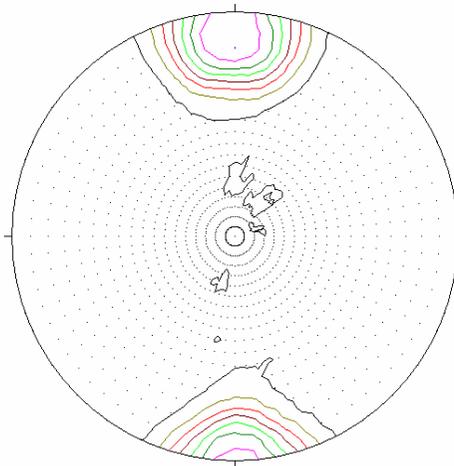
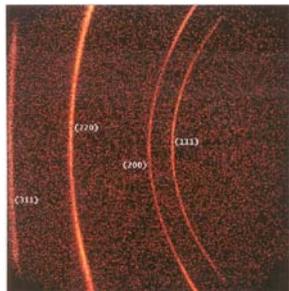
$$n\lambda = 2d_{hkl} \sin \theta$$

$$\text{where } k = \frac{2\pi}{\lambda}$$

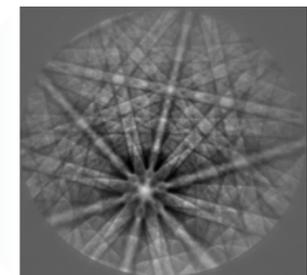
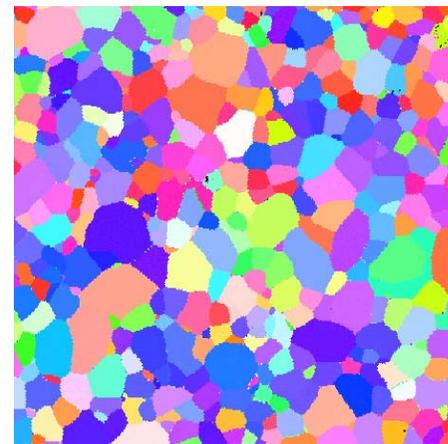


- x-ray, neutrons, synchrotron (pole figures)
- neutrons (pole figures)
- electrons (Kikuchi patterns)

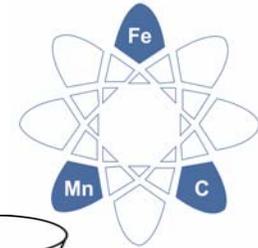
pole figure



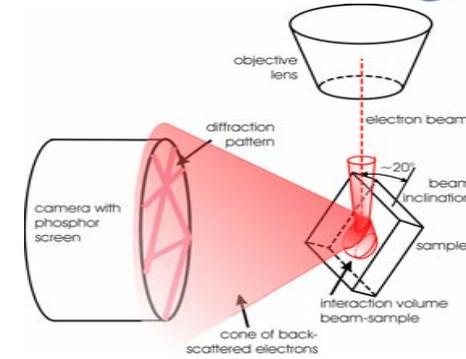
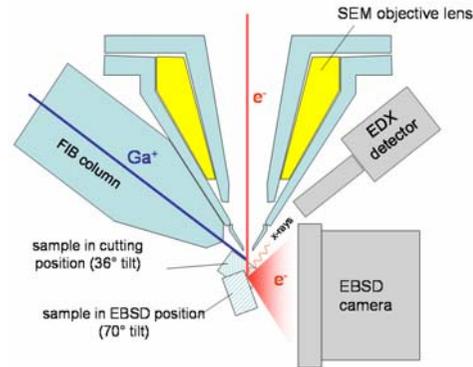
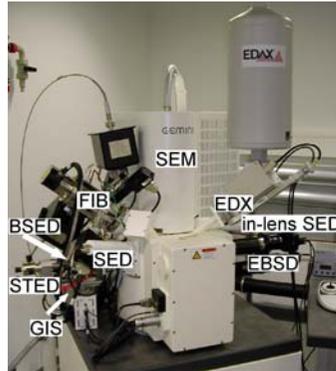
EBSD maps



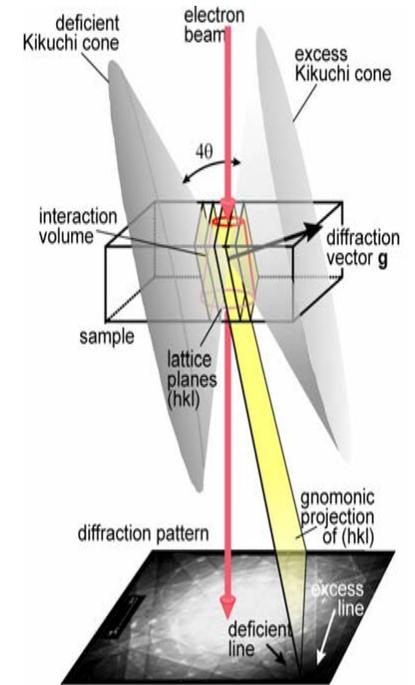
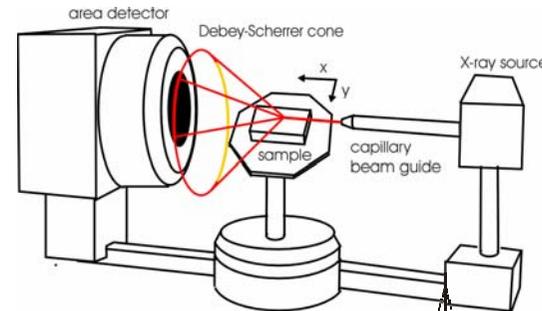
Experimental



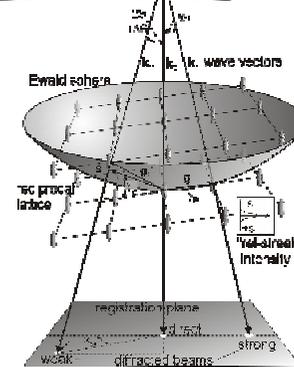
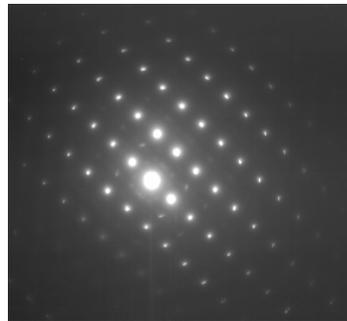
EBSD



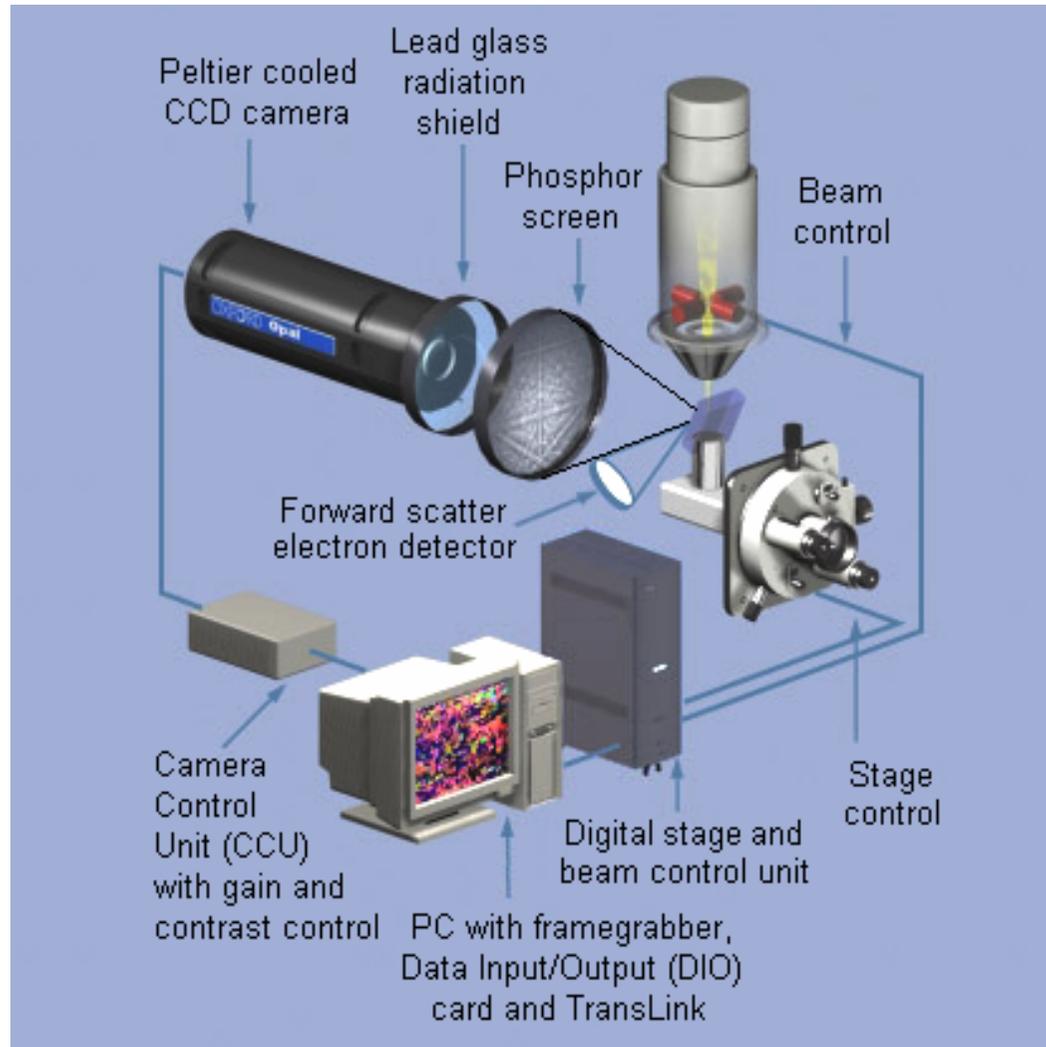
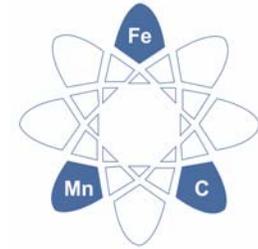
x-ray



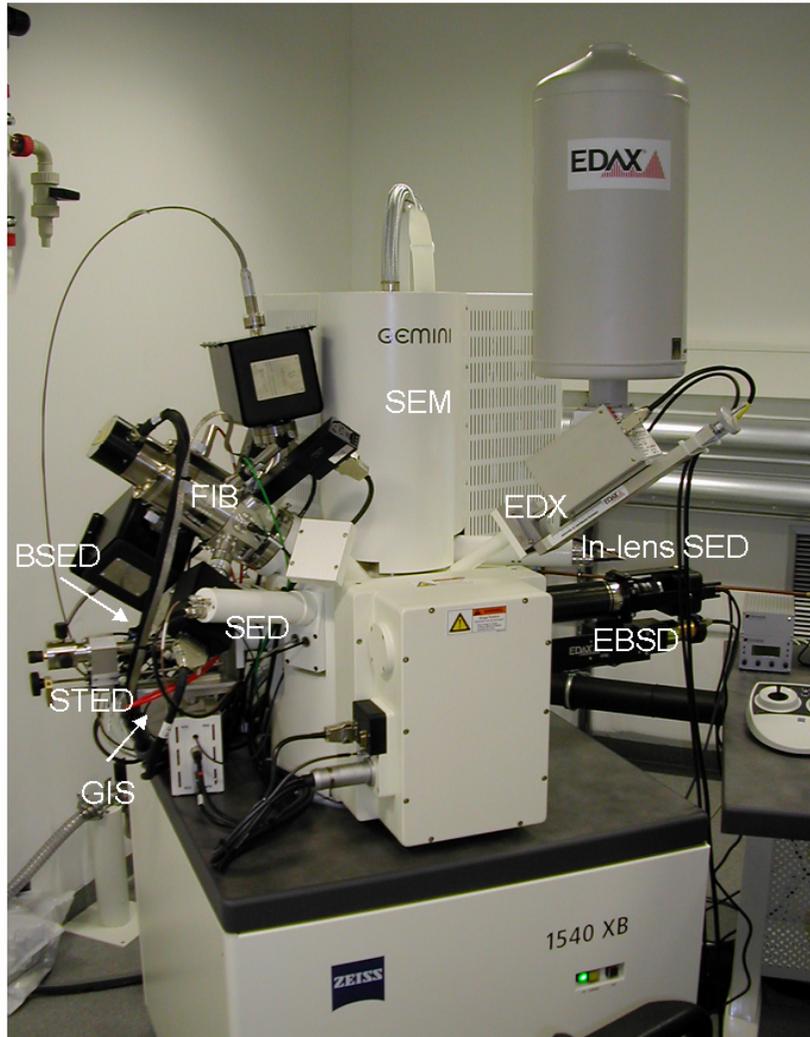
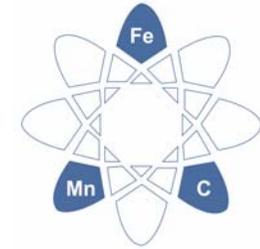
TEM



Texture measurement



Serial sectioning and 3D-EBSD in a FIB-SEM

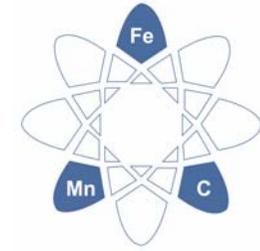


scanning electron microscope

- observation with SE, BSE, STEM
- quantitative analysis with EBSD and EDX

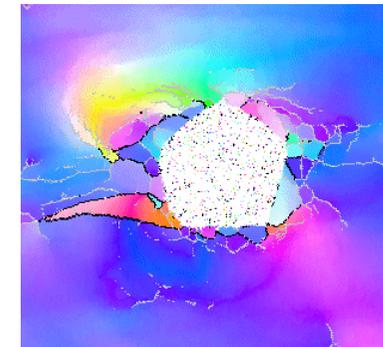
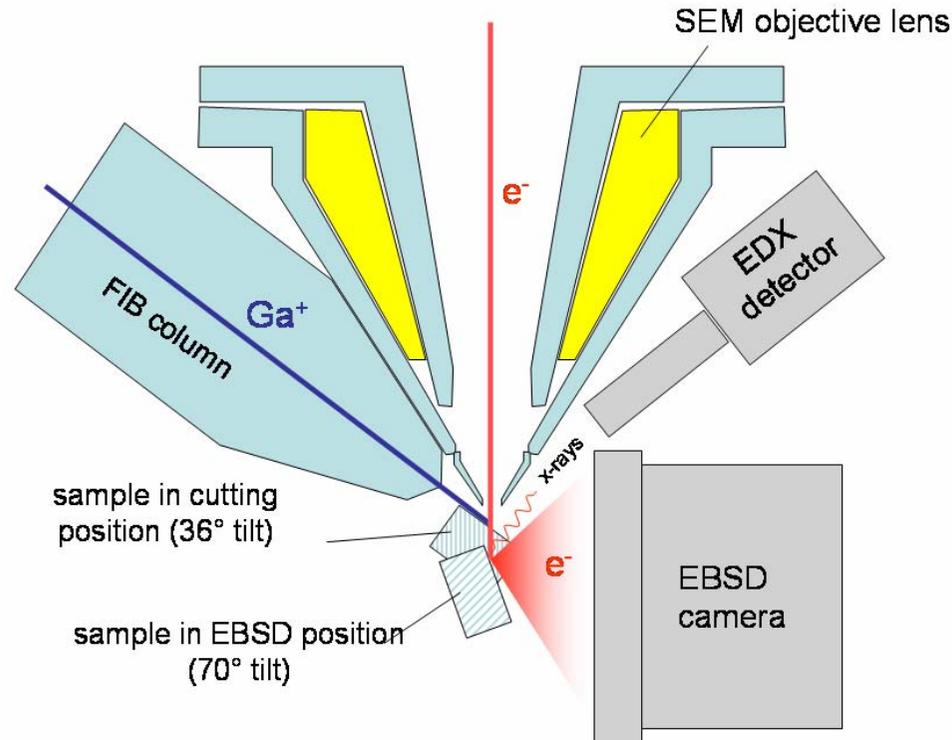
scanning Ga⁺-ion microscope (FIB = focused ion beam)

- beam current 10 pA... 50 nA
- ion energies 1 ... 30 keV
- observation with ion-induced SE
- sputtering (milling) for serial sectioning, TEM thin-foil preparation, surface structuring
- deposition of various films (W, Pt, SiO₂) from organic precursor gasses



Serial sectioning and 3D-EBSD in a FIB-SEM

J. Konrad, S. Zaefferer, D. Raabe, "Investigation of orientation gradients around a hard Laves particle in a warm rolled Fe₃Al-based alloy by a 3D EBSD-FIB technique", Acta Materialia, Volume 54, Issue 5, March 2006, Pages 1369-1380

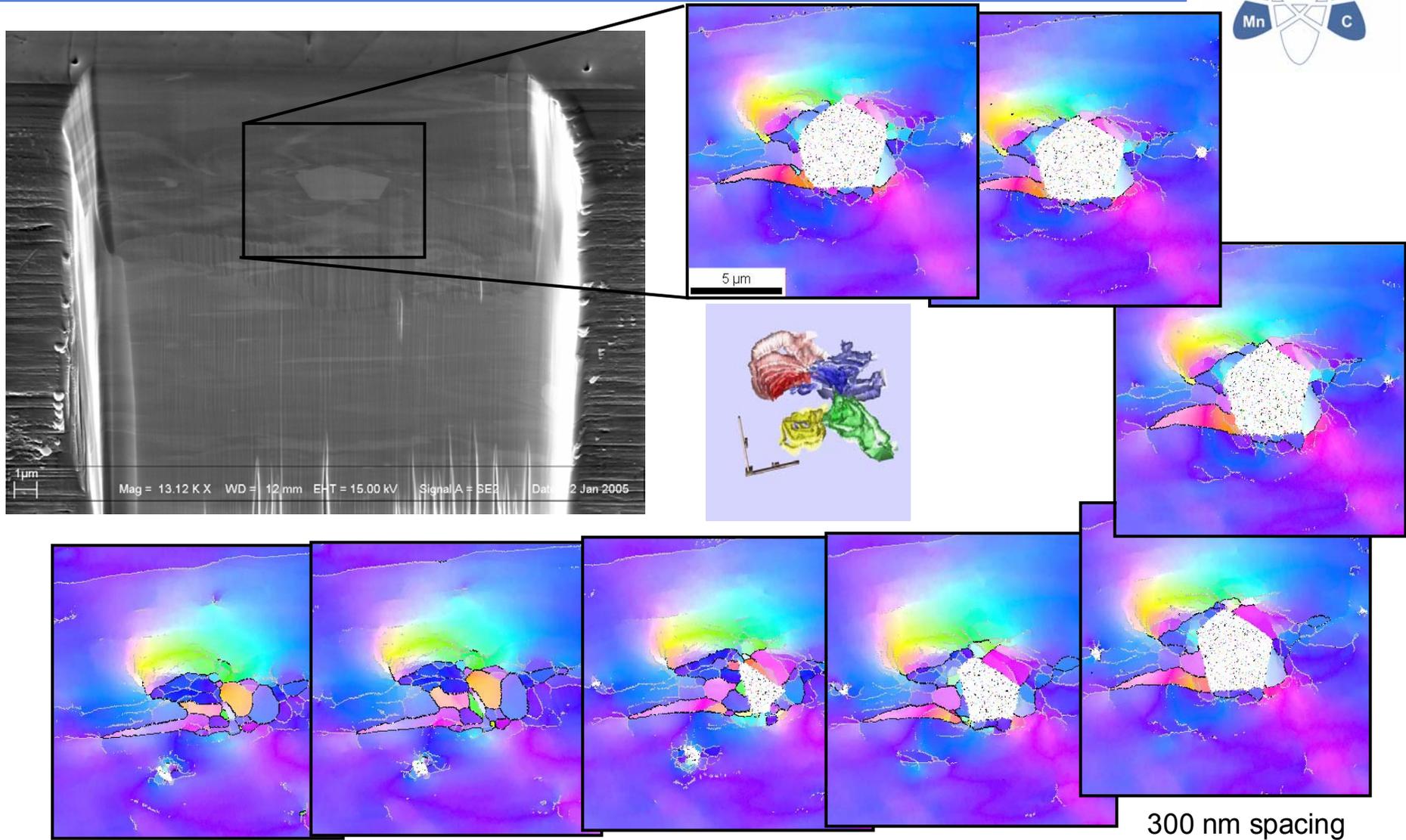
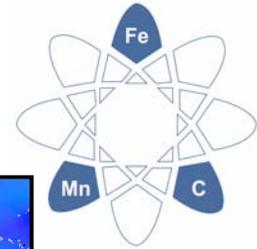


EBSD camera opposite to the FIB gun:

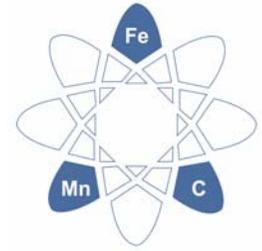
- ⇒ Only two axes (tilt & y-shift) need to move
- ⇒ Quick and precise change between milling for serial sectioning (sample at 36°) and EBSD-mapping (sample at 70°).

3D EBSD

J. Konrad, S. Zaefferer, D. Raabe, "Investigation of orientation gradients around a hard Laves particle in a warm rolled Fe3Al-based alloy by a 3D EBSD-FIB technique", Acta Materialia, Volume 54, Issue 5, March 2006, Pages 1369-1380

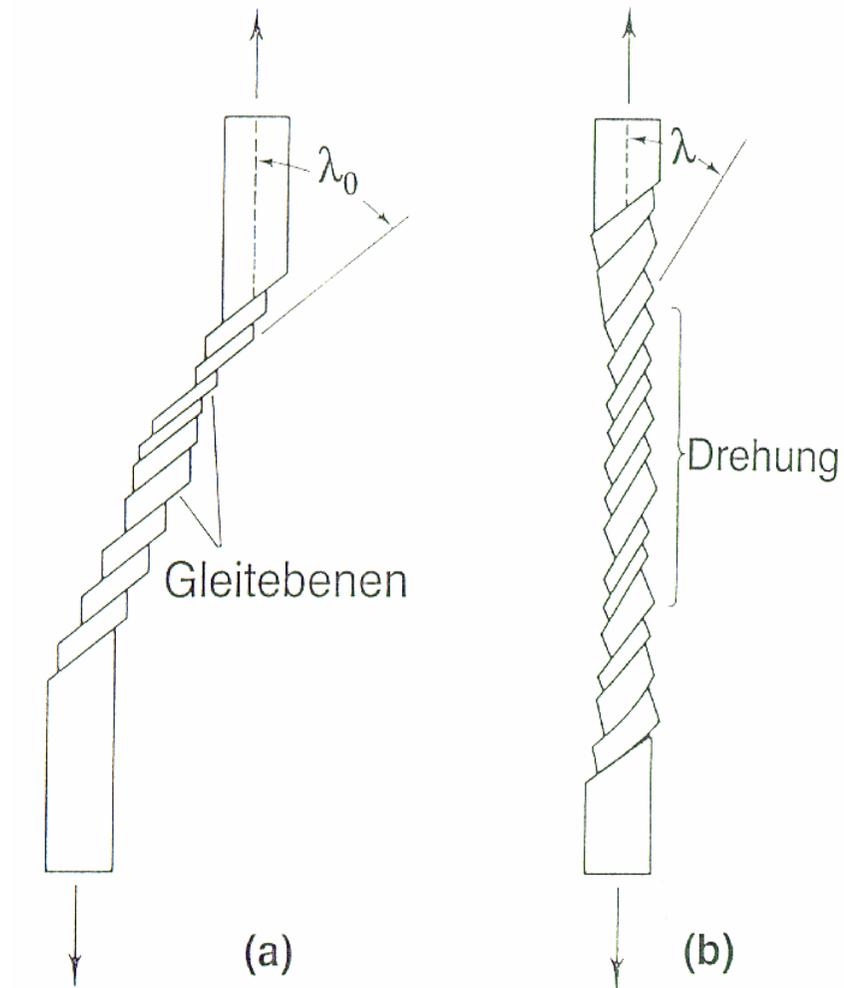
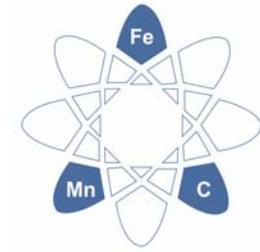


Overview

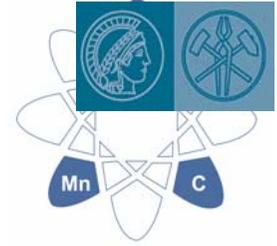


- Anisotropy
- Presentation
- Measurement
- **Textures and Mechanics**
- Examples of Texture Research

