



Max-Planck-Institut für Eisenforschung GmbH
Düsseldorf



MAX-PLANCK-GESELLSCHAFT

VDEh

Grundlagen der Kristallographie und Mikrostruktur von Stählen

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1





Grundbegriffe

Kristallographie

Textur

Anisotropie

- **Mikrostruktur / Gefüge:** Gesamtheit aller Gitterfehler, die sich nicht im thermodynamischen Gleichgewicht befinden (*kompensiert die Entropie die Bildungsenthalpie ?*)
- **Textur:** Volumengewichtete Gesamtheit aller Kristallorientierungen in einer Probe
- **OVF:** Orientierungsverteilungsfunktion, 3D Textur, quantitativ
- **Polfigur:** 2D Projektion der Orientierungsverteilungsfunktion, qualitativ
- **Isotropie:** Richtungsunabhängigkeit (*Tropos (gr.): Richtung*)
- **Anisotropie:** Richtungsabhängigkeit (Gefügezeiligkeit, Textur, etc.)
- **Fließort:** Gesamtheit aller Spannungszustände, bei denen plastisches Fließen auftritt
- **R-Wert:** Verhältnis von Breiten- zu Dickenabnahme an einer Stelle des Fließortes



Grundbegriffe

Kristallographie

Textur

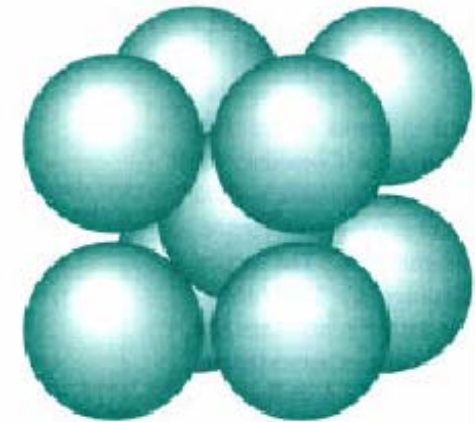
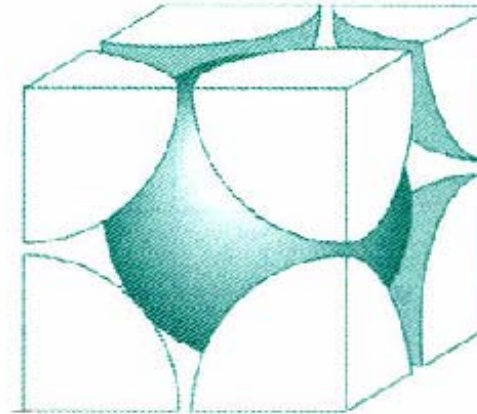
Anisotropie

Fe, Cr, Mo, Ta, Nb, Mo, W

Atome pro Zelle = $(8 \times 1/8) + 1 = 2$

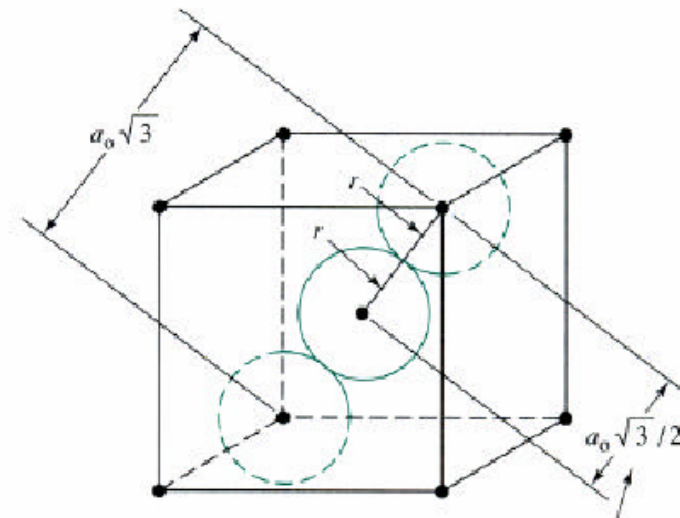
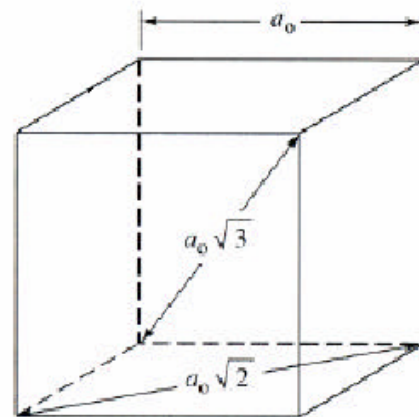
Koordinationszahl = $4 + 4 = 8$