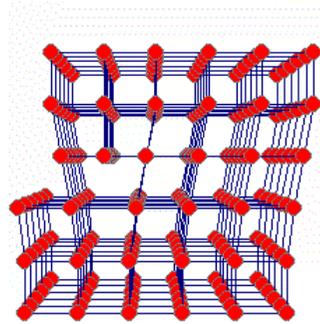
Single crystal plasticity



Single and polycrystal crystal plasticity

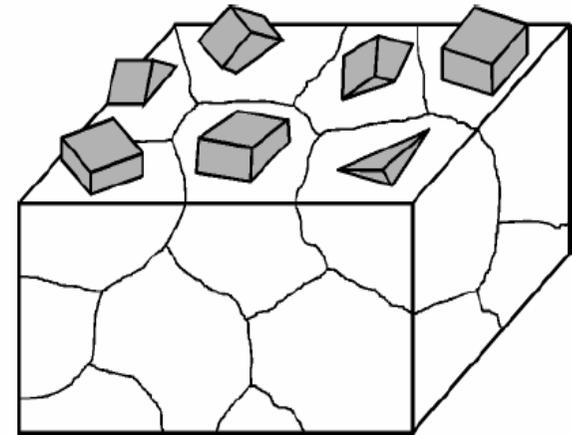


dynamics, kinematics



one dislocation

mesoscopic boundary conditions
(grain / orientation neighborhood)

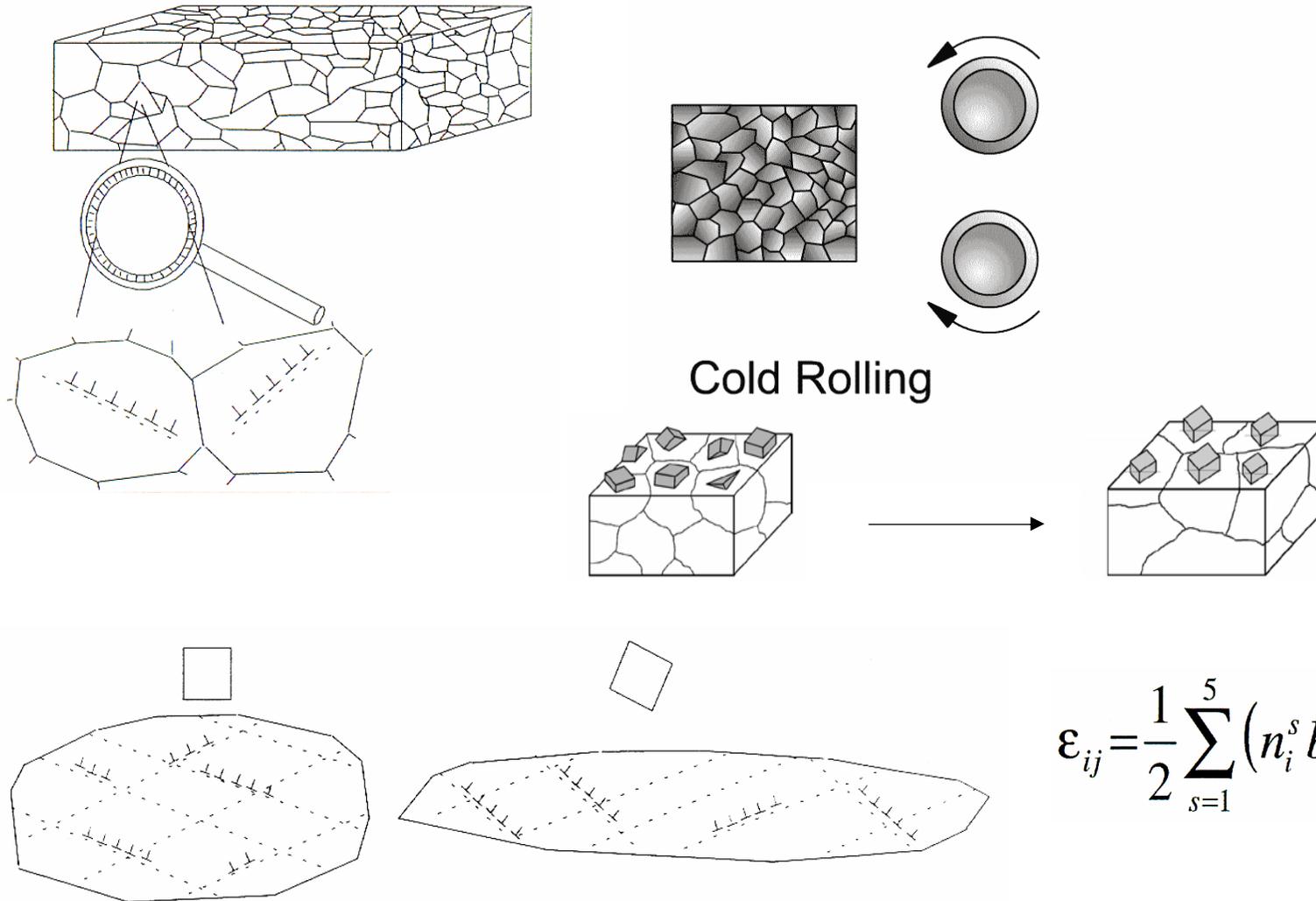
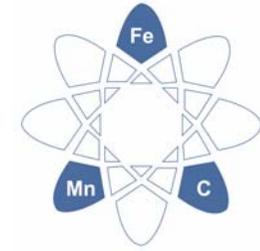


orientation change



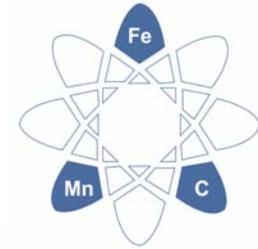
Shear and rotation

Single and polycrystal crystal plasticity



$$\epsilon_{ij} = \frac{1}{2} \sum_{s=1}^5 (n_i^s b_j^s + n_j^s b_i^s) \gamma^s$$

Single and polycrystal crystal plasticity



strain rates and displacement gradients in crystals

$$\dot{\varepsilon}_{ij}^K = D_{ij}^K = \frac{1}{2}(\dot{u}_{i,j}^K + \dot{u}_{j,i}^K) = \sum_{s=1}^N m_{ij}^{\text{sym},s} \dot{\gamma}^s \quad \text{mit} \quad m_{ij}^{\text{sym}} = m_{ji}^{\text{sym}} = \frac{1}{2}(n_i b_j + n_j b_i)$$

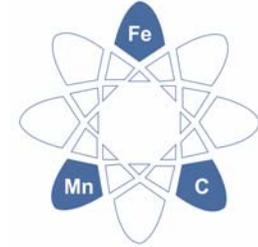
plastic spin from polar decomposition

$$\dot{\omega}_{ij}^K = W_{ij}^K = \frac{1}{2}(\dot{u}_{i,j}^K - \dot{u}_{j,i}^K) = \sum_{s=1}^N m_{ij}^{\text{asym},s} \dot{\gamma}^s \quad \text{mit} \quad m_{ij}^{\text{asym}} = -m_{ji}^{\text{asym}} = \frac{1}{2}(n_i b_j - n_j b_i)$$

example

$$\mathbf{n} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{L} = \frac{\dot{\gamma}}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{D} = \frac{\dot{\gamma}}{2\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad \mathbf{W} = \frac{\dot{\gamma}}{2\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ -1 & -1 & 0 \end{pmatrix}$$

Single and polycrystal crystal plasticity



Gleitsystem s :

$$n_i^s, b_i^s$$

Orientierungsfaktor für s (Gleitsystem \rightarrow Kristall):

$$m_{ij}^s = n_i^s b_j^s$$

symmetrischer Anteil:
$$m_{ij}^{\text{sym},s} = \frac{1}{2} (n_i^s b_j^s + n_j^s b_i^s)$$

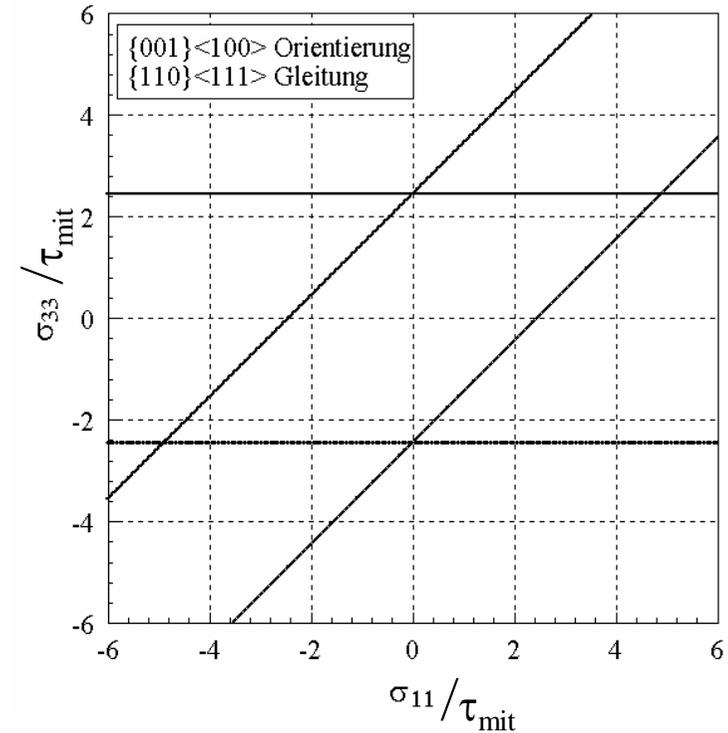
Orientierungsfaktor für s (Kristall \rightarrow Probe): $m_{kl}^s = a_{ki}^c n_i^s a_{lj}^c b_j^s$

symmetrischer Anteil:
$$m_{kl}^{\text{sym},s} = \frac{1}{2} (a_{ki}^c n_i^s a_{lj}^c b_j^s + a_{lj}^c n_j^s a_{ki}^c b_i^s)$$

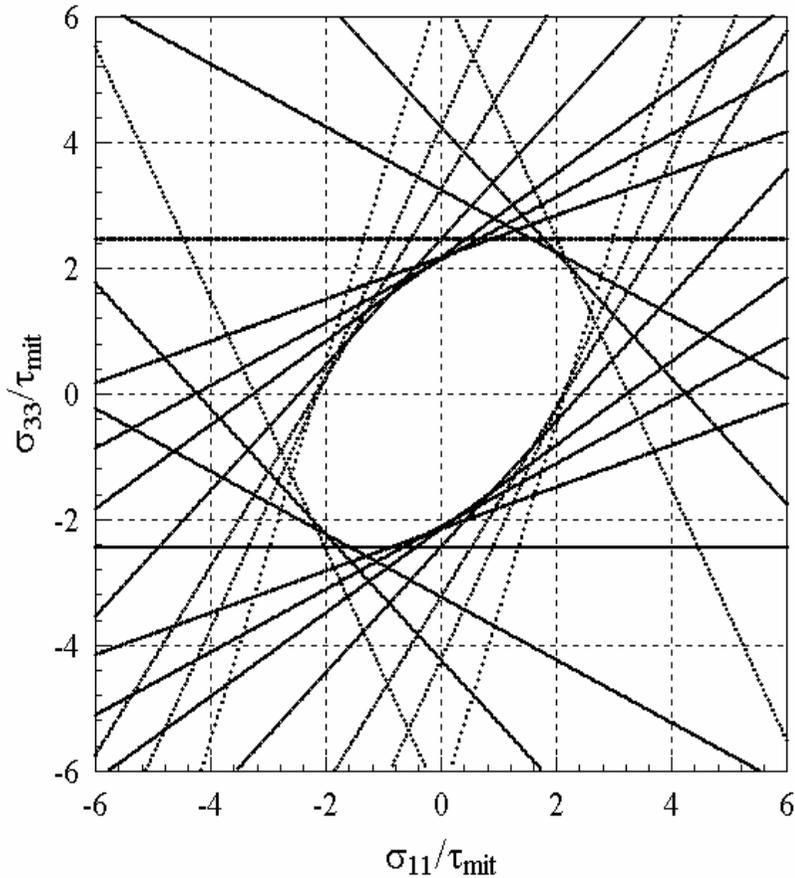
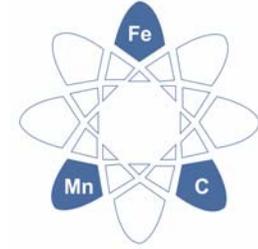
Fließort der aktiven Systeme:
$$m_{kl}^{\text{sym},s=\text{aktiv}} \sigma_{kl} = \sigma_{\text{aufg}}^s = \tau_{\text{krit},(+)}^{s=\text{aktiv}}$$

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

Nicht-aktive Systeme:
$$m_{kl}^{\text{sym},s=\text{inaktiv}} \sigma_{kl} = \sigma_{\text{aufg}}^s < \tau_{\text{krit},(\pm)}^{s=\text{inaktiv}}$$



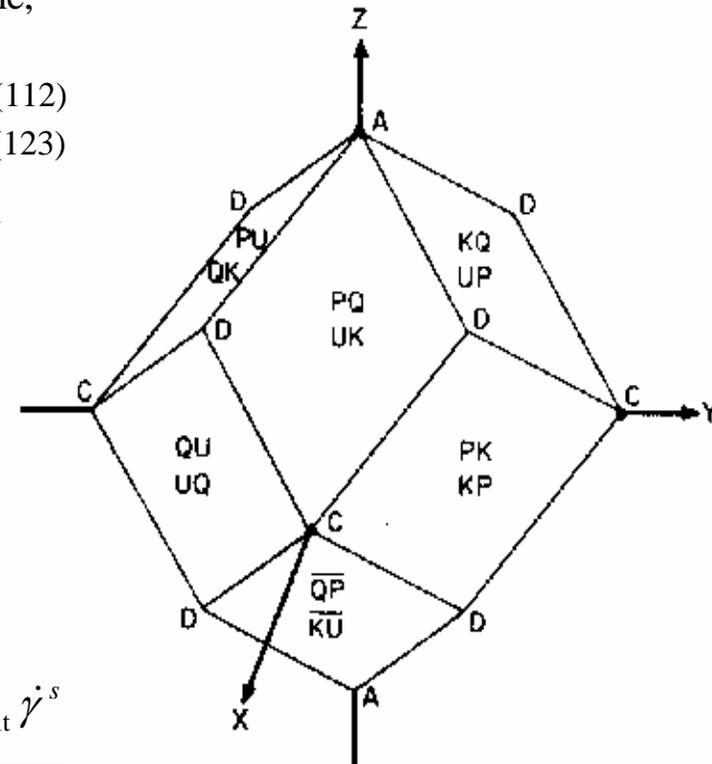
Single and polycrystal crystal plasticity



krz, 48 Systeme,
Schnitt

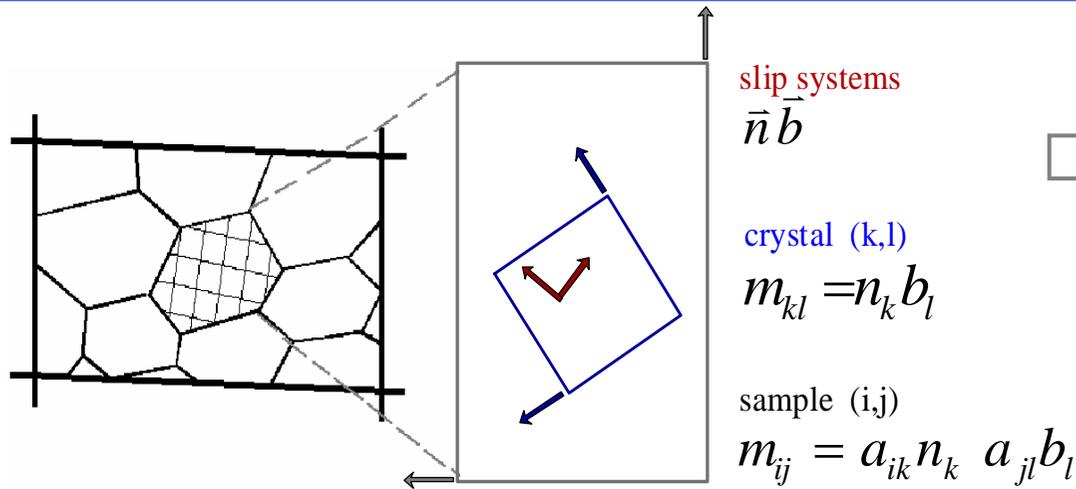
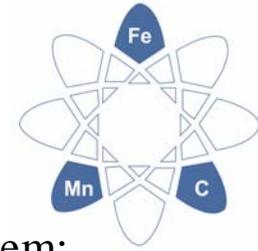
$$\tau_{krit}(110) = \tau_{krit}(112) = \tau_{krit}(123)$$

$$\tau_{mit} = \sum \tau_{krit}(i)/N$$



$$\bar{\tau}_{krit} = \frac{\sum_{s=1}^N \tau_{krit}^s \dot{\gamma}^s}{\dot{\Gamma}}$$

Single and polycrystal crystal plasticity



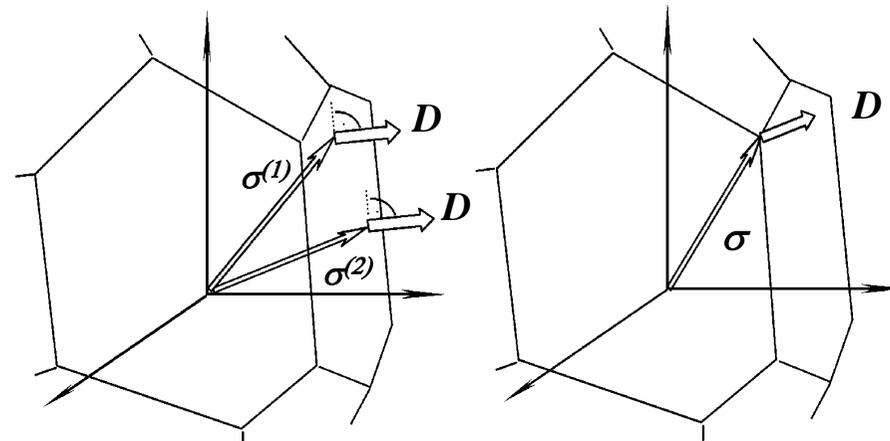
Ein Korn, ein System:

Kinematik

Kinetik

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

Ein Korn, viele Systeme:



Fließort:

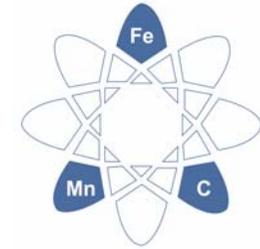
auf FO: elastisches und plastisches Fließen

unterhalb FO: elastisches Fließen

oberhalb FO: existiert nicht

Größe:

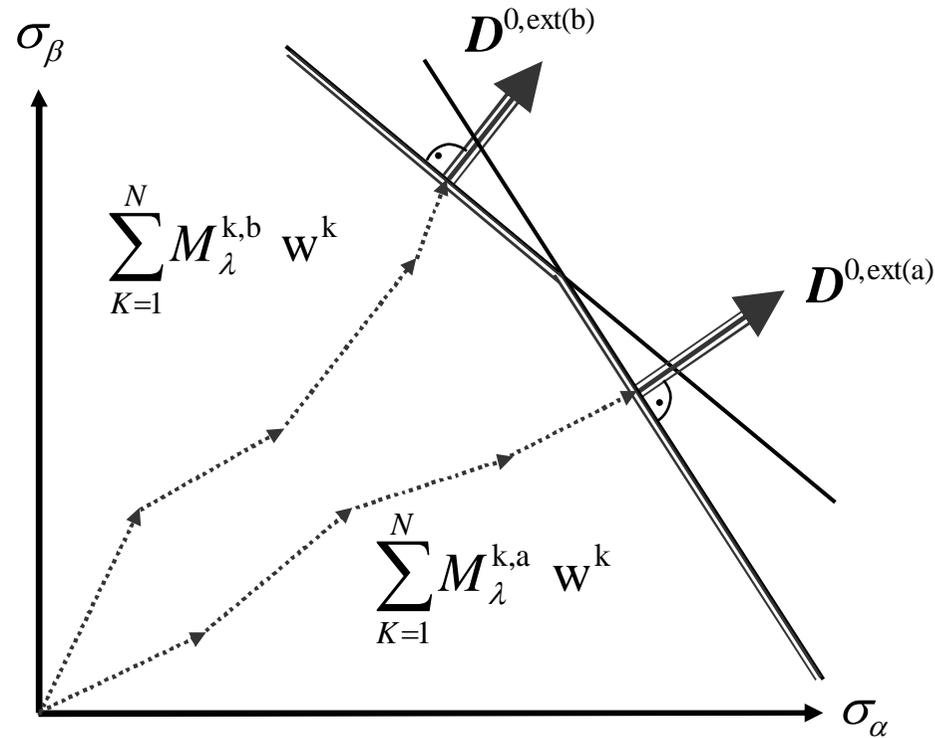
M: 2.1 - 4.5



Single and polycrystal crystal plasticity



Viele Körner, viele Systeme:



$$R_{ij}^P = \frac{1}{V} \int_V \underbrace{M_{ij}^{\text{hom}}(\mathbf{g}, D_{ij})}_{\text{Kinematik}} \underbrace{\tau_{\text{crit}}(s^1, \dots, s^m, S_{ij}^1, \dots, S_{ij}^n, T, D_{ij}^{\text{Kon}}, \mathbf{g})}_{\text{Kinetik}} dV \approx \sum_{k=1}^N M_{ij}^{\text{hom},k} \tau_{\text{crit}}^k w^k$$

Kinematik

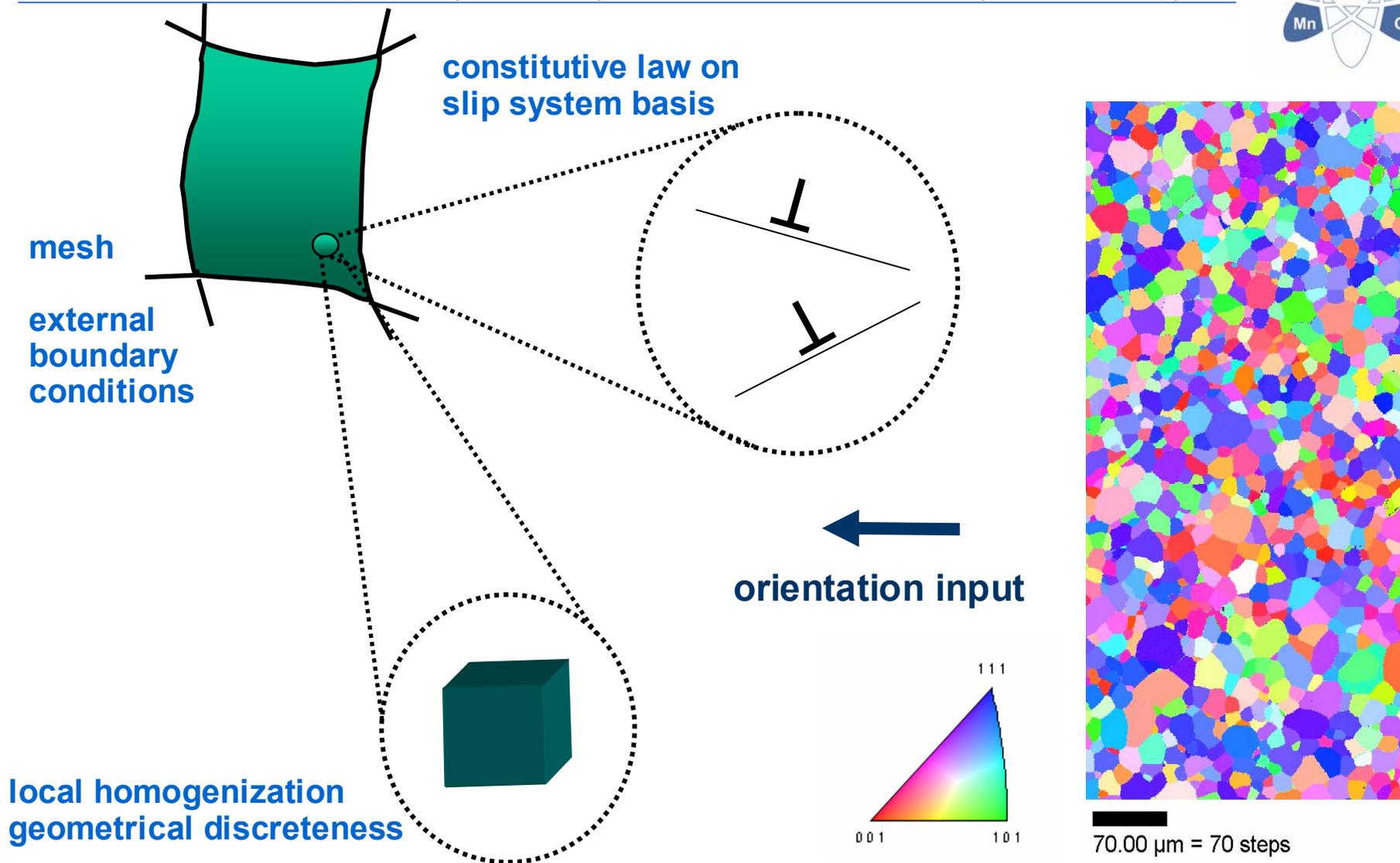
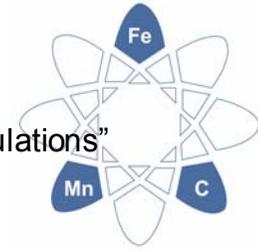
Kinetik



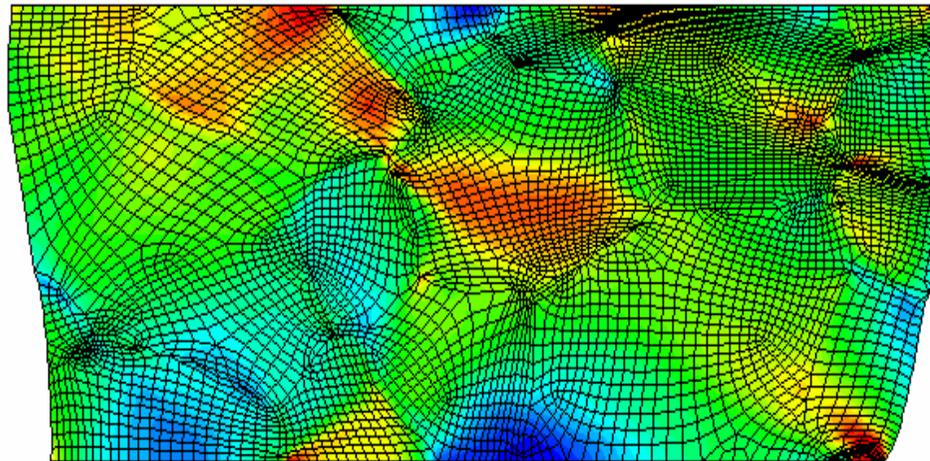
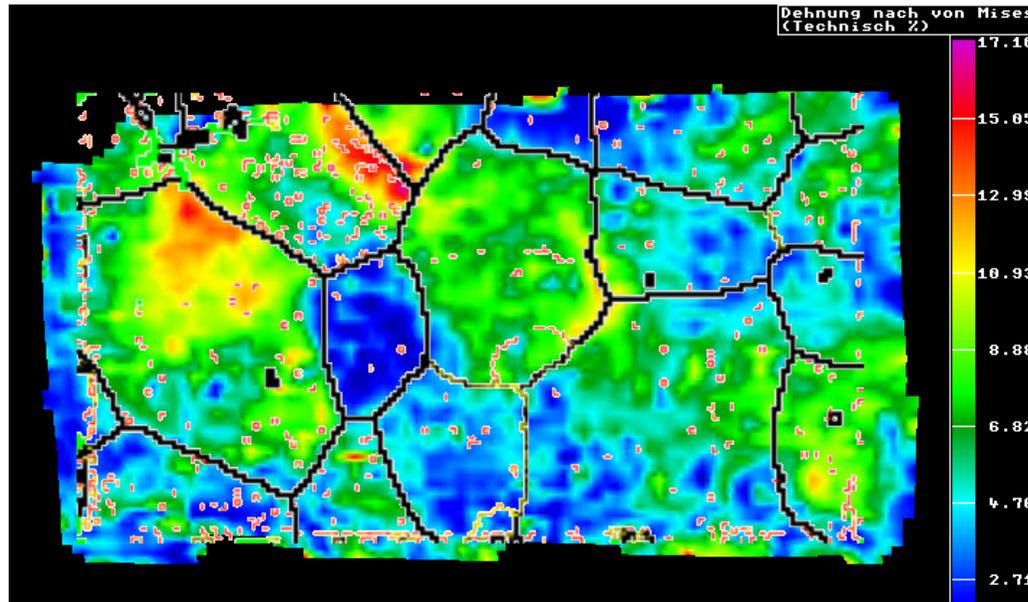
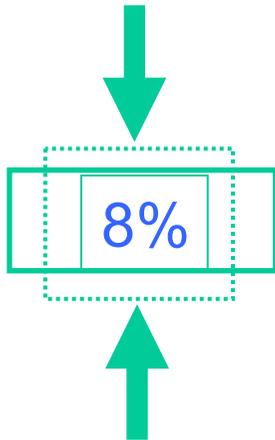
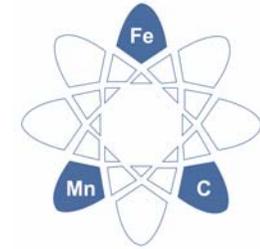
Crystal Mechanics FEM (General)

Z. Zhao, F. Roters, W. Mao, D. Raabe: Adv. Eng. Mater. 3 (2001) p.984/990

„Introduction of A Texture Component Crystal Plasticity Finite Element Method for Industry-Scale Anisotropy Simulations”



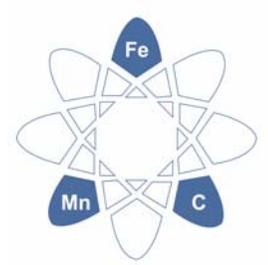
Crystal Mechanics



D. Raabe, M. Sachtleber, Z. Zhao, F. Roters, S. Zaefferer: Acta Materialia 49 (2001) 3433–3441
„Micromechanical and macromechanical effects in grain scale polycrystal plasticity experimentation and simulation”

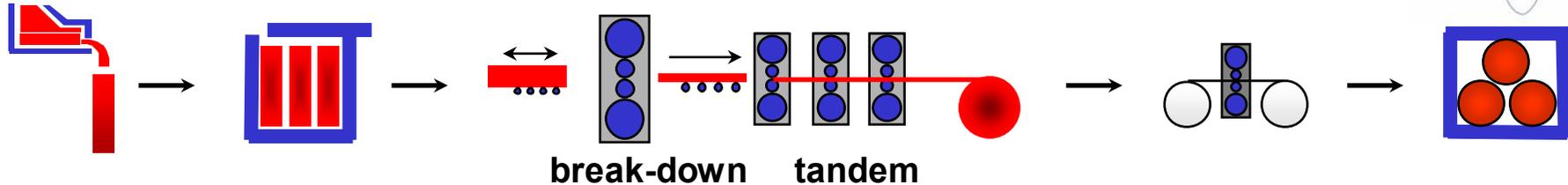
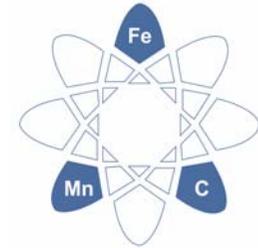
M. Sachtleber, Z. Zhao, D. Raabe: Materials Science and Engineering A 336 (2002) 81–87, “Experimental investigation of plastic grain interaction”

Overview

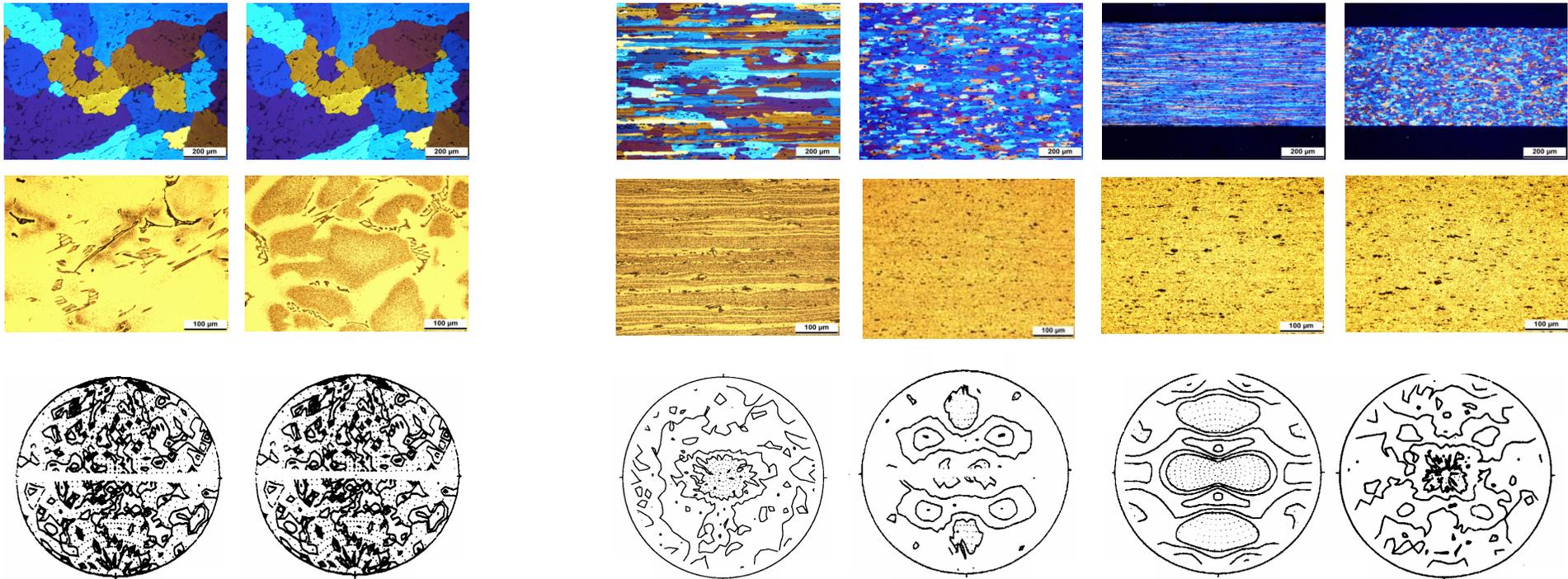


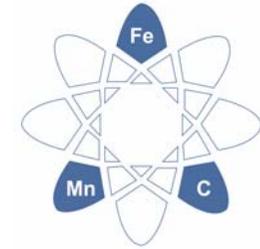
- Anisotropy
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- **Examples of Texture Research**

Texture evolution during processing

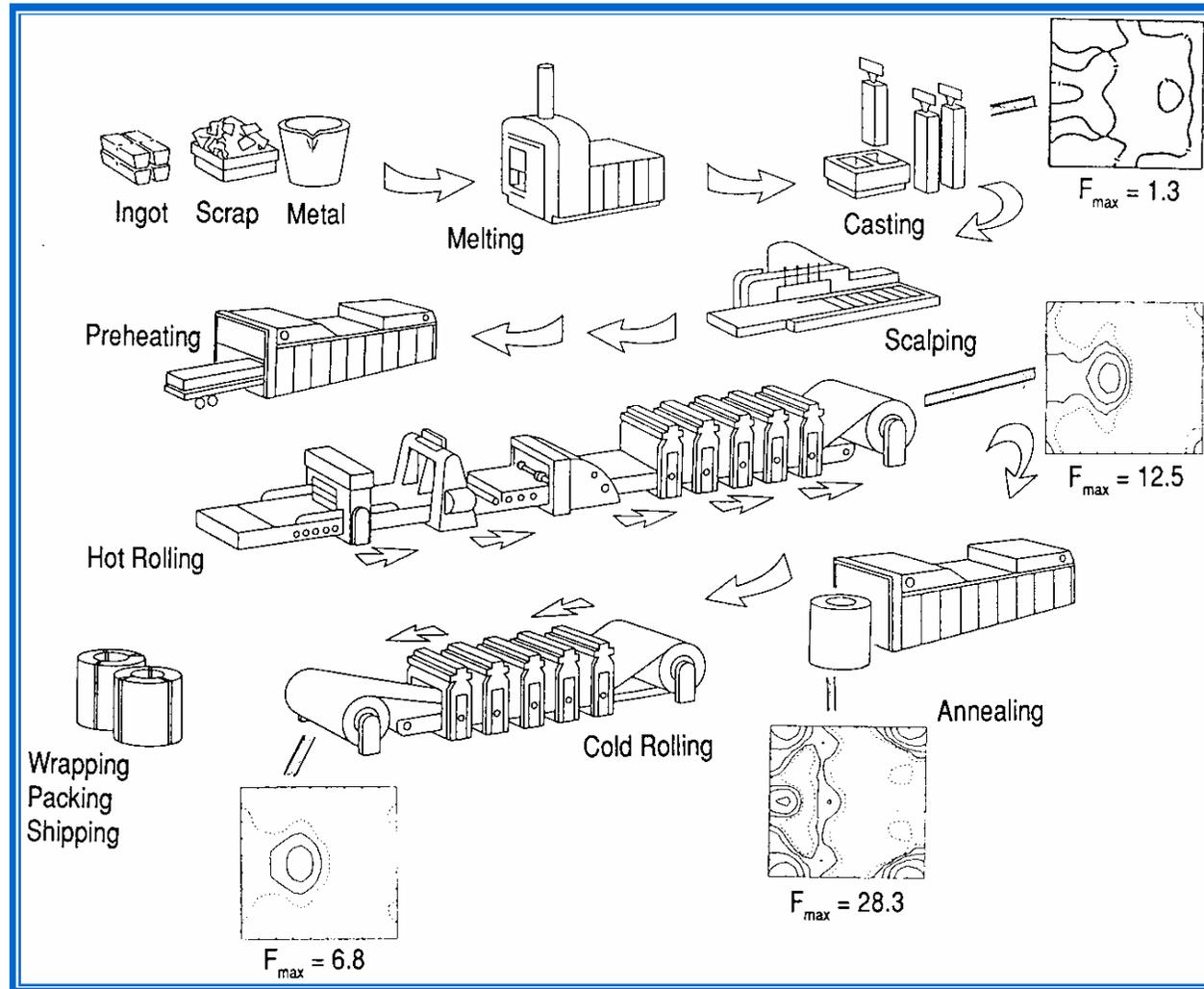


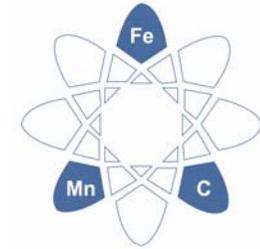
Barrenguß - Homogenisierung - Warmwalzen - Kaltwalzen - Glühen



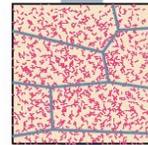
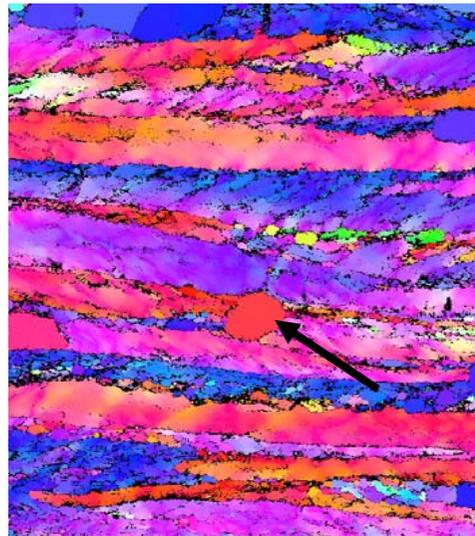


Texture evolution during processing

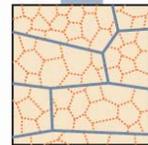




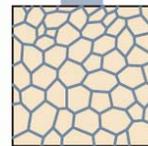
Texture evolution during processing



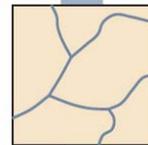
Ausgangslage:
Gefüge von verformtem Material
→ viele **Gitterbaufehler** (Versetzungen)



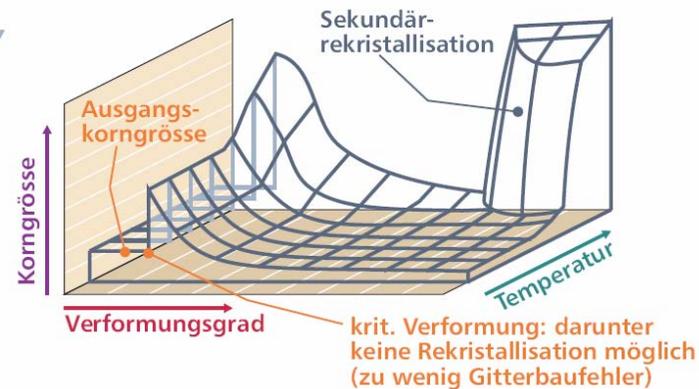
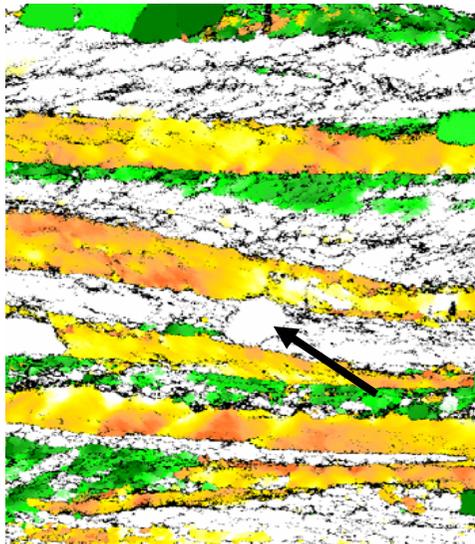
Erholung: teilweiser Abbau von Versetzungen (Bildung von Subkörnern), Korngrenzen bleiben bestehen. Bildung von Keimen für Rekristallisation



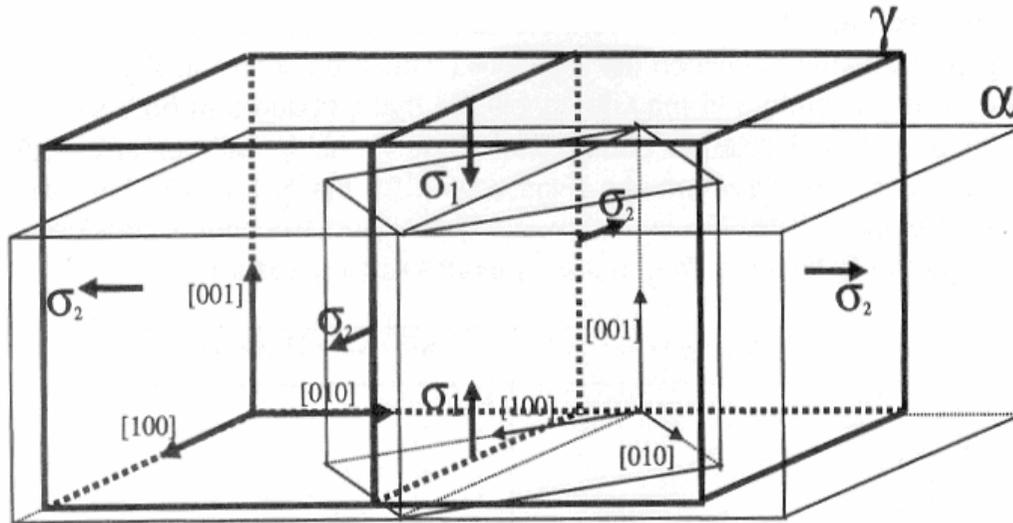
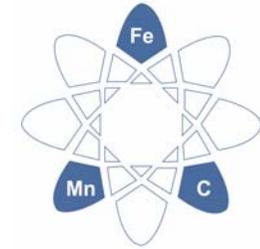
Rekristallisation: an Keimstellen Bildung neuer Körner, die durch das ursprüngliche Gefüge wachsen und dieses ersetzen.



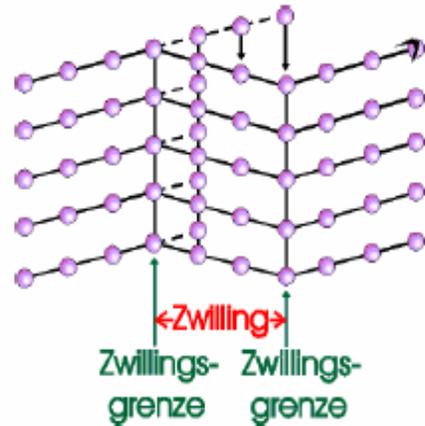
Kornwachstum: in späterer Phase der Rekristallisation Wachstum einzelner Körner, starke Vergrößerung des Gefüges (meist unerwünscht)



Texture evolution during processing

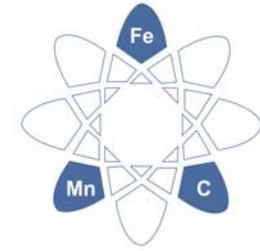


Umwandlung



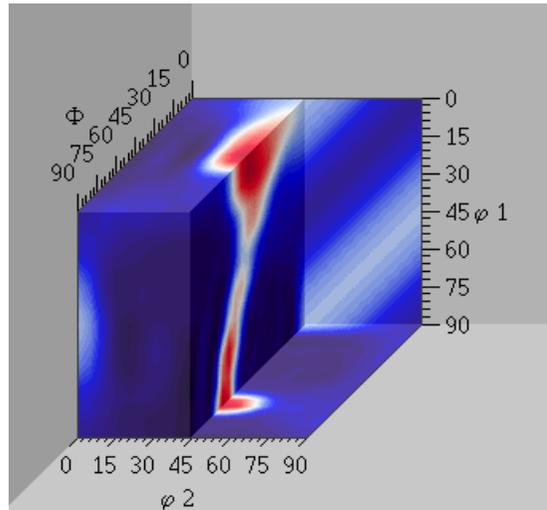
Texture component	Origin
$\{332\}\langle 113\rangle_{\alpha}$	$\{110\}\langle 112\rangle_{\gamma}$, rolled γ texture component (brass component)
$\{113\}\langle 110\rangle_{\alpha}$	$\{112\}\langle 111\rangle_{\gamma}$, rolled γ texture component (copper component)
$\{100\}\langle 011\rangle_{\alpha}$	$\{100\}\langle 001\rangle_{\gamma}$, recrystallised γ texture component (cube component)