atomare Packungsdichte = 0.68



$$4r = \sqrt{3}a$$

$$a = \frac{4}{\sqrt{3}}r$$



Fe, Al, Ni, Pt, Ir, Ag, Cu, Ag

Atome pro Zelle

$$= (8 \times 1/8) + (6 \times 1/2) = 4$$

Koordinationszahl

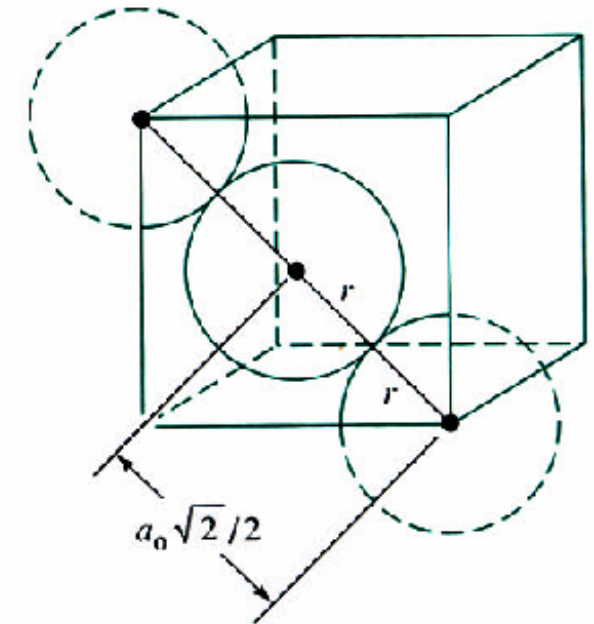
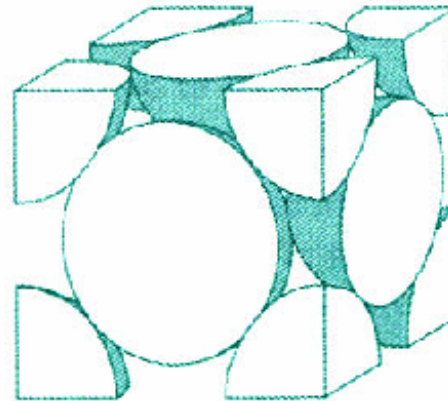
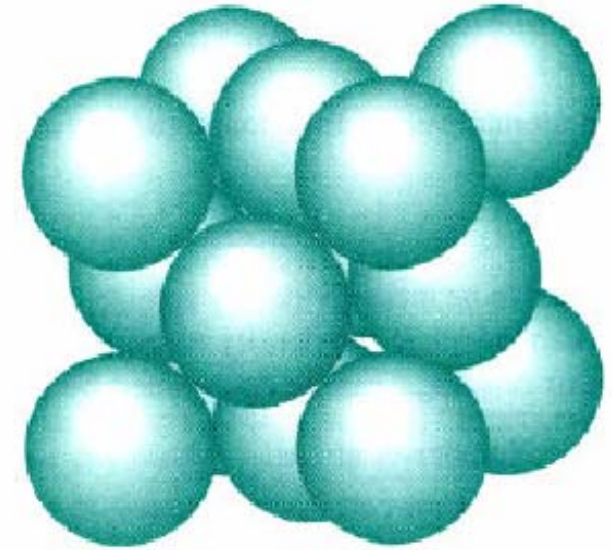
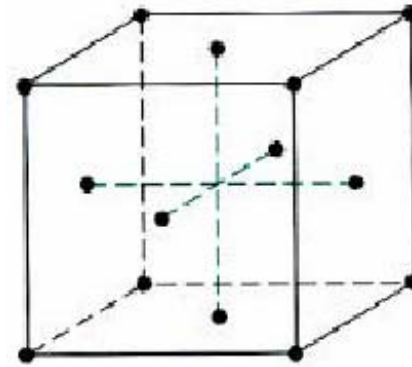
$$= 4 + 4 + 4 = 12$$