Texture evolution during processing

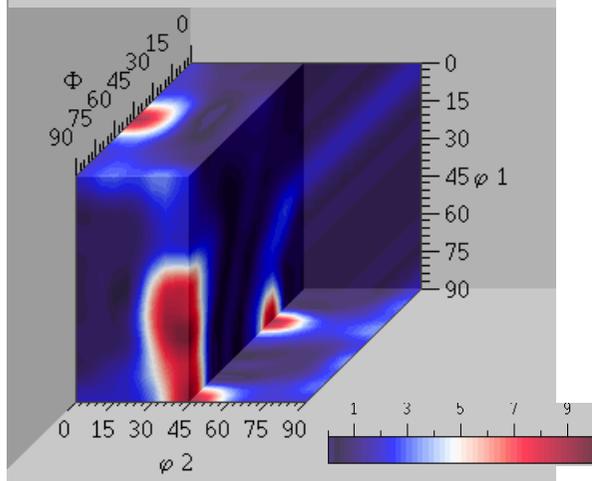


Simulation

Bandmitte

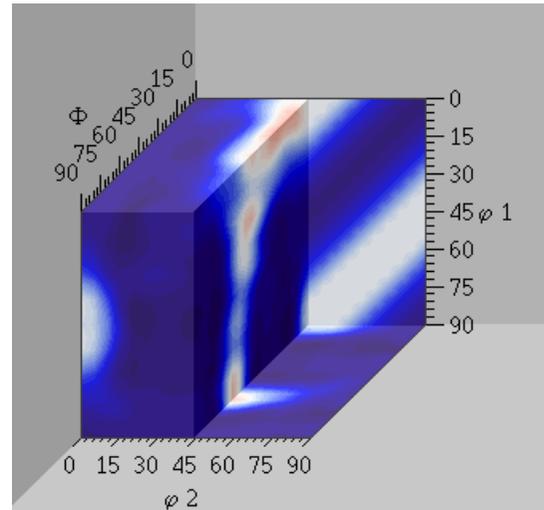


Band-
oberfläche



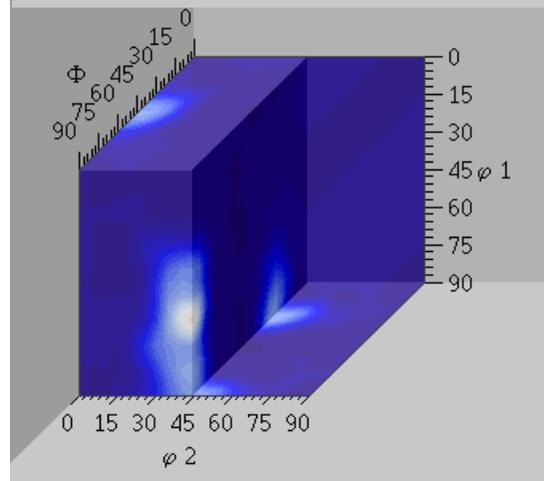
Experiment

Bandmitte

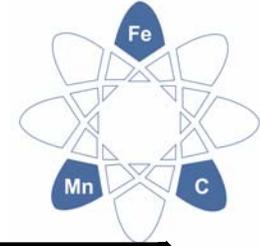


$\Delta d/d_0=40\%$
 $\mu=0.3$

Band-
oberfläche

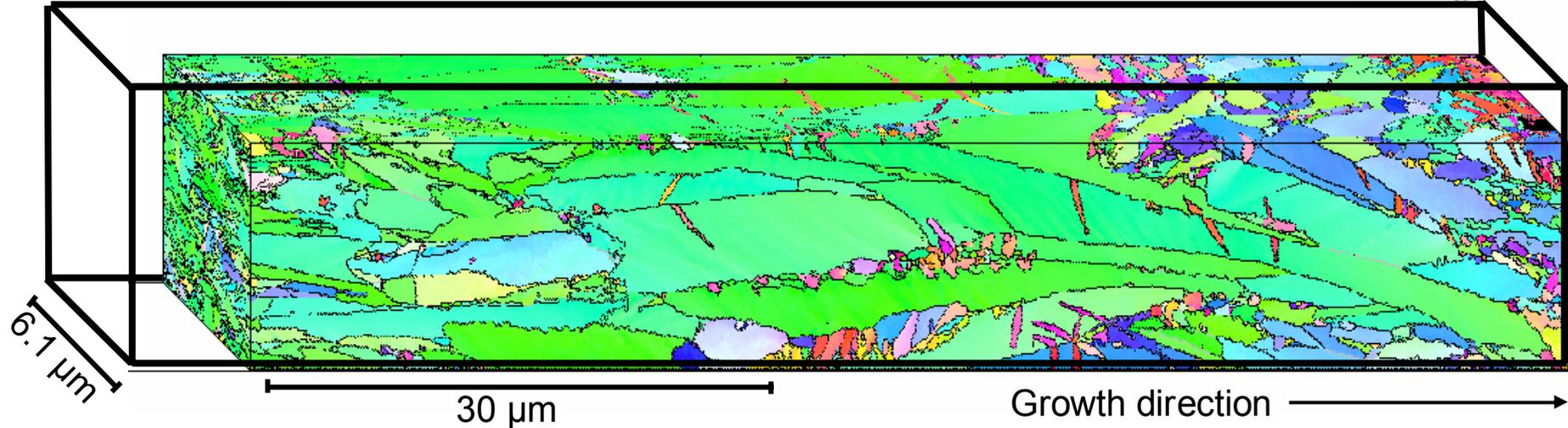


D. Raabe, K. Lücke: Materials Science and Technology 9 (1993) 302–312
„Textures of ferritic stainless steels“

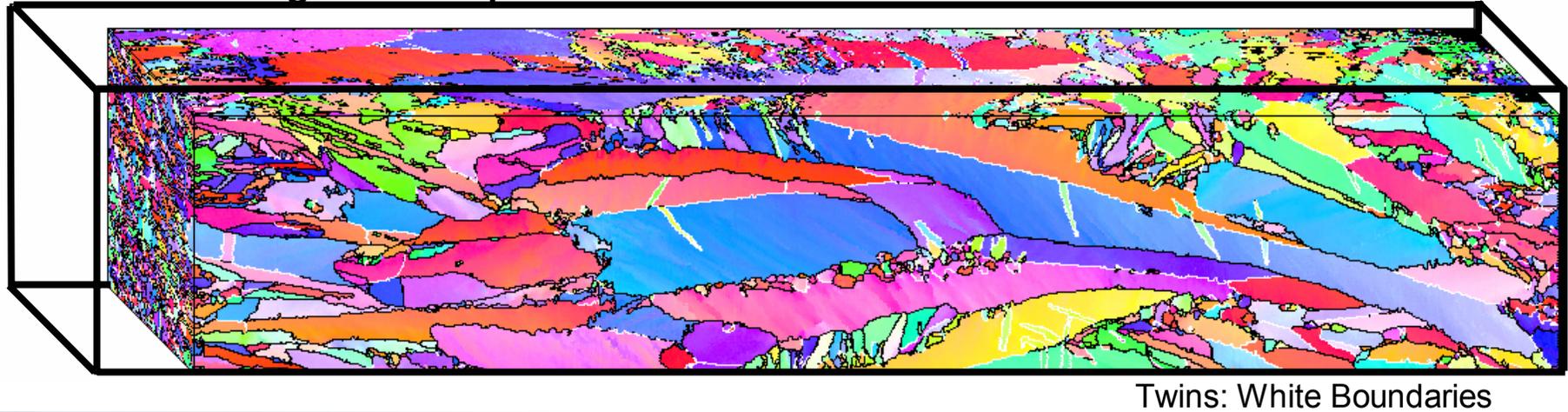


3D texture evolution in nanocrystals

Inverse Pole Figure 3D map – ND direction

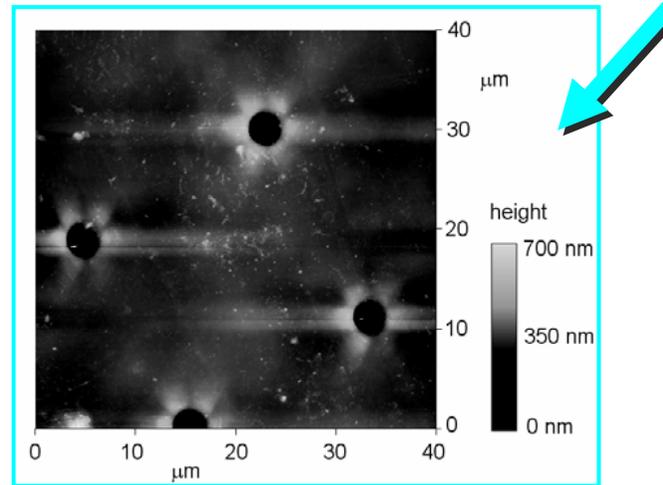
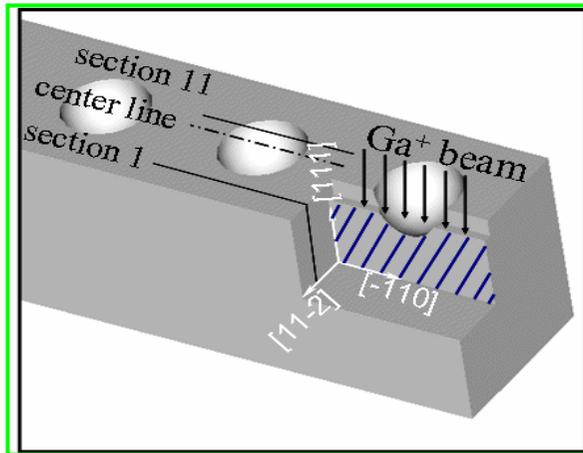
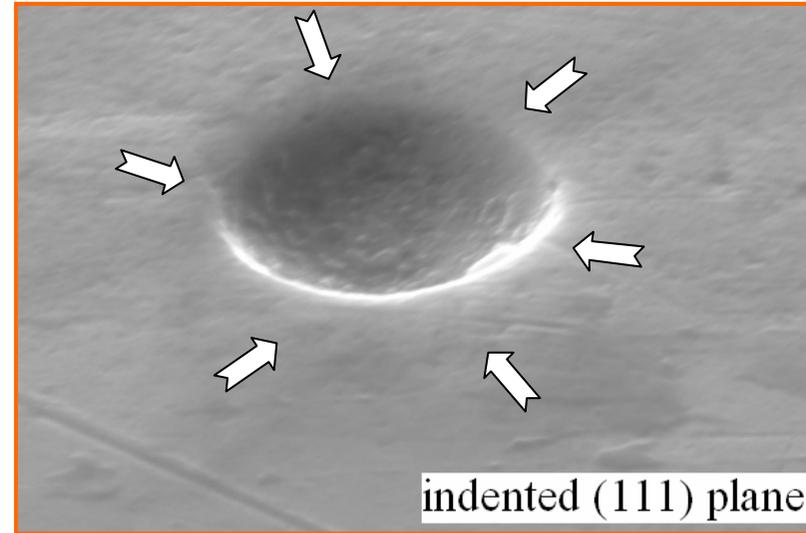
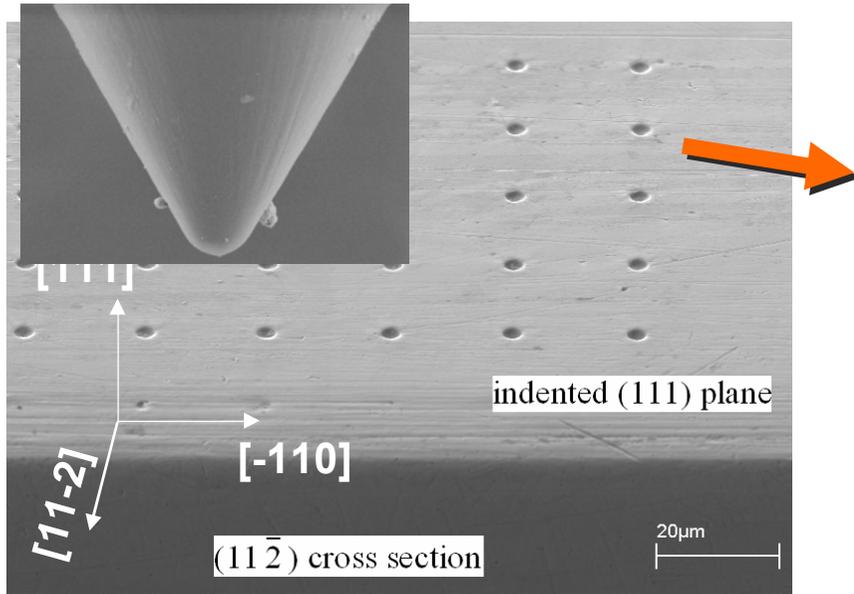
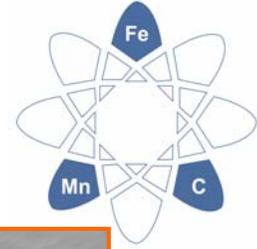


Inverse Pole Figure 3D map – RD direction

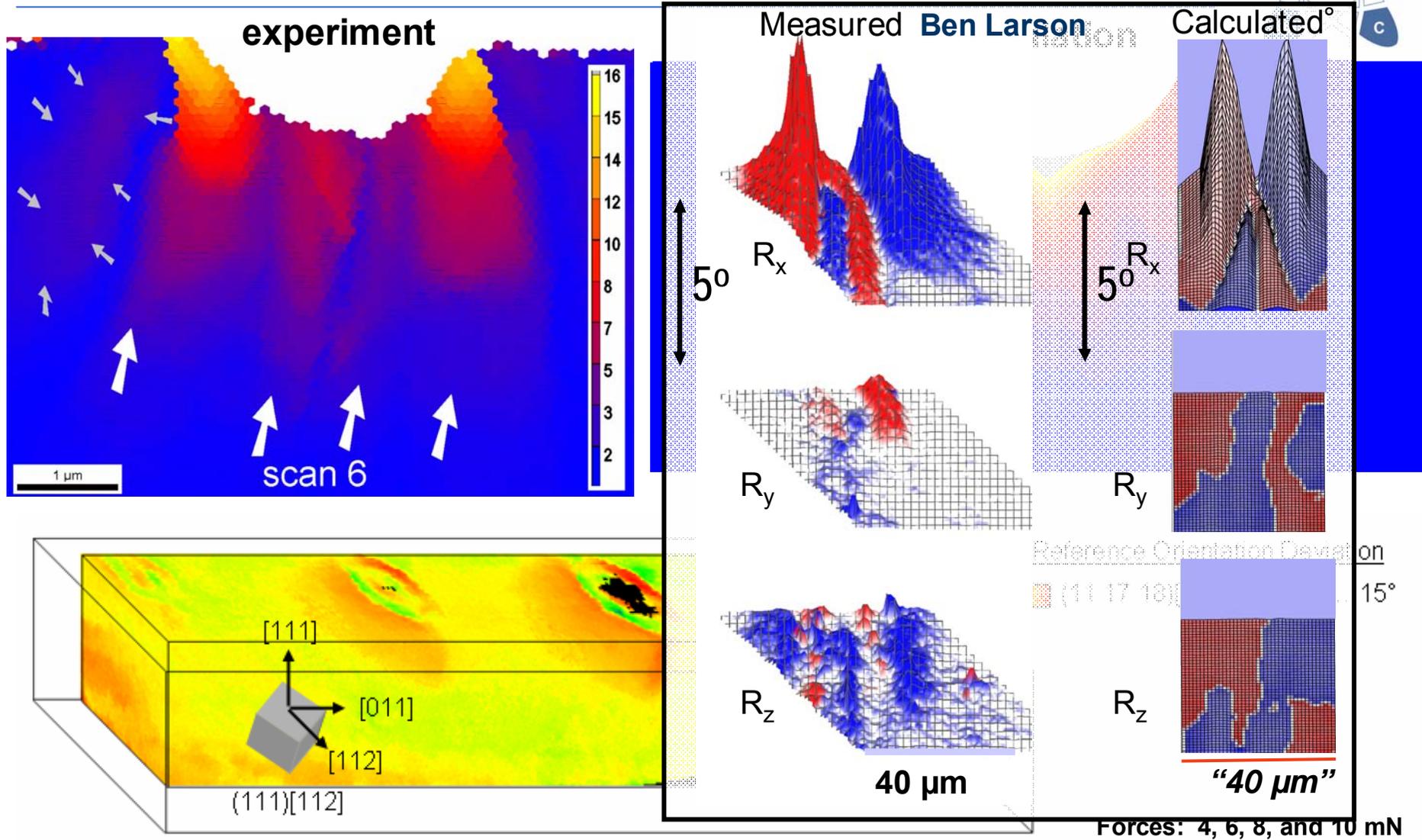
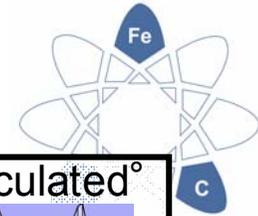


Twins: White Boundaries

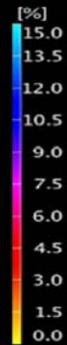
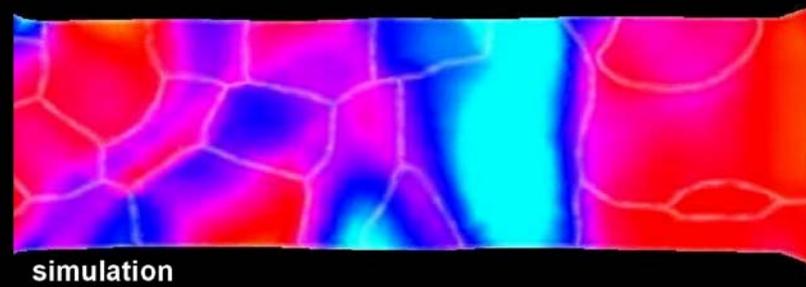
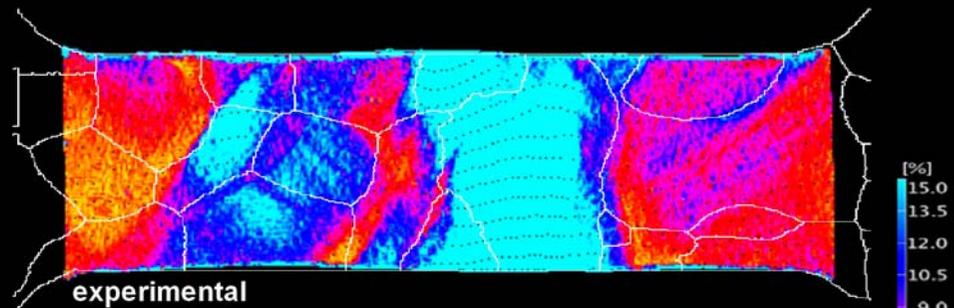
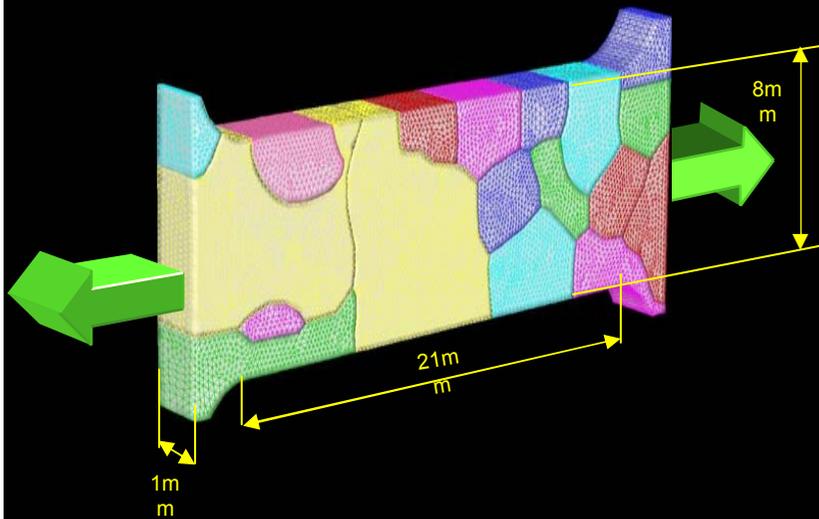
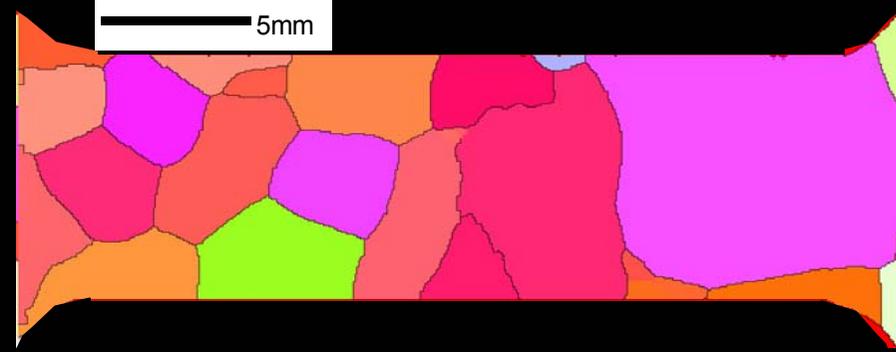
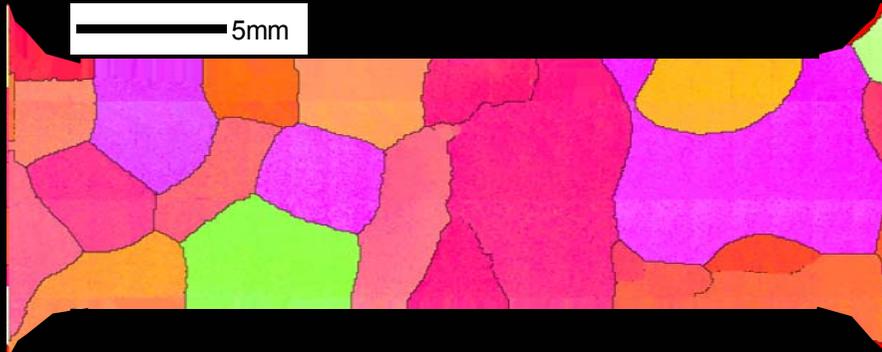
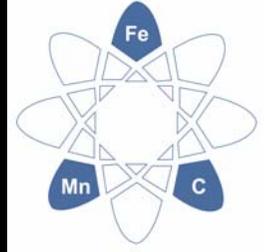
Crystal mechanics FEM, nanoindentation



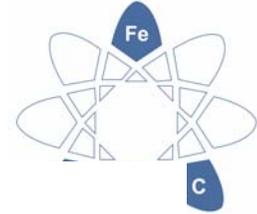
Crystal mechanics, nanoindentation



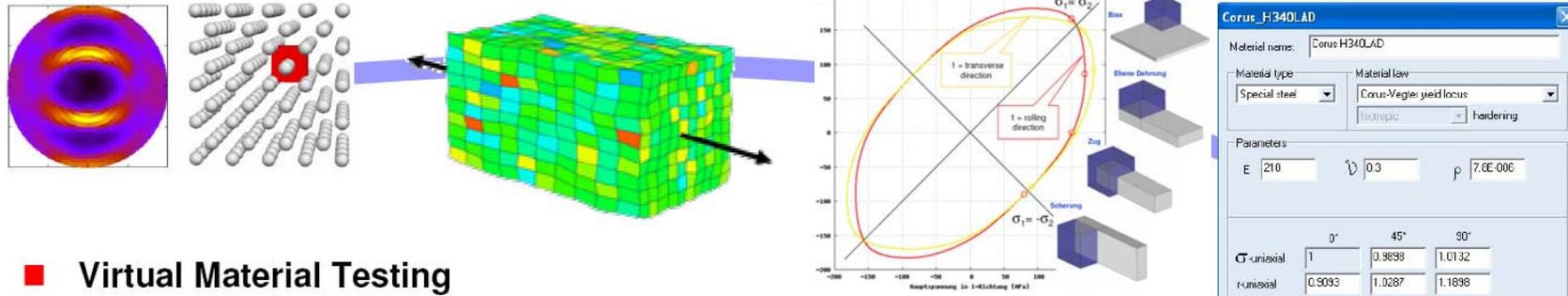
Crystal Mechanics FEM and experiment, 3D



Example: automotive modeling

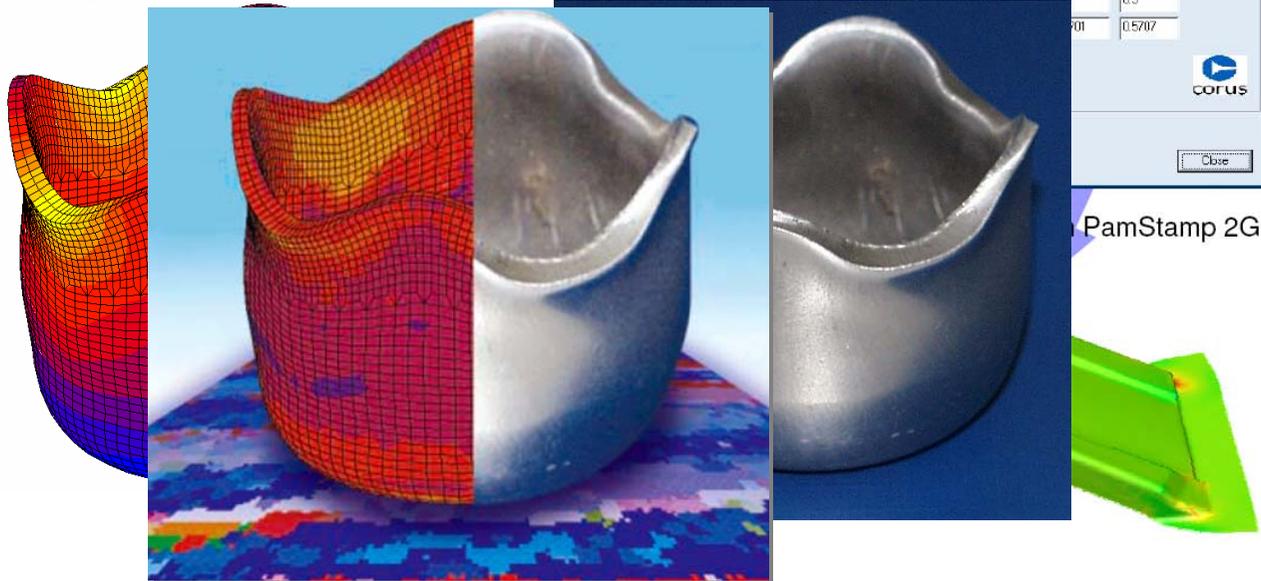


From Crystal Plasticity to Deep Drawing



Virtual Material Testing

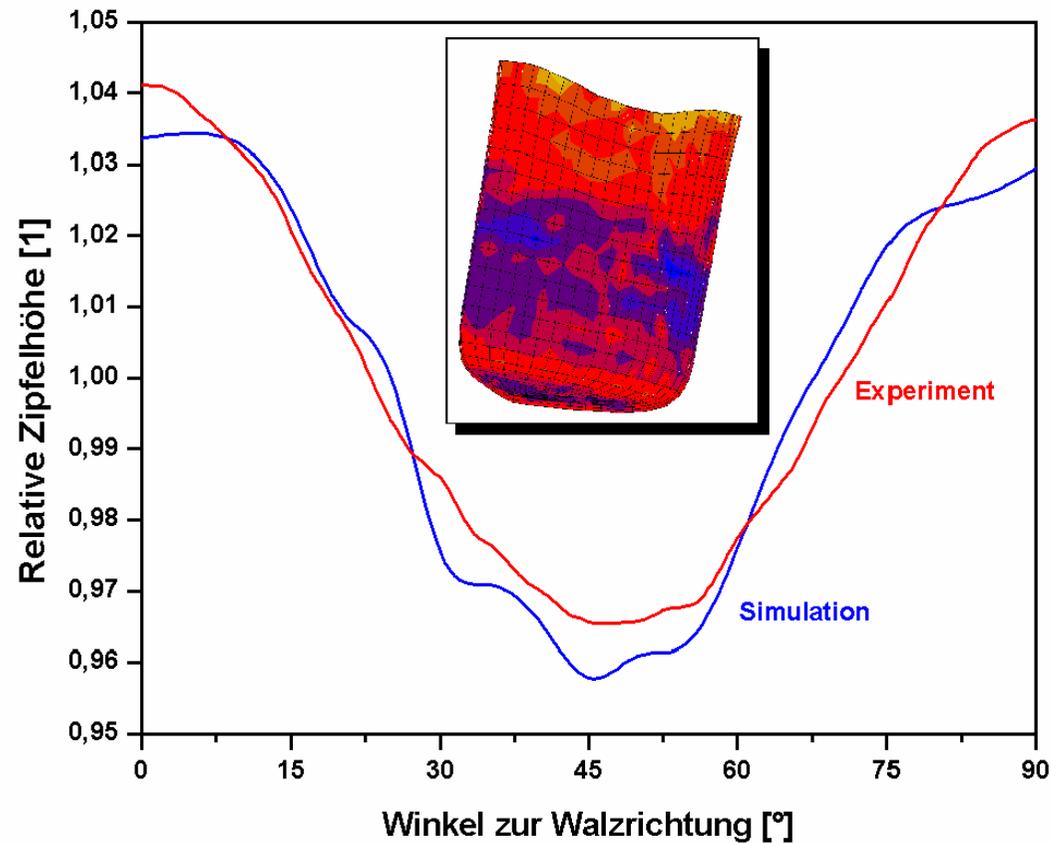
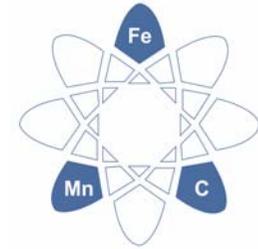
- Representative Volume Element
- Virtual test program
- Parameter fit of the material model
- No performance loss in deep drawing simulation
- Material behaviour from commercial FE code
- Demonstrated by IFA for (bcc) HSLA steel



PamStamp 2G

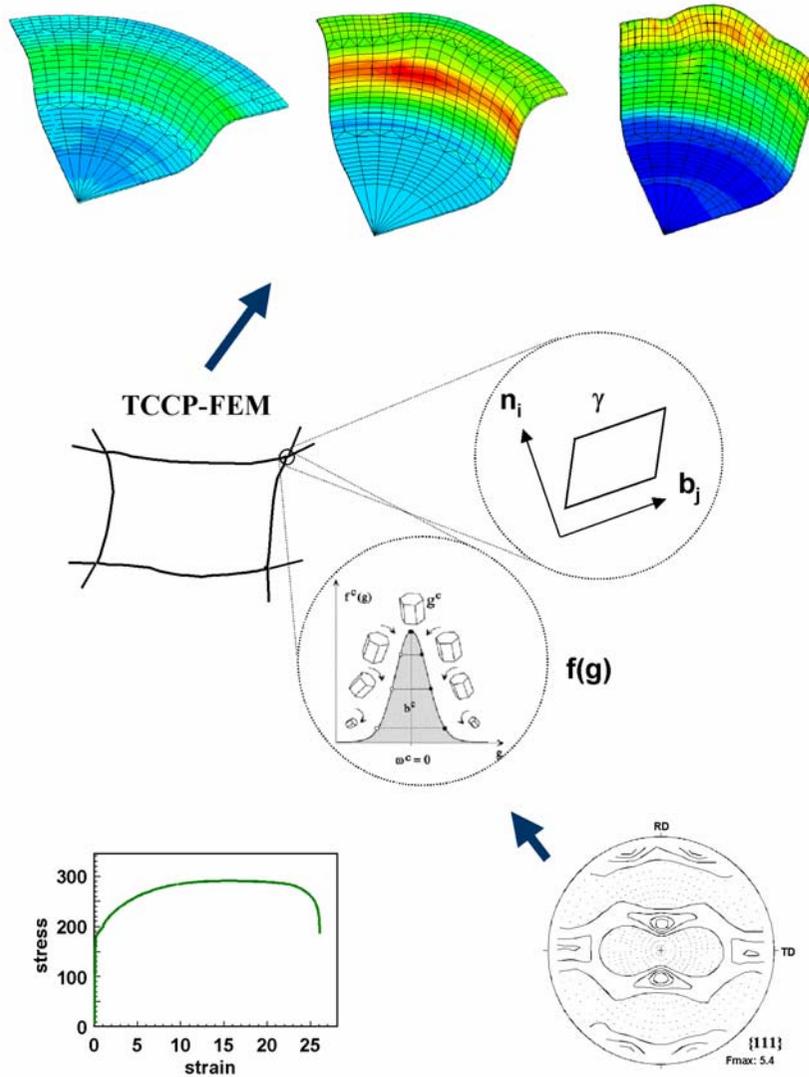
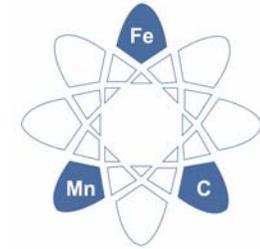


Example: automotive modeling



D. Raabe, P. Klose, B. Engl, K.-P. Imlau, F. Friedel, F. Roters: Advanced Engineering Materials 4 (2002) 169-180 „Concepts for integrating plastic anisotropy into metal forming simulations”

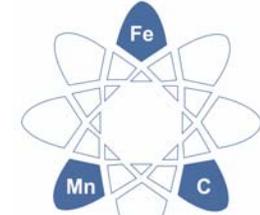
Example: automotive modeling



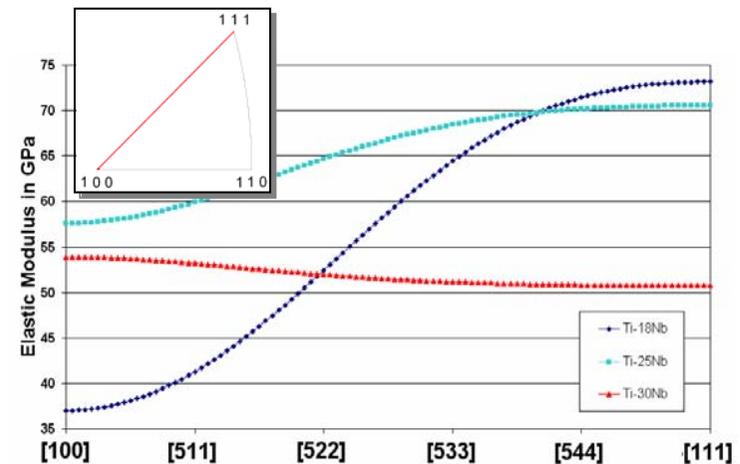
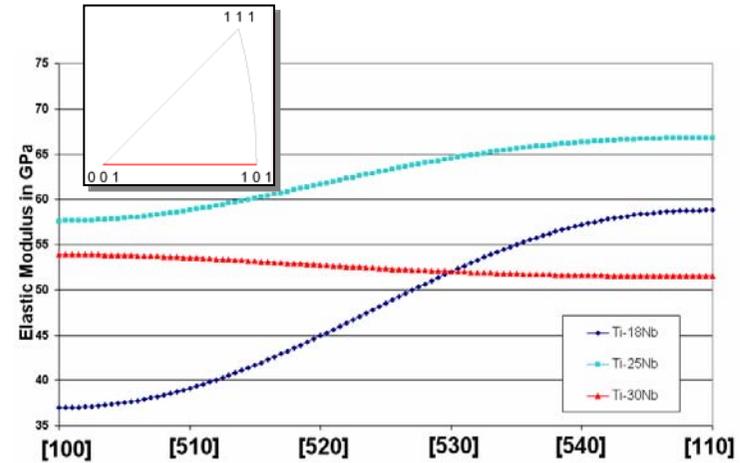
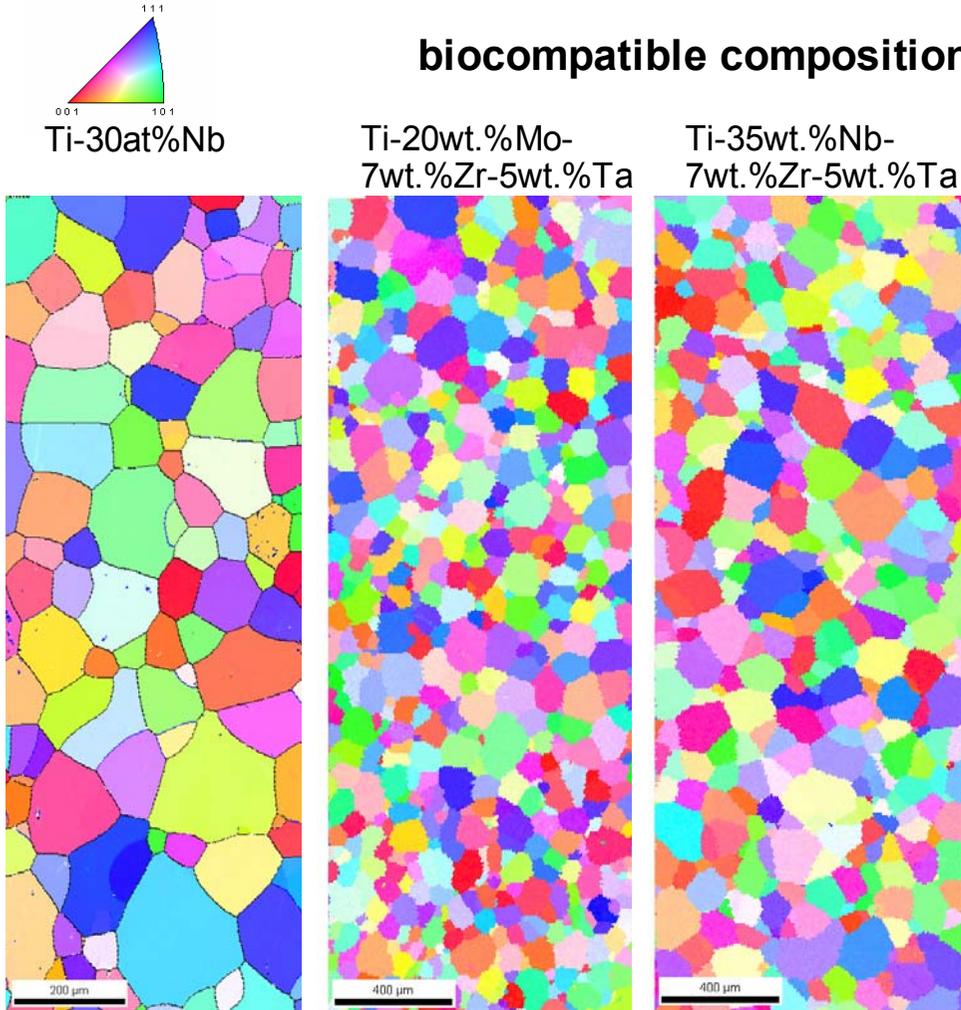
D. Raabe, P. Klose, B. Engl, K.-P. Imlau, F. Friedel, F. Roters: Advanced Engineering Materials 4 (2002) 169-180
 „Concepts for integrating plastic anisotropy into metal forming simulations”

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

Ab initio inspired alloy design

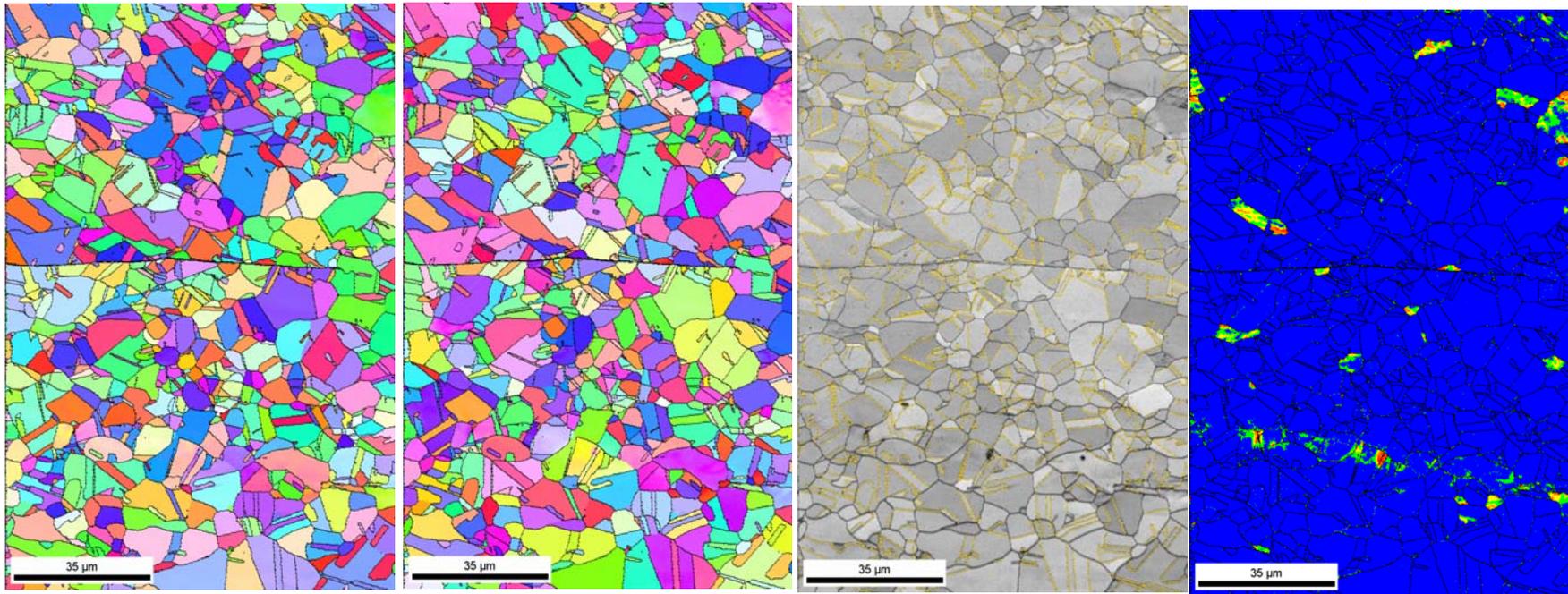
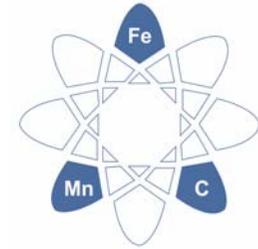


biocompatible composition; low stiffness; isotropy; texture design



D. Raabe, B. Sander, M. Friák, D. Ma, J. Neugebauer
 "Theory-guided bottom-up design of beta-titanium alloys as biomaterials based on first principles calculations: theory and experiments"
 Acta Materialia 55 (2007) 4475–4487

TWIP steel analysis



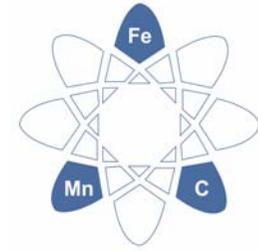
ND

RD

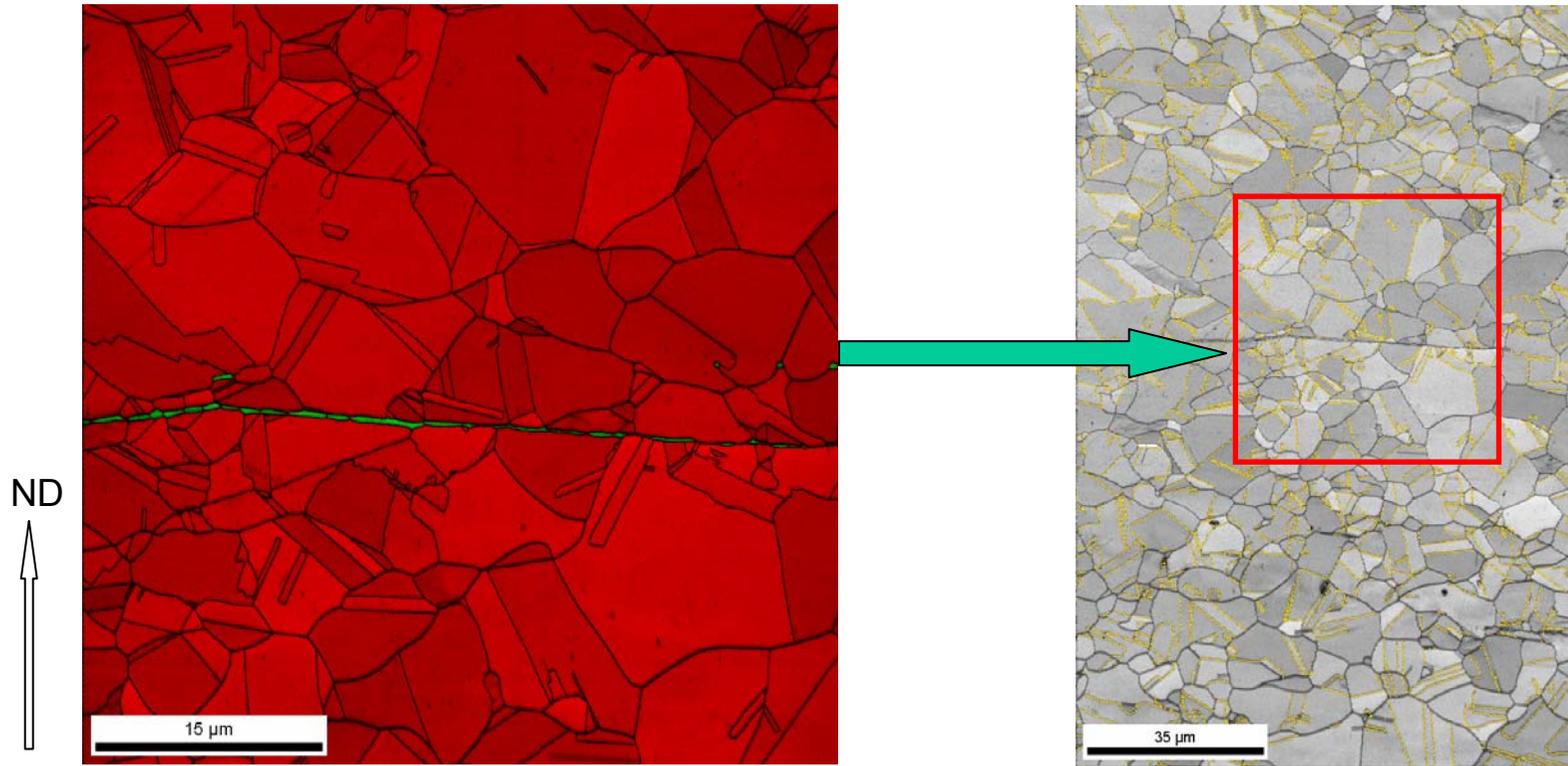
IQ + Sigma3

Kernel Average
Misorientation

TWIP steel analysis

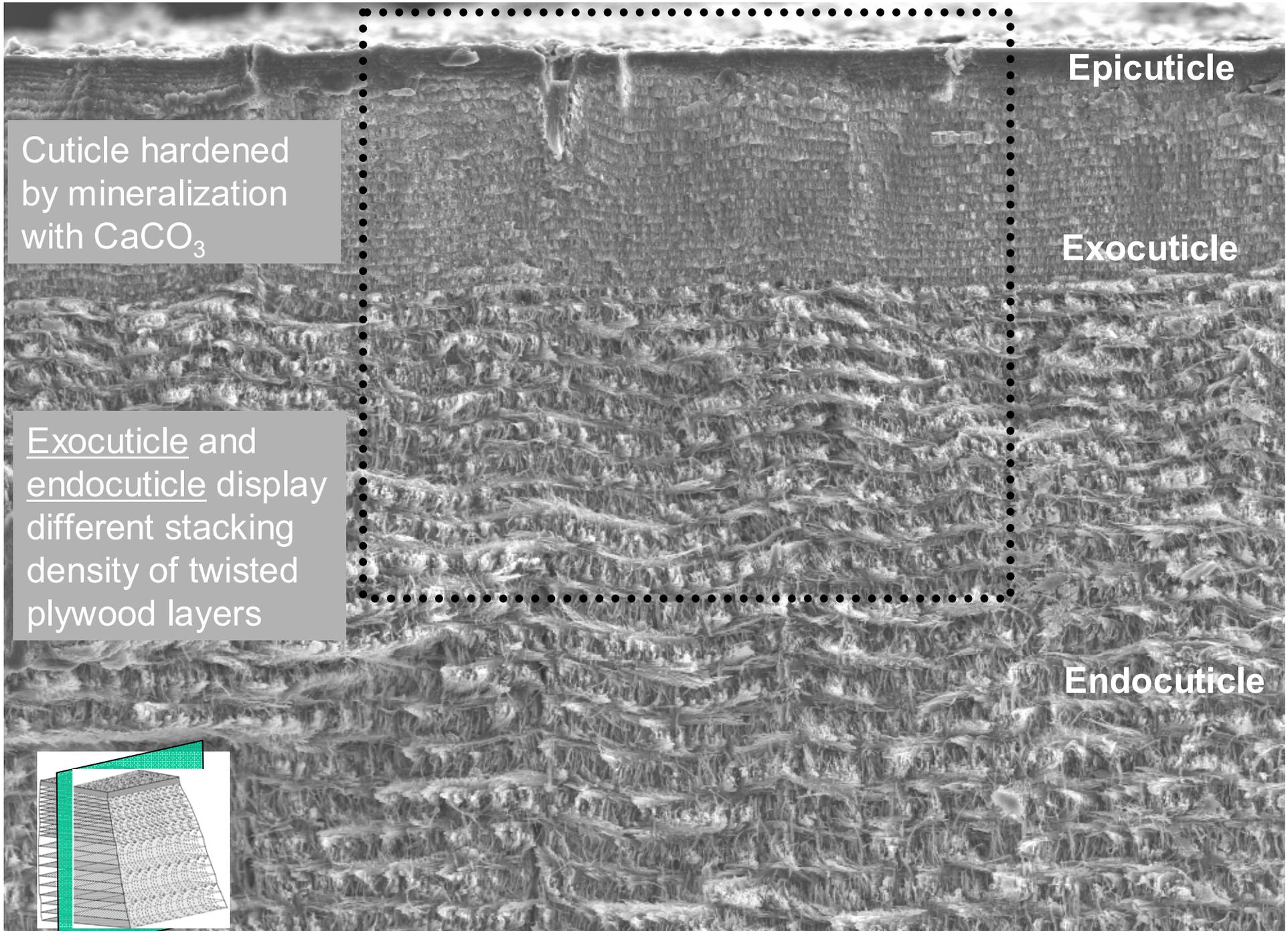


Finescan
(50nm)



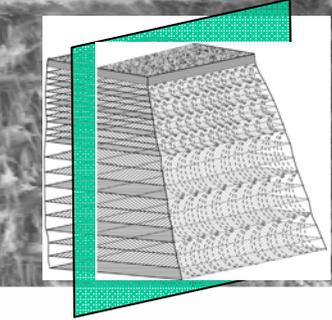
Phase	Total Fraction	Partition Fraction
Iron (Gamma)	0.995	0.995
Iron (Alpha)	0.005	0.005

Boundaries: Rotation Angle				
Min	Max	Fraction	Number	Length
15°	180°	0.968	73580	2.12 mm



Cuticle hardened by mineralization with CaCO_3

Exocuticle and endocuticle display different stacking density of twisted plywood layers