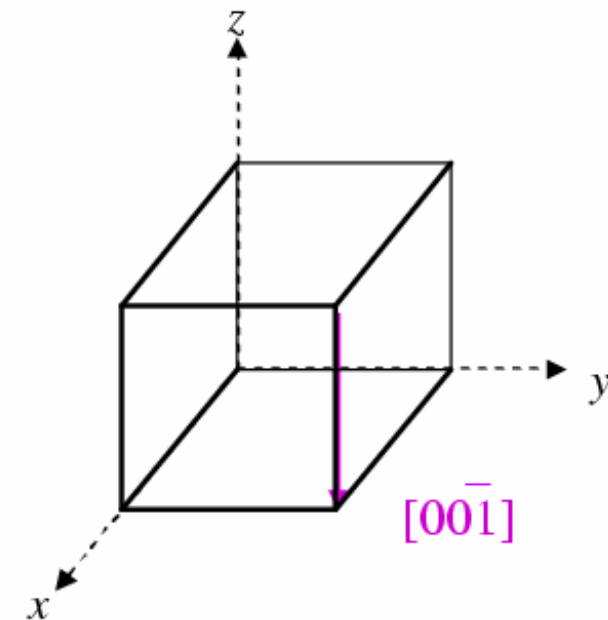
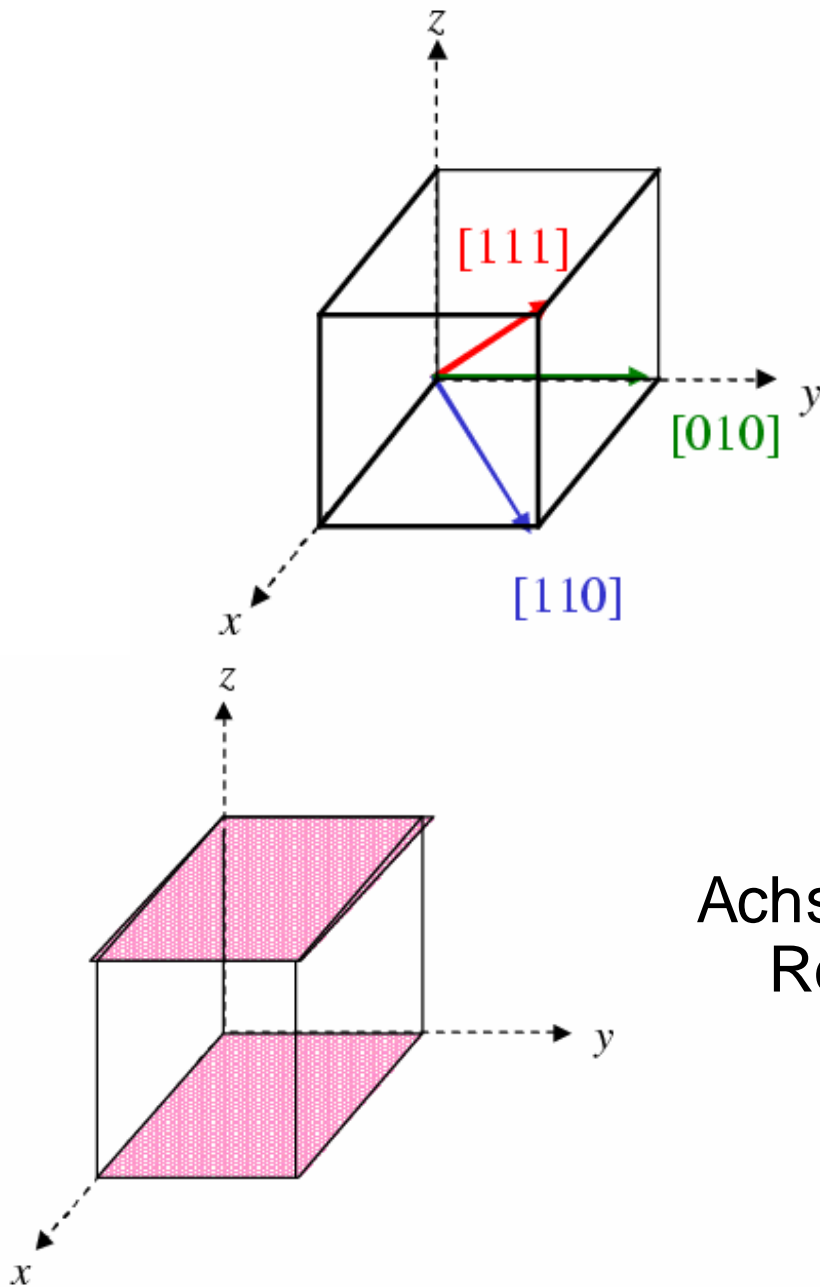
atomare Packungsdichte