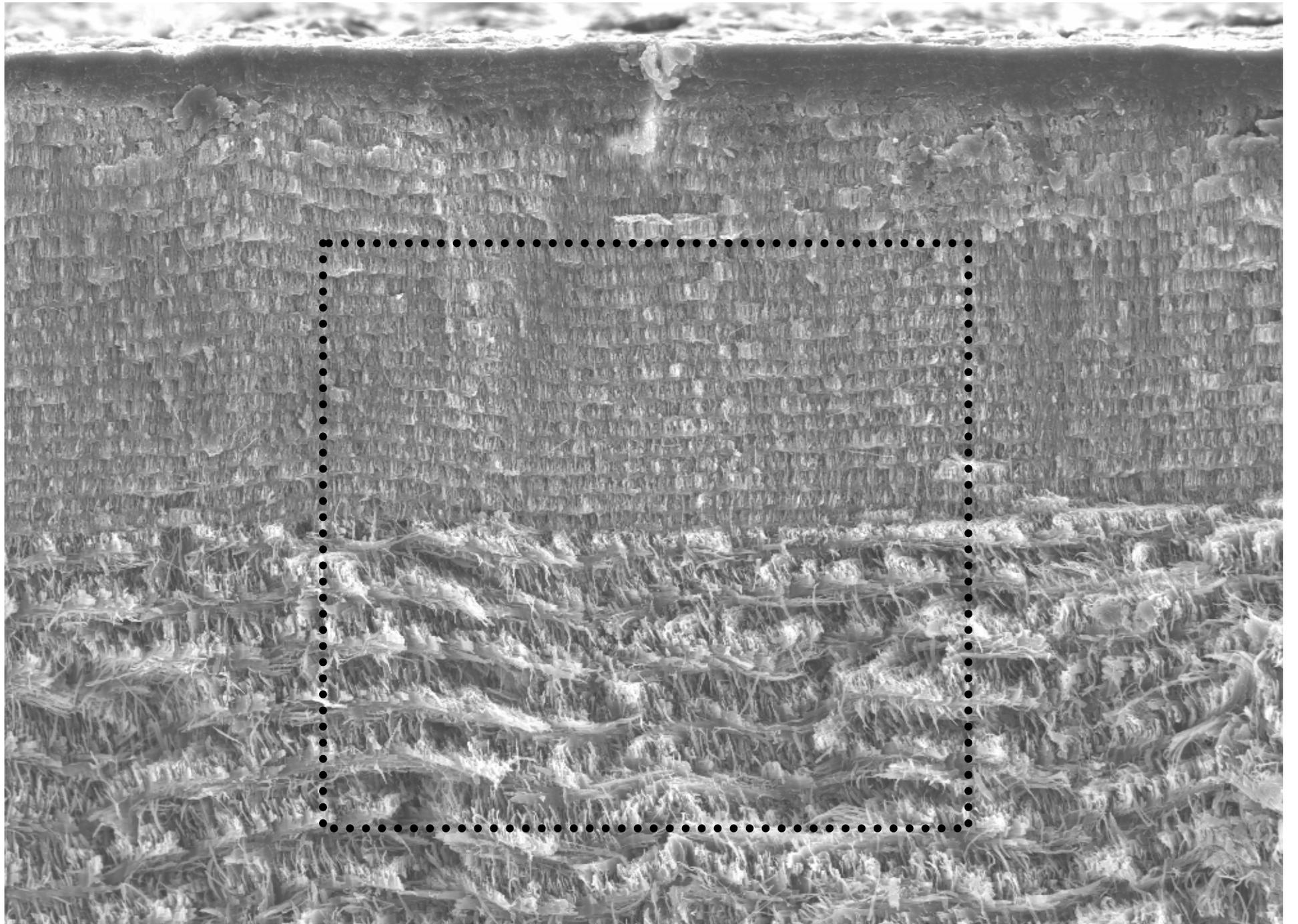


Epicuticle

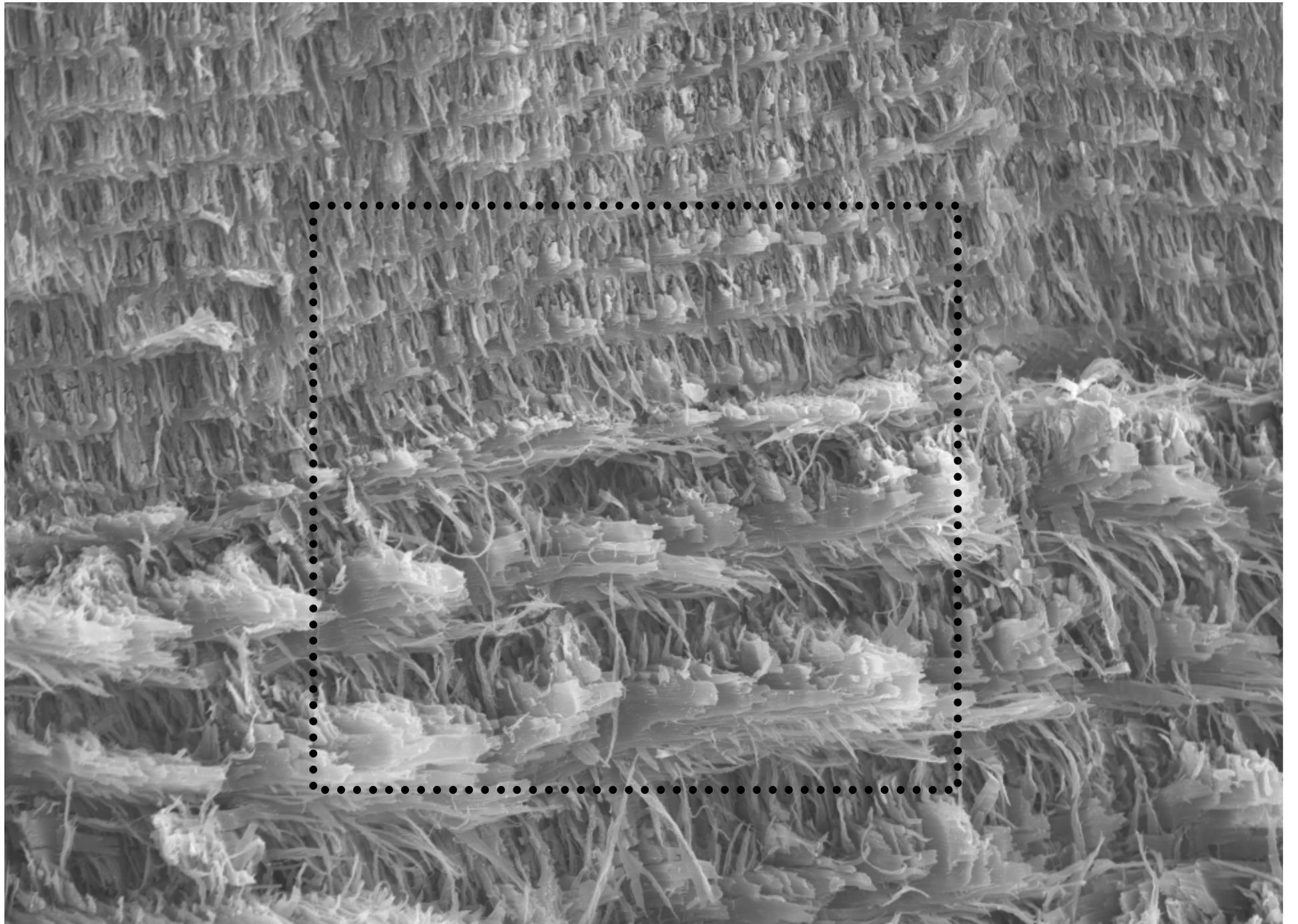
Exocuticle

Endocuticle

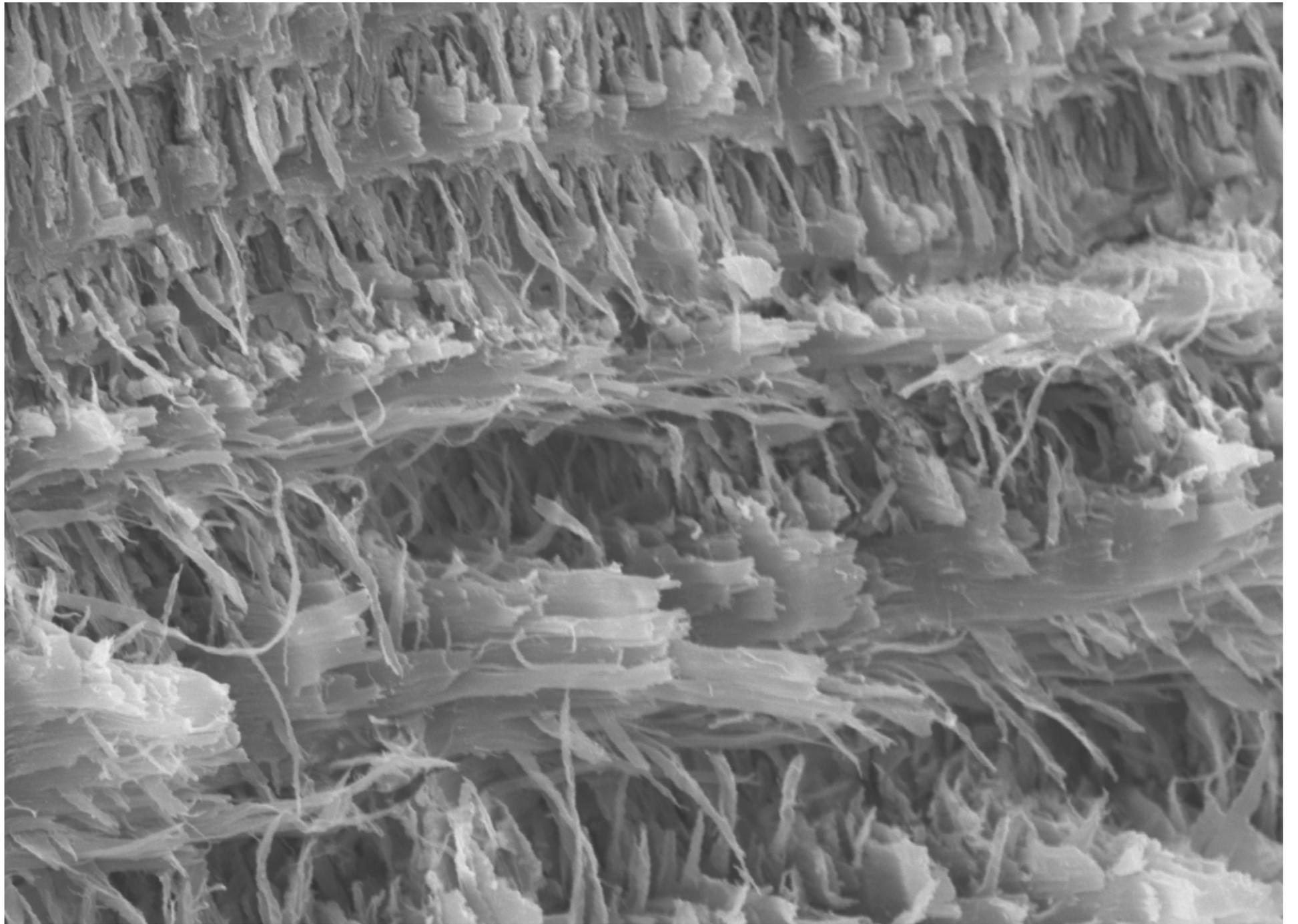
— 200 μm —



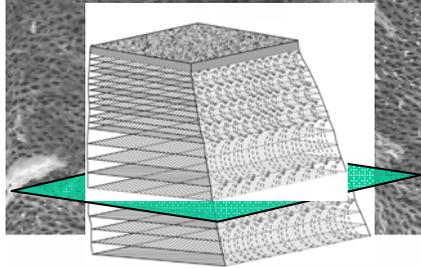
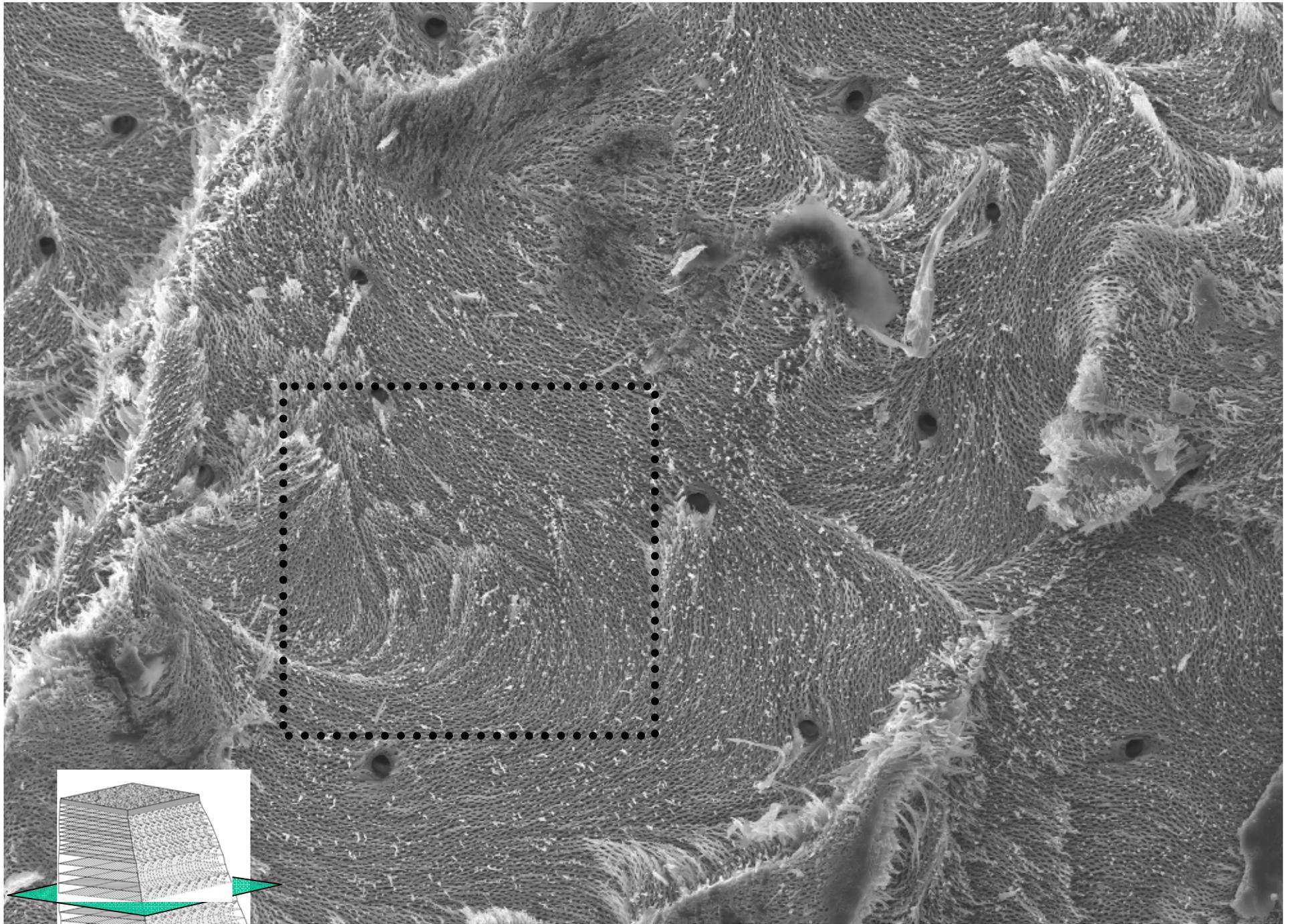
— 100 μm —



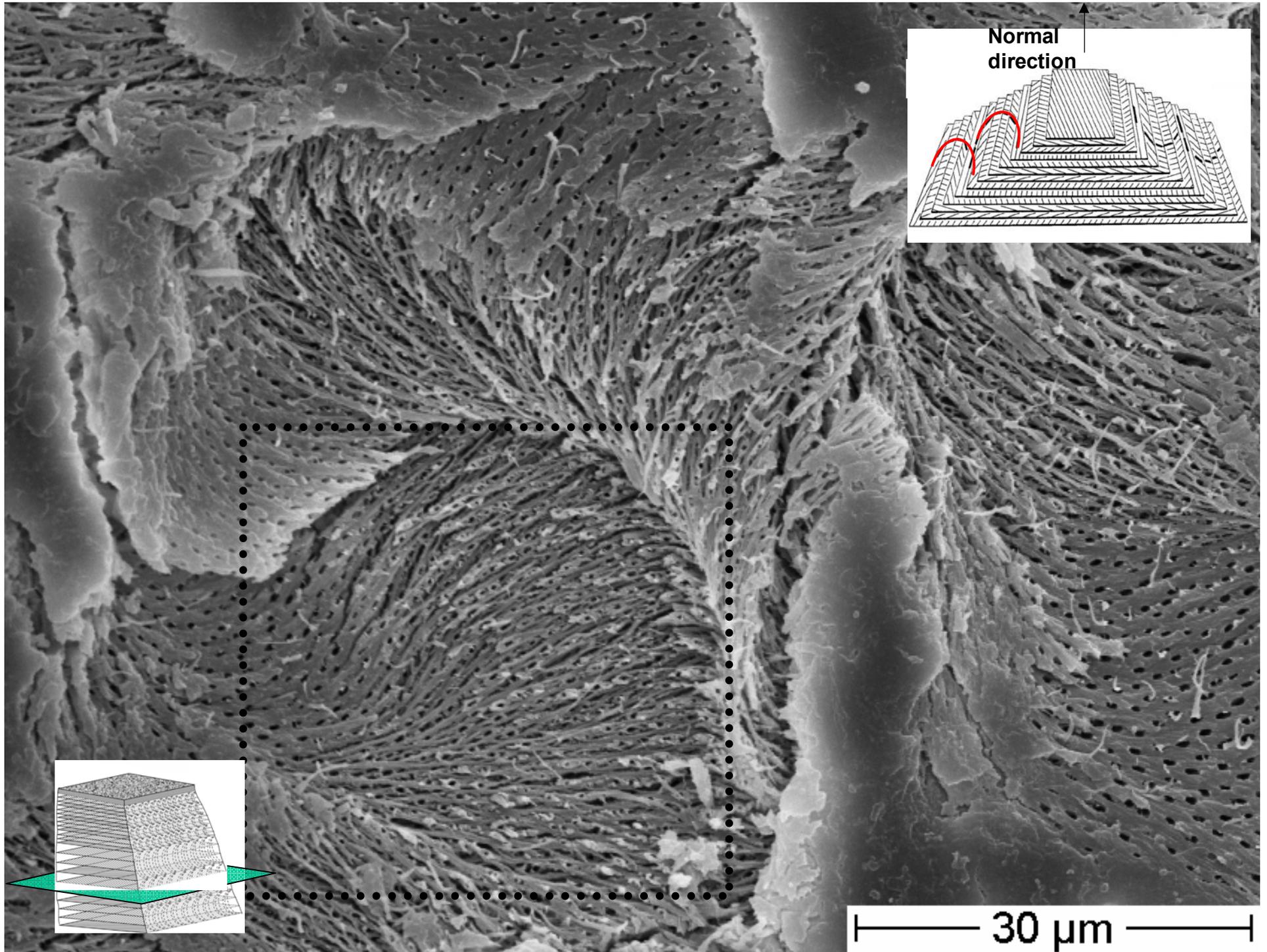
— 30 μm —



┌ 10 μ m ┐

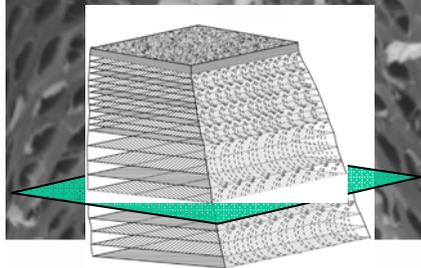
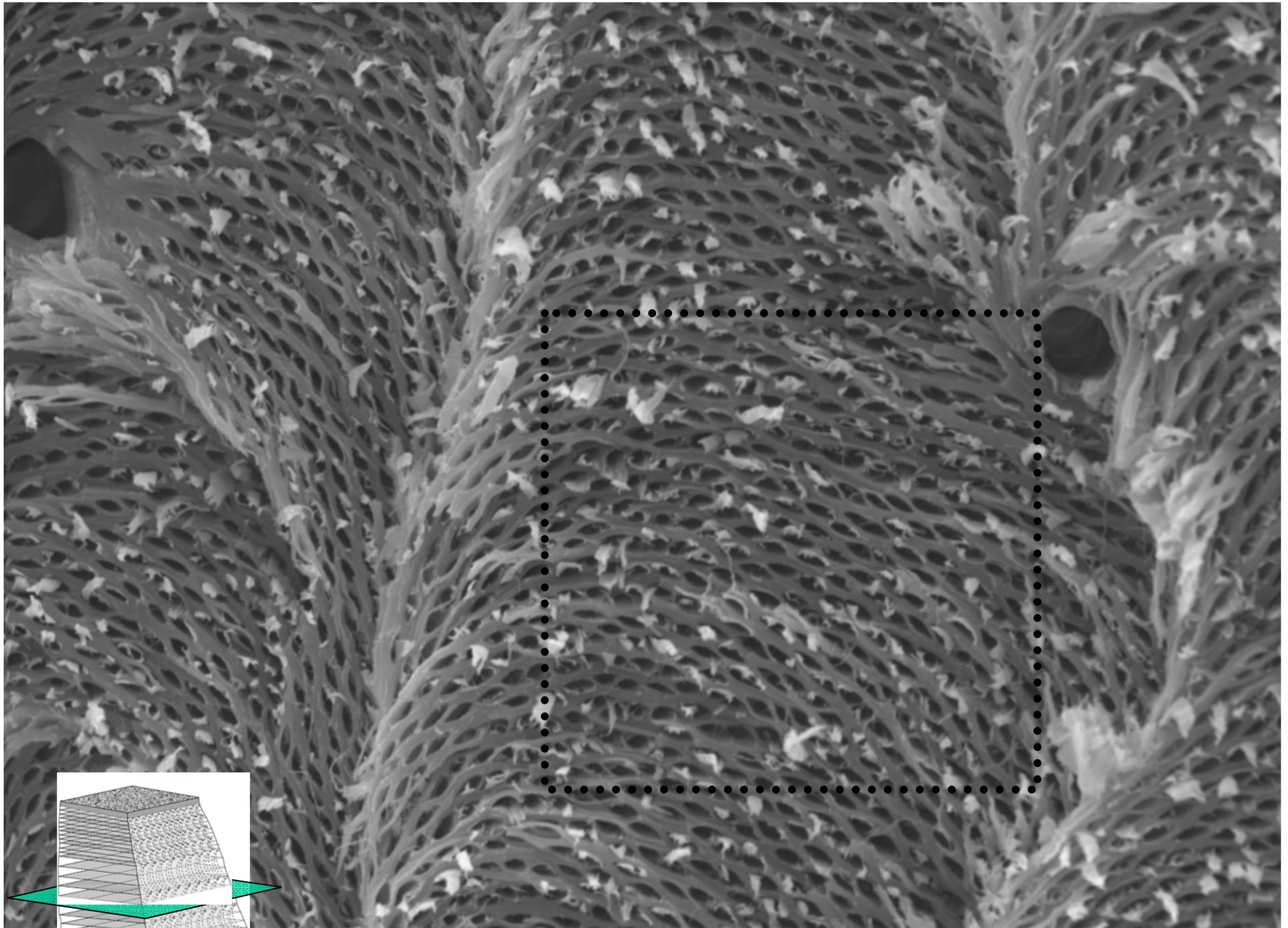