$$= 0.74$$

$$4r = \sqrt{2}a$$

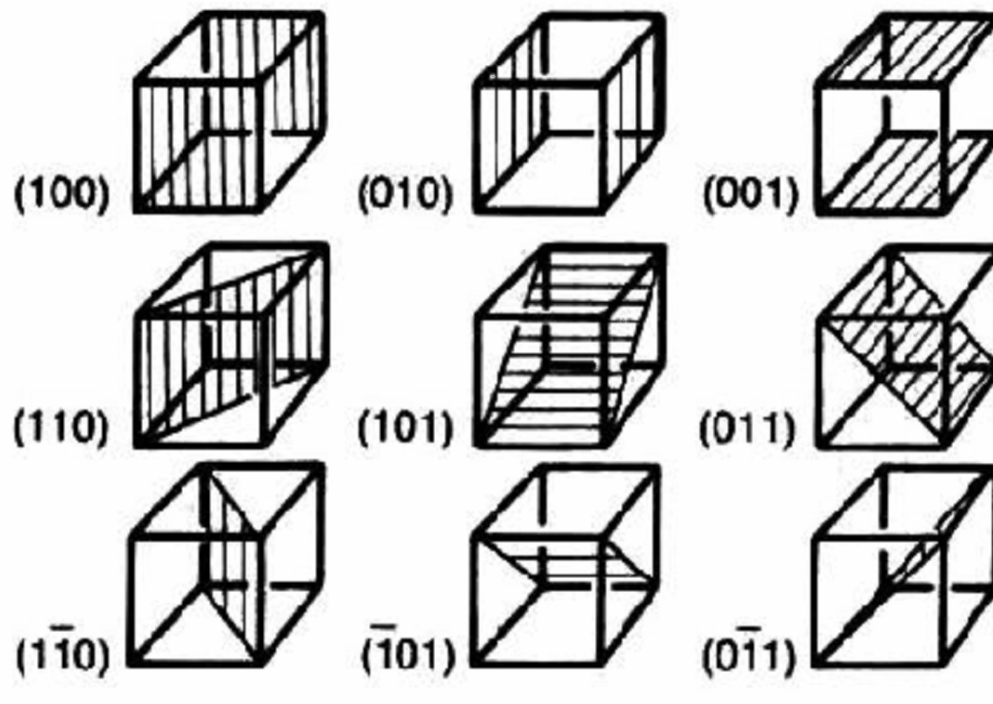
$$a = 2\sqrt{2}r$$





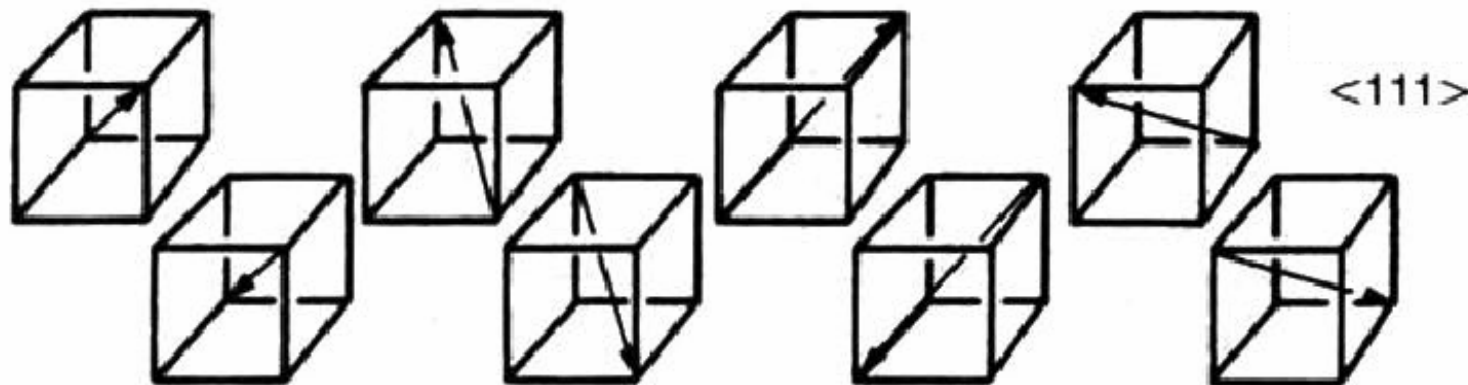
	x	y	z
Achsenabschnitte	∞	∞	1
Reziprokwerte	0	0	1
Indizes	(001)		