— 100 μm —

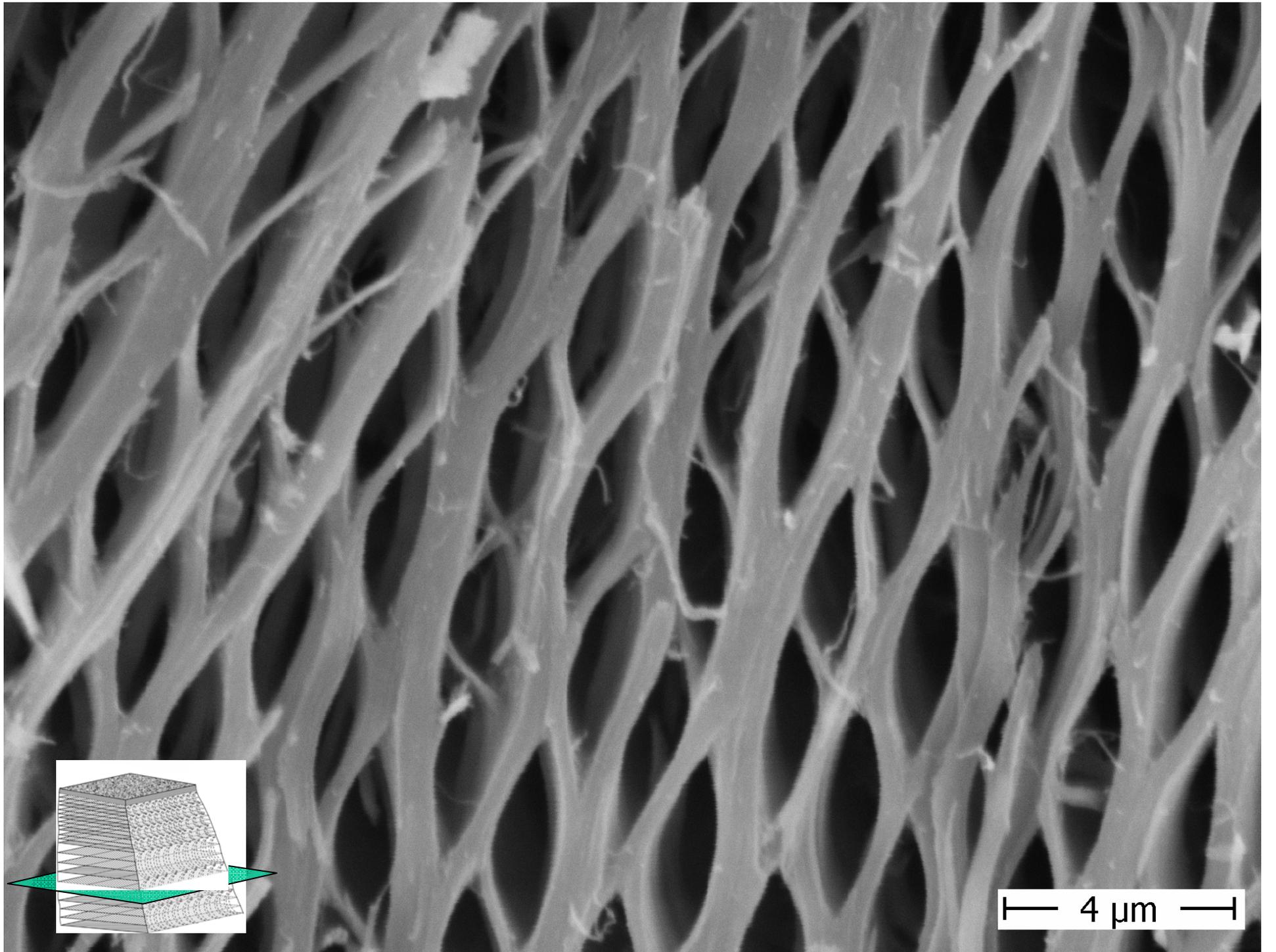


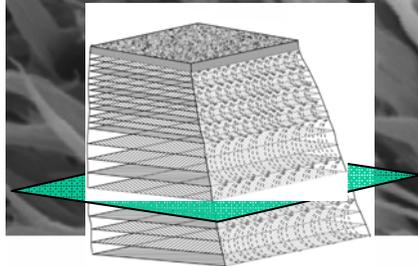
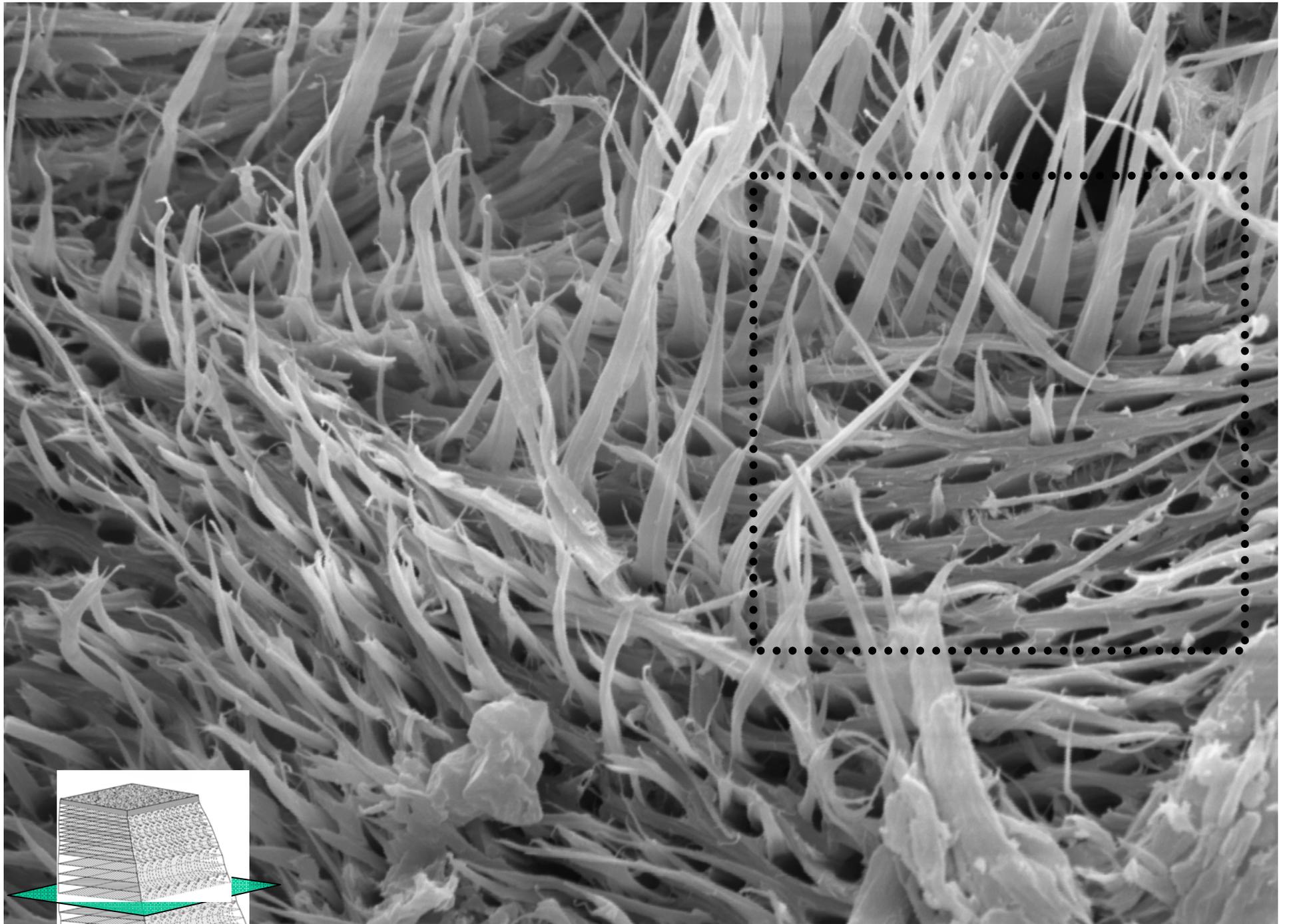
Normal
direction

30 μm

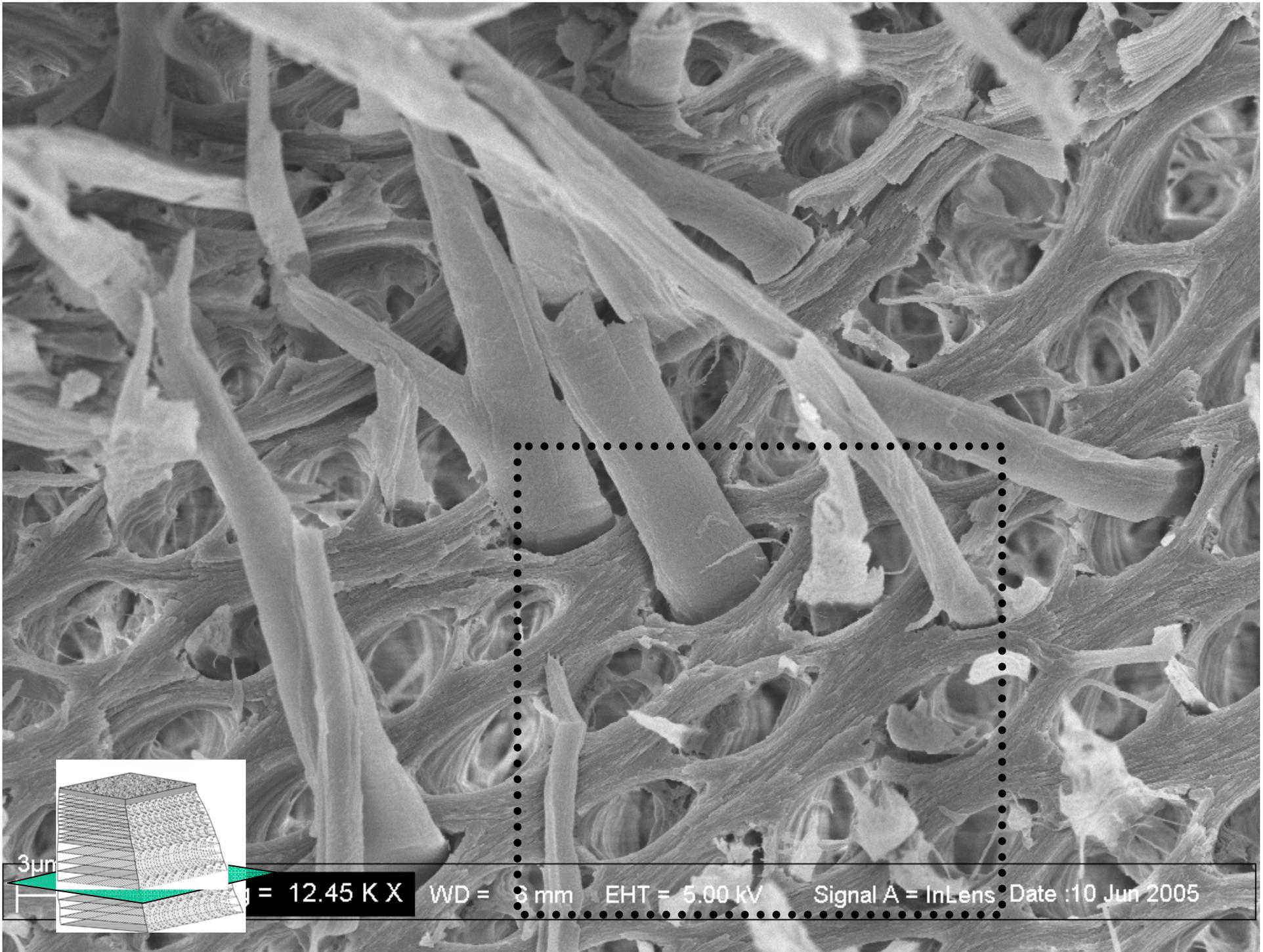


— 20 μm —





— 10 μm —



3µm

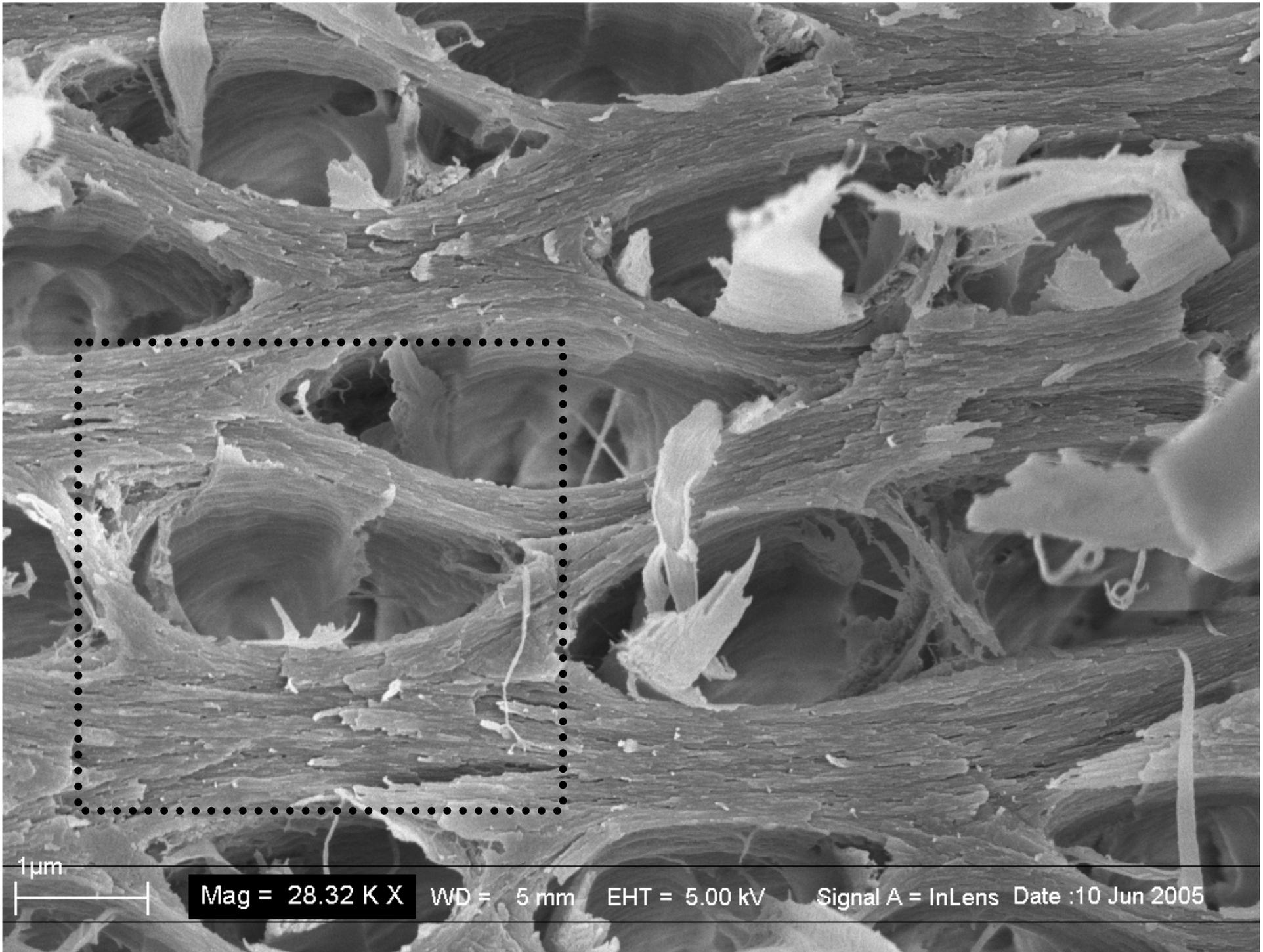
Magnification = 12.45 K X

WD = 3 mm

EHT = 5.00 kV

Signal A = InLens

Date : 10 Jun 2005



1µm

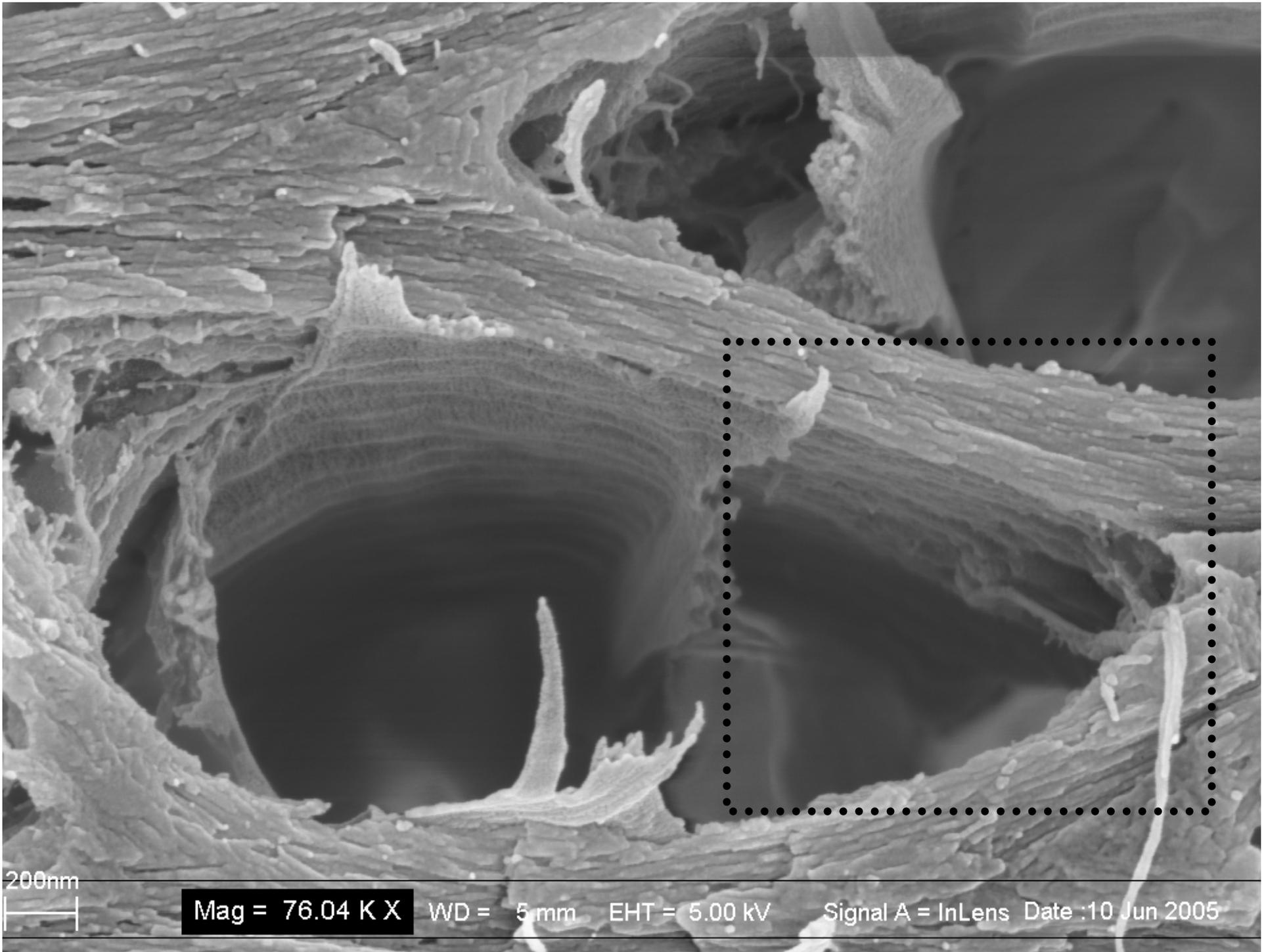
Mag = 28.32 K X

WD = 5 mm

EHT = 5.00 kV

Signal A = InLens

Date :10 Jun 2005



200nm
|
|

Mag = 76.04 K X WD = 5mm EHT = 5.00 kV Signal A = InLens Date :10 Jun 2005

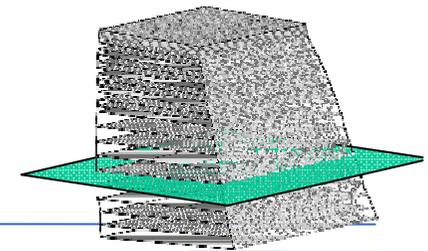
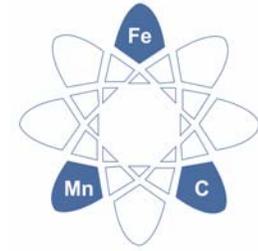


100nm

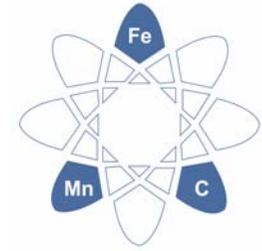


Mag = 133.31 K X WD = 5 mm EHT = 5.00 kV Signal A = InLens Date :9 Jun 2005

SEM chemical deproteinization



X-ray wide angle diffraction, lobster

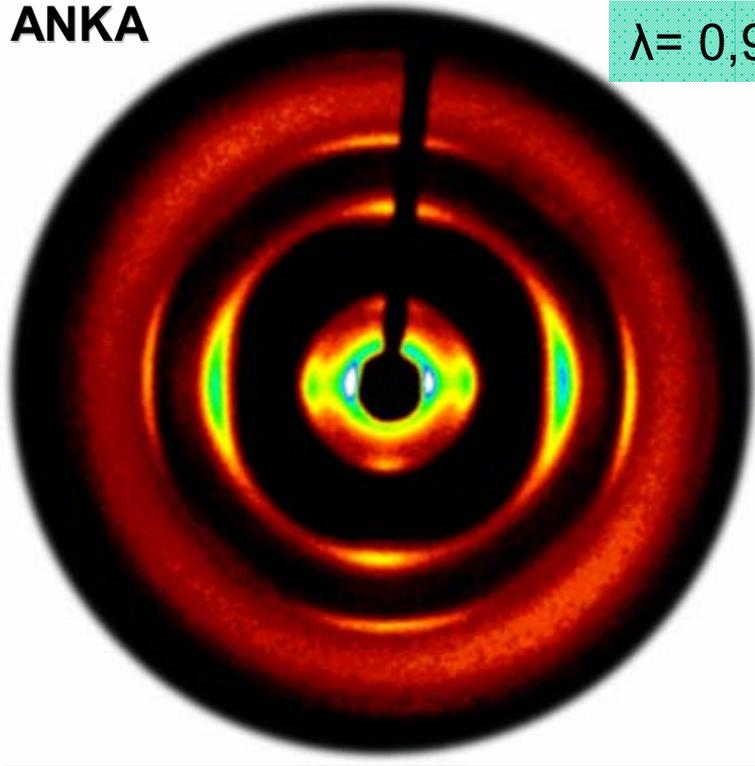


Co-target

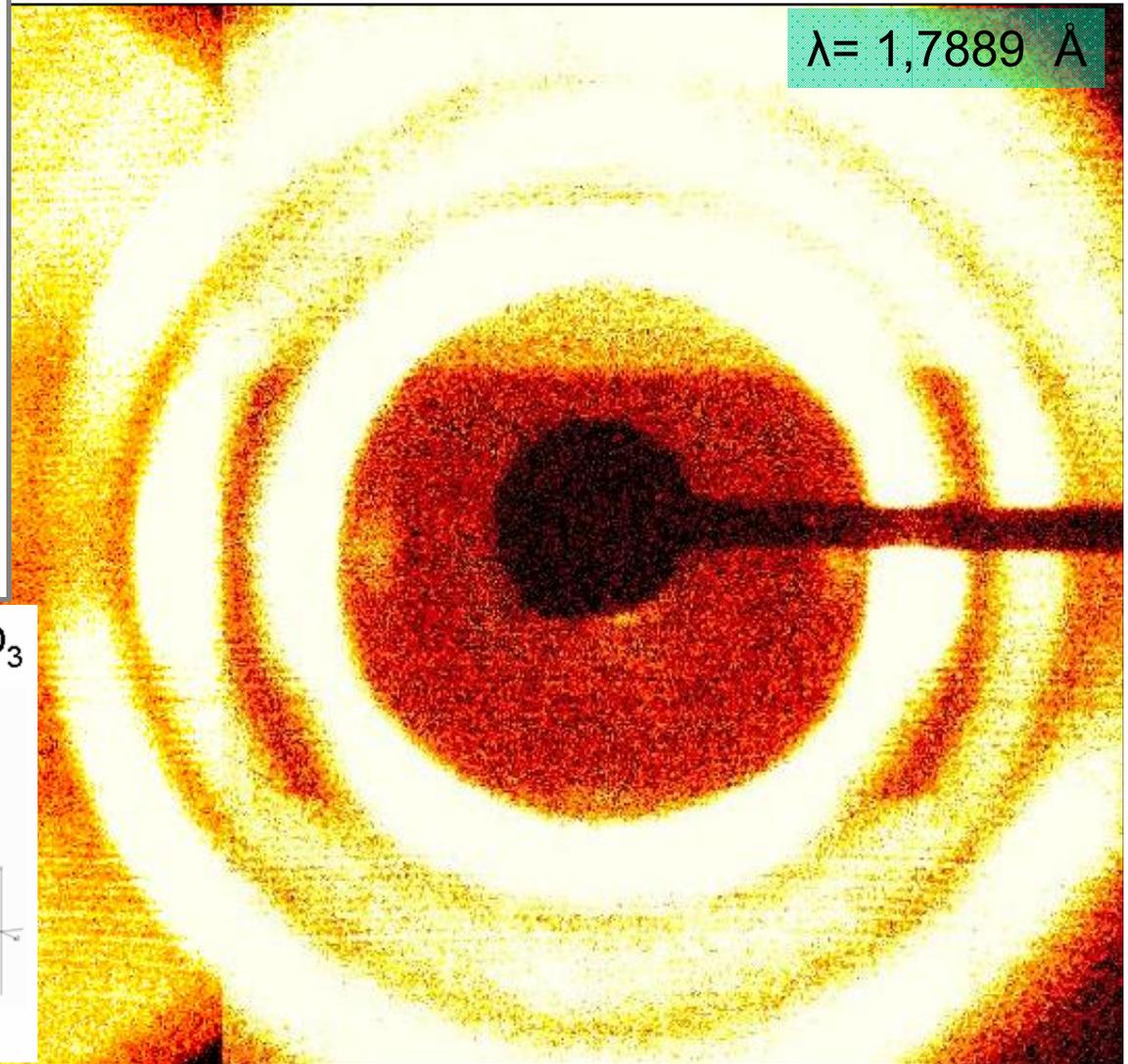
ANKA

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

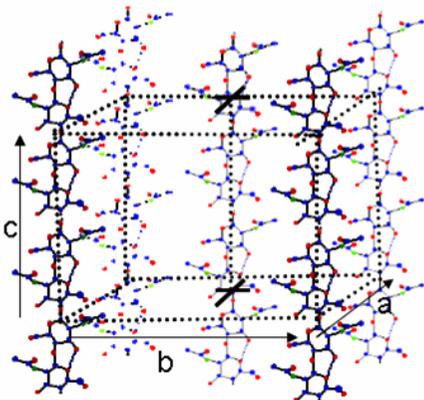
very strong chitin textures



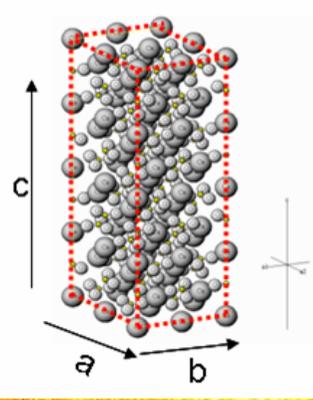
$\lambda = 1,7889 \text{ \AA}$



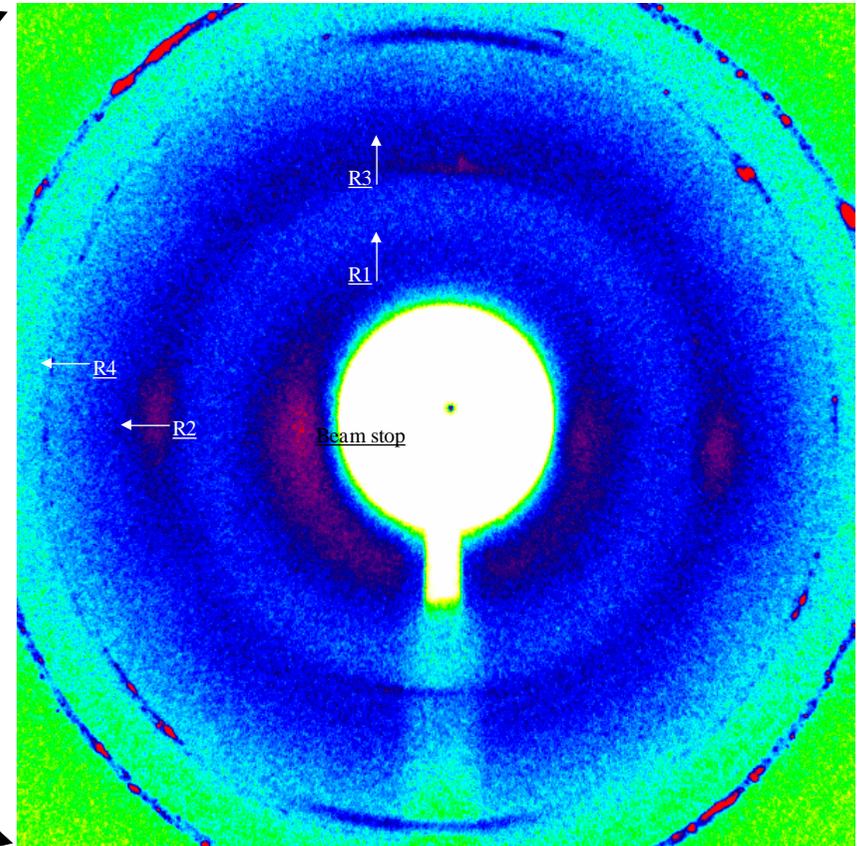
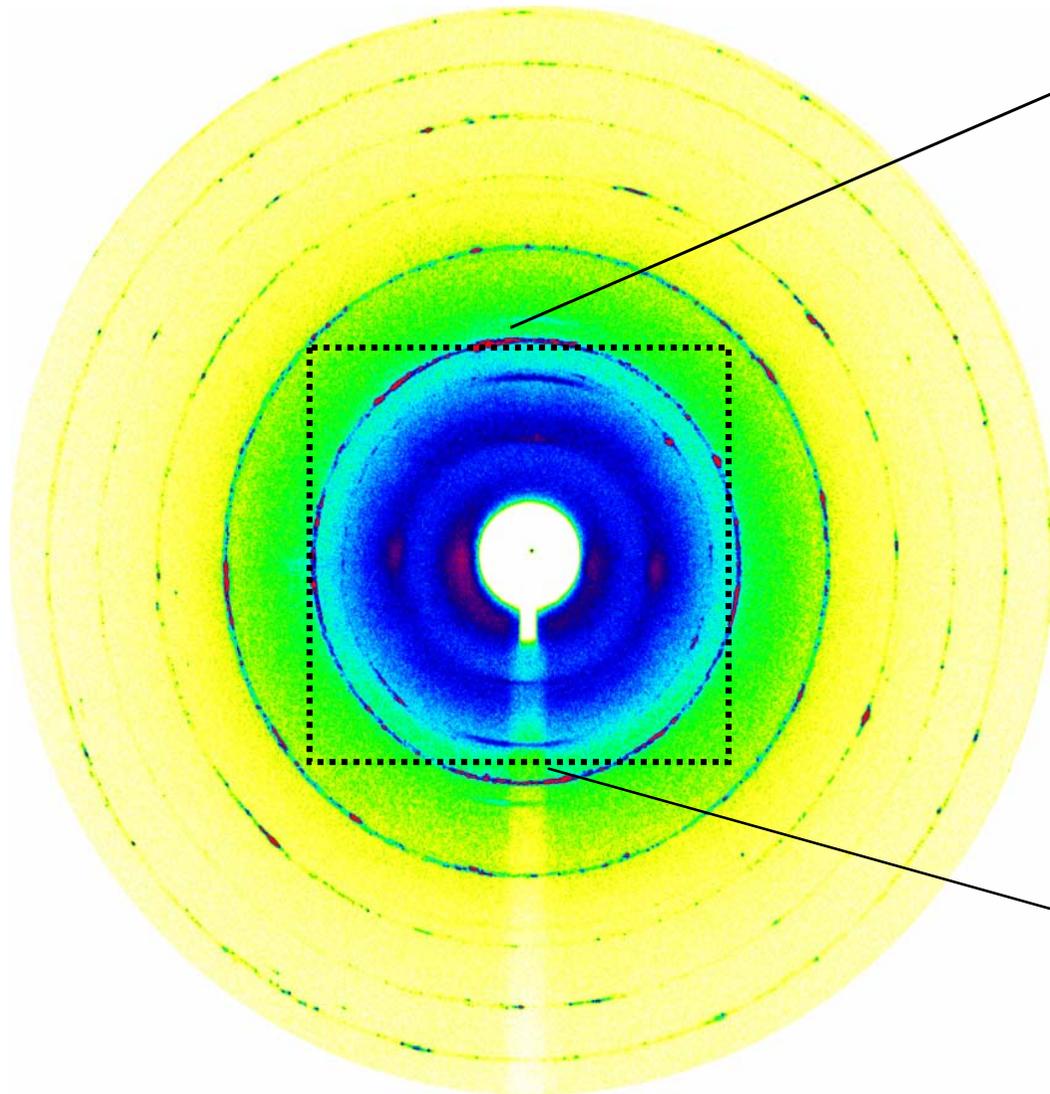
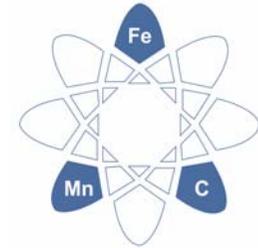
α -Chitin $C_8H_{13}NO_5$



Calcite $CaCO_3$

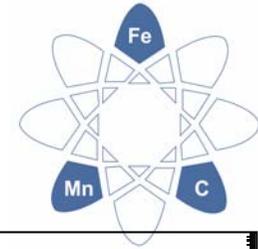


Synchrotron x-ray, wide angle, lobster

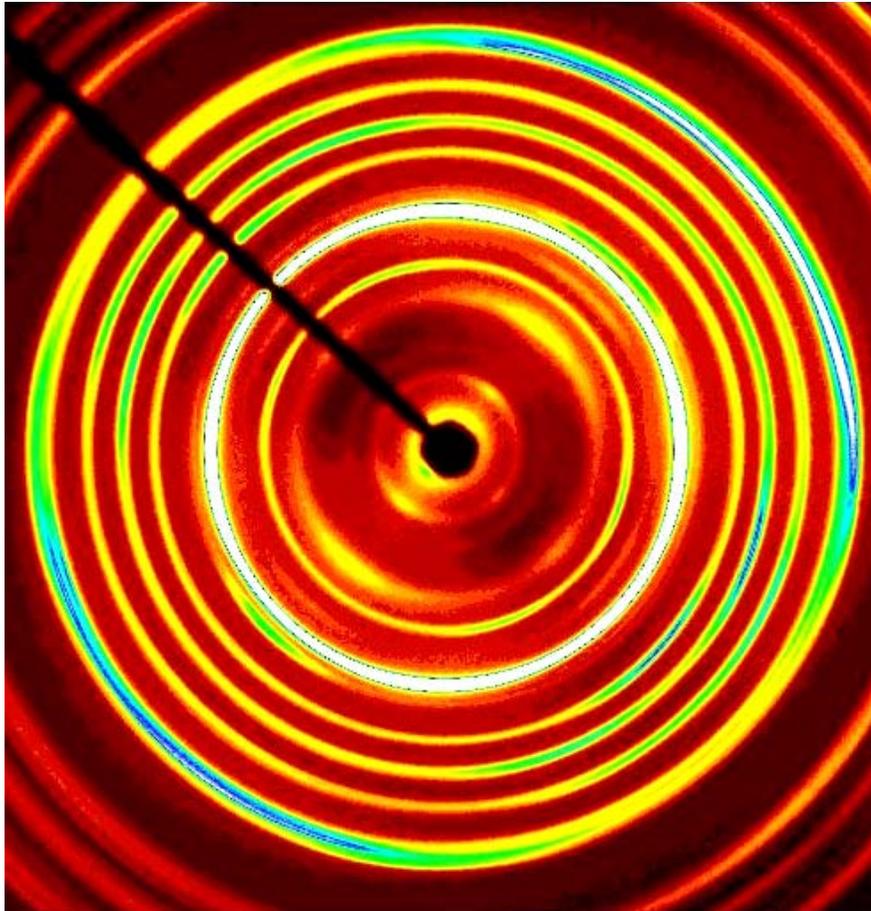


**very strong chitin textures
clusters of calcite ?**

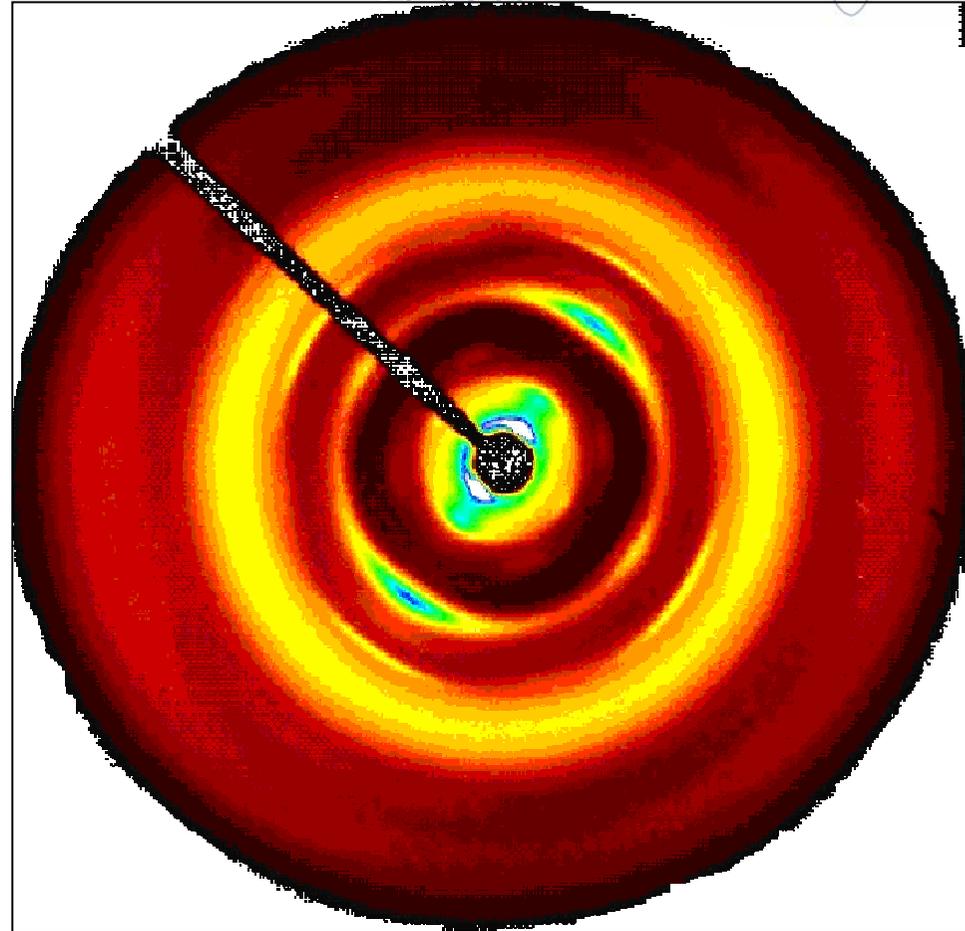
Synchrotron x-ray, wide angle, crab vs. lobster



crab

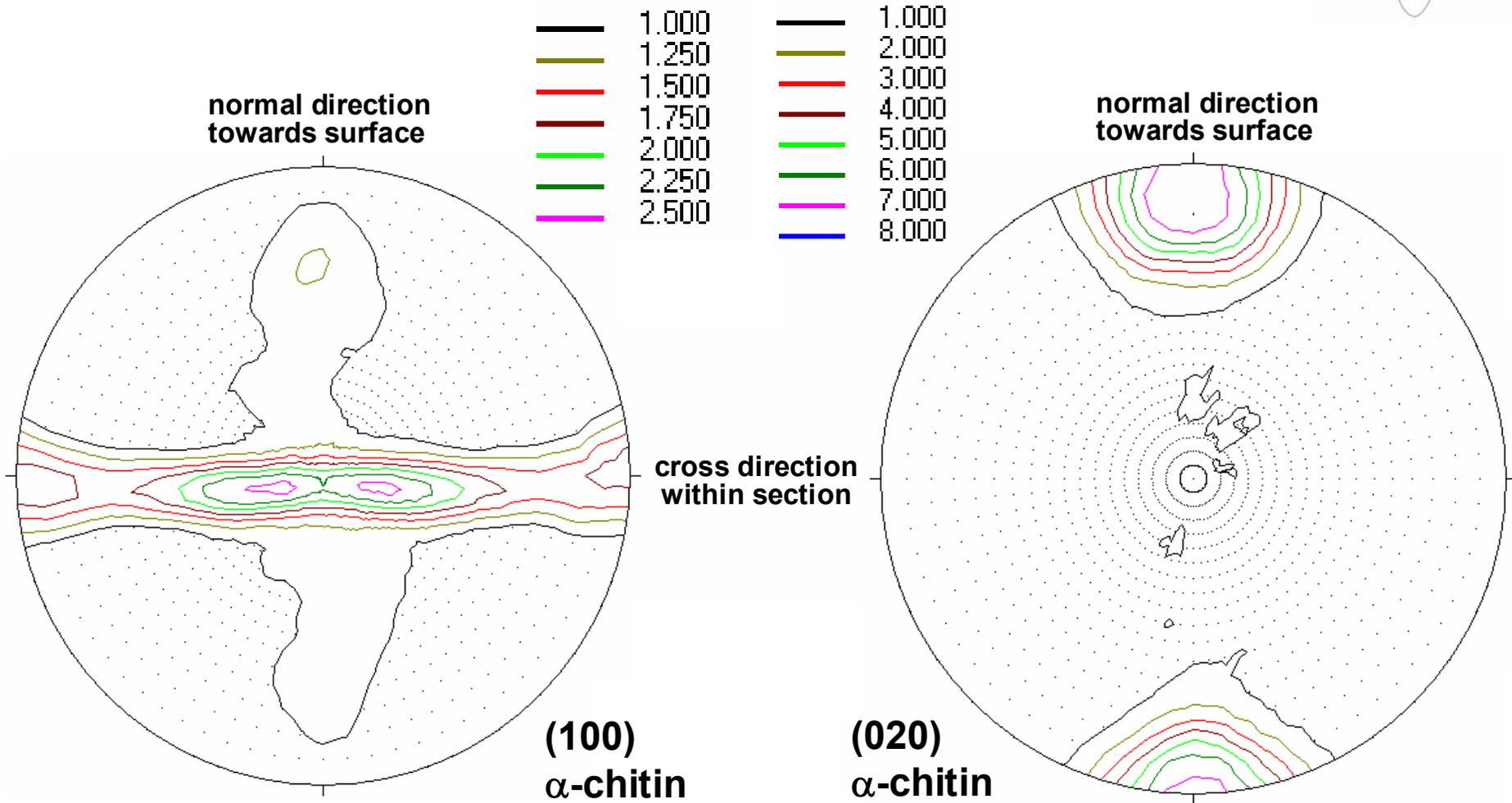
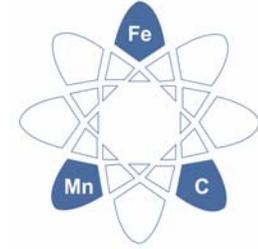


lobster

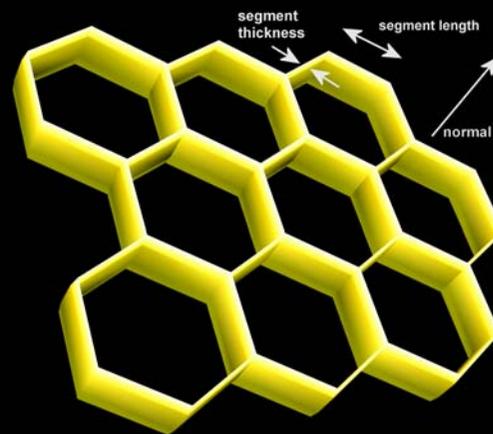
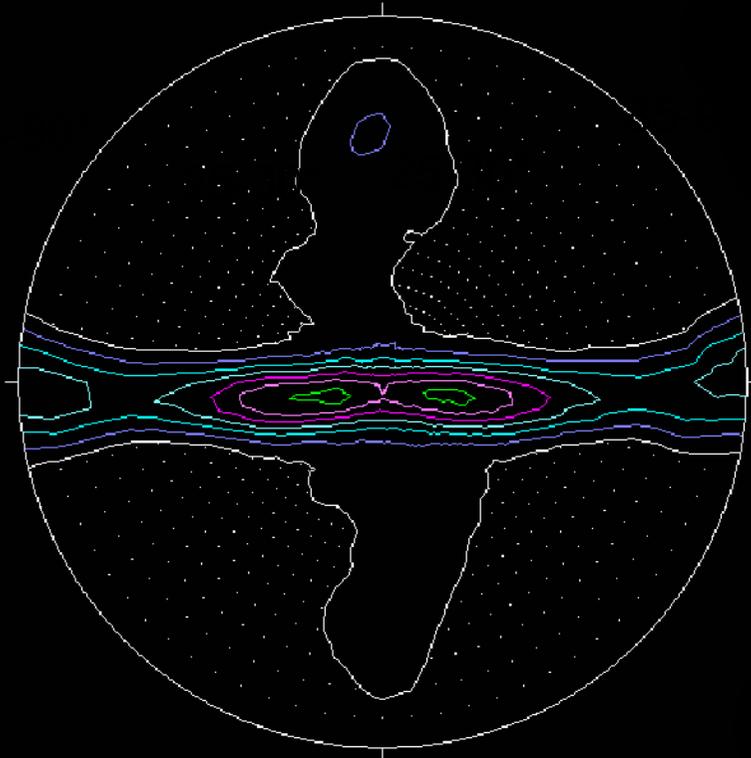
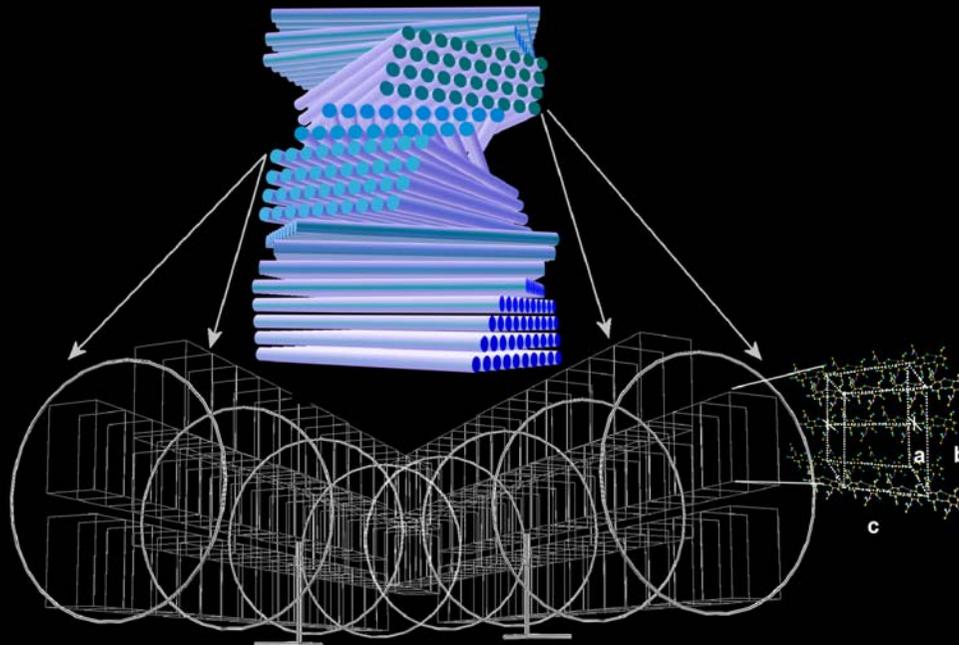
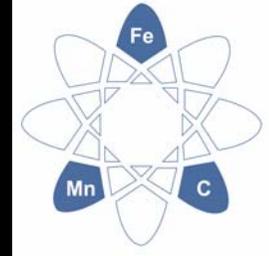


D. Raabe, P. Romano, C. Sachs, H. Fabritius, A. Al-Sawalmih, S.-B. Yi, G. Servos, H.G. Hartwig, Materials Science and Engineering A Vol. 421 (2006) pages 143–153., “Microstructure and crystallographic texture of the chitin-protein network in the biological composite material of the exoskeleton of the lobster *Homarus americanus*”

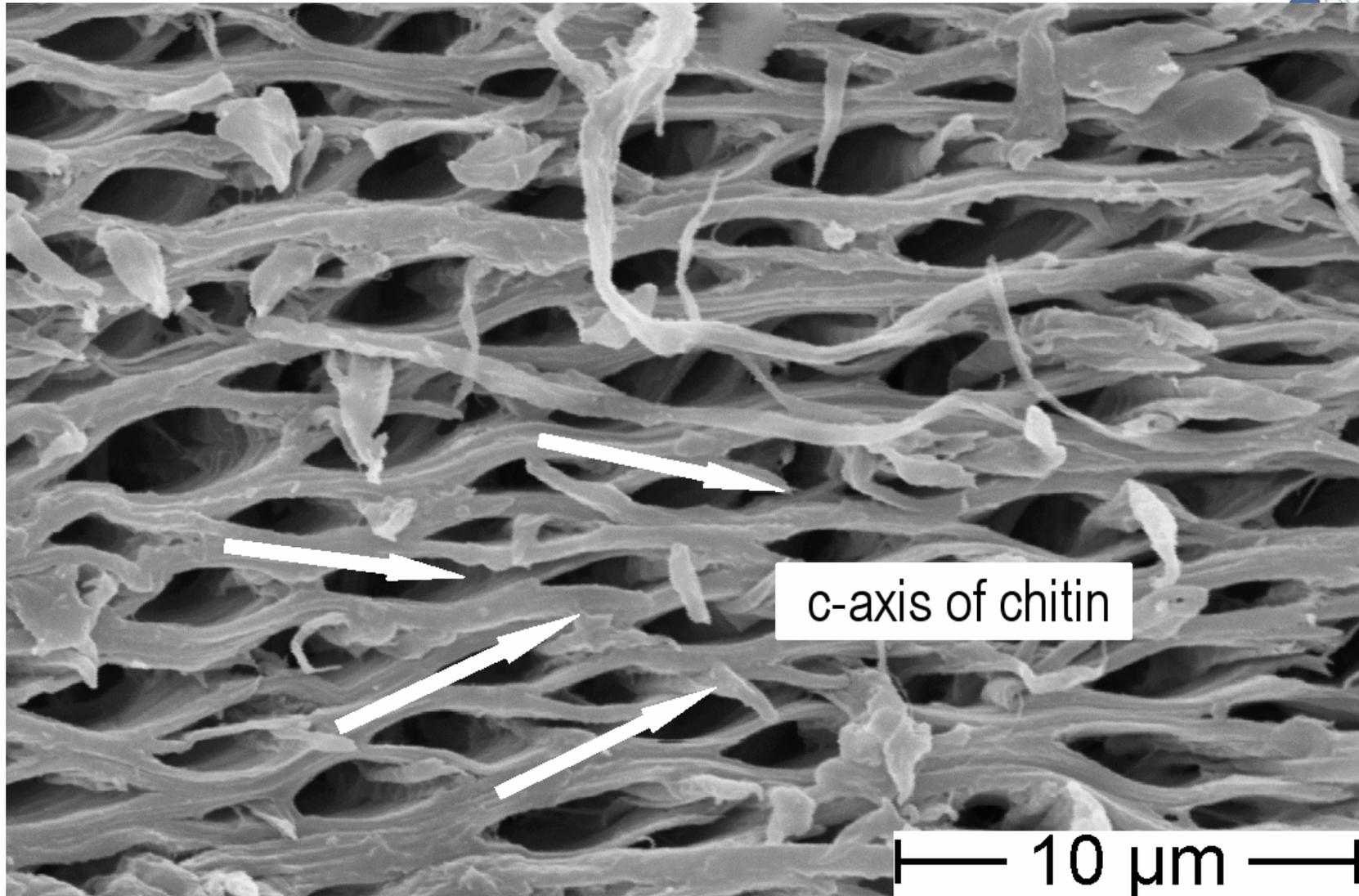
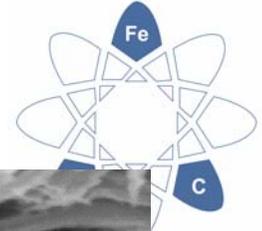
Synchrotron x-ray wide angle, lobster, chitin



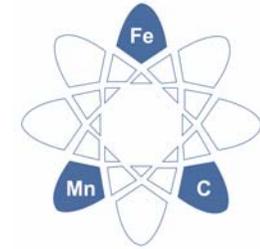
Structure and texture of α -chitin



Structure and texture of α -chitin



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