Familie



{001}

{011}



$\langle 111 \rangle$

spezifisch

allgemein

Richtung

[]

< >

Ebene

()

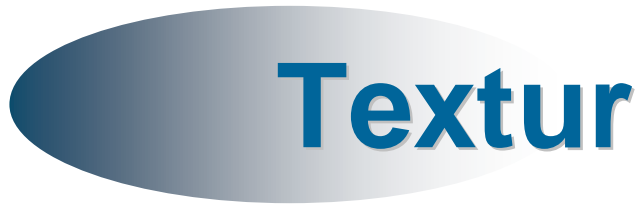
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Grundbegriffe

Kristallographie

Textur

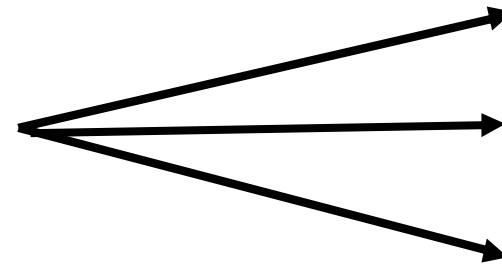
Anisotropie



Grundbegriffe

Kristallographie

Textur

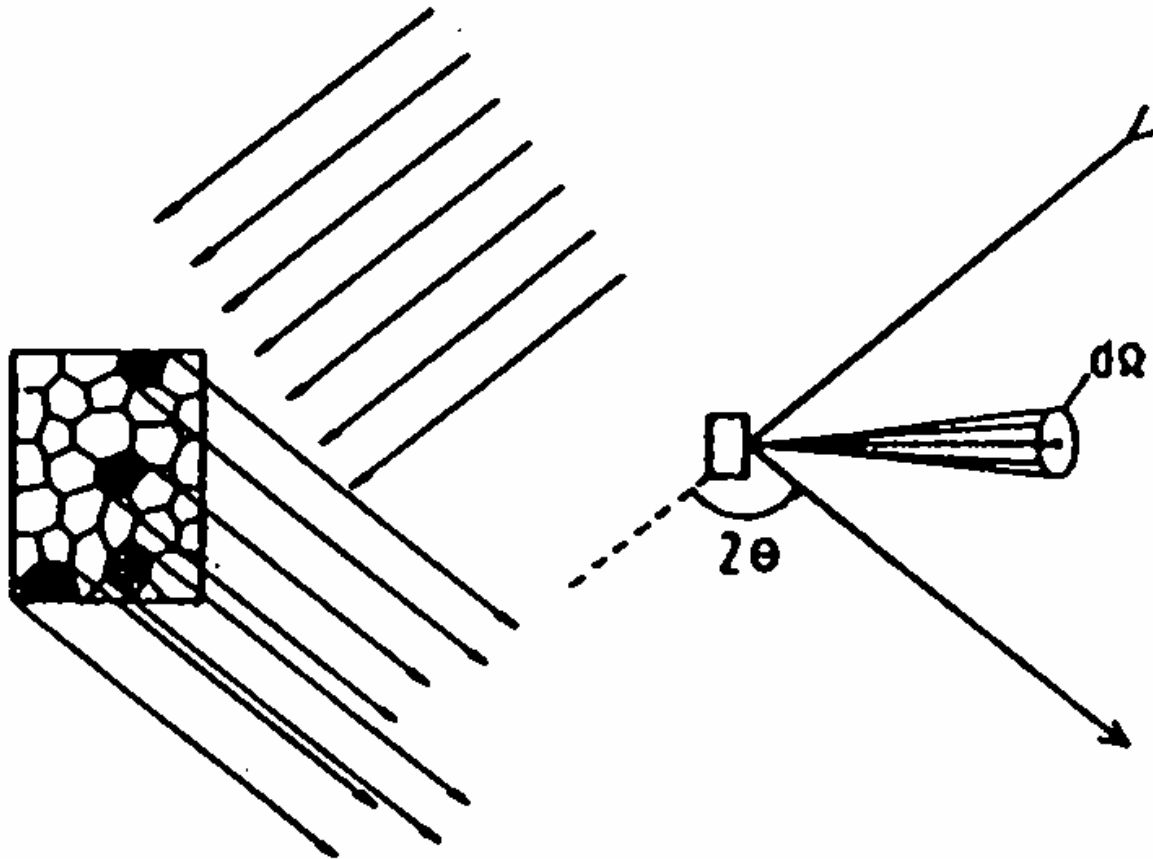


Messung
Grundlagen
Entstehung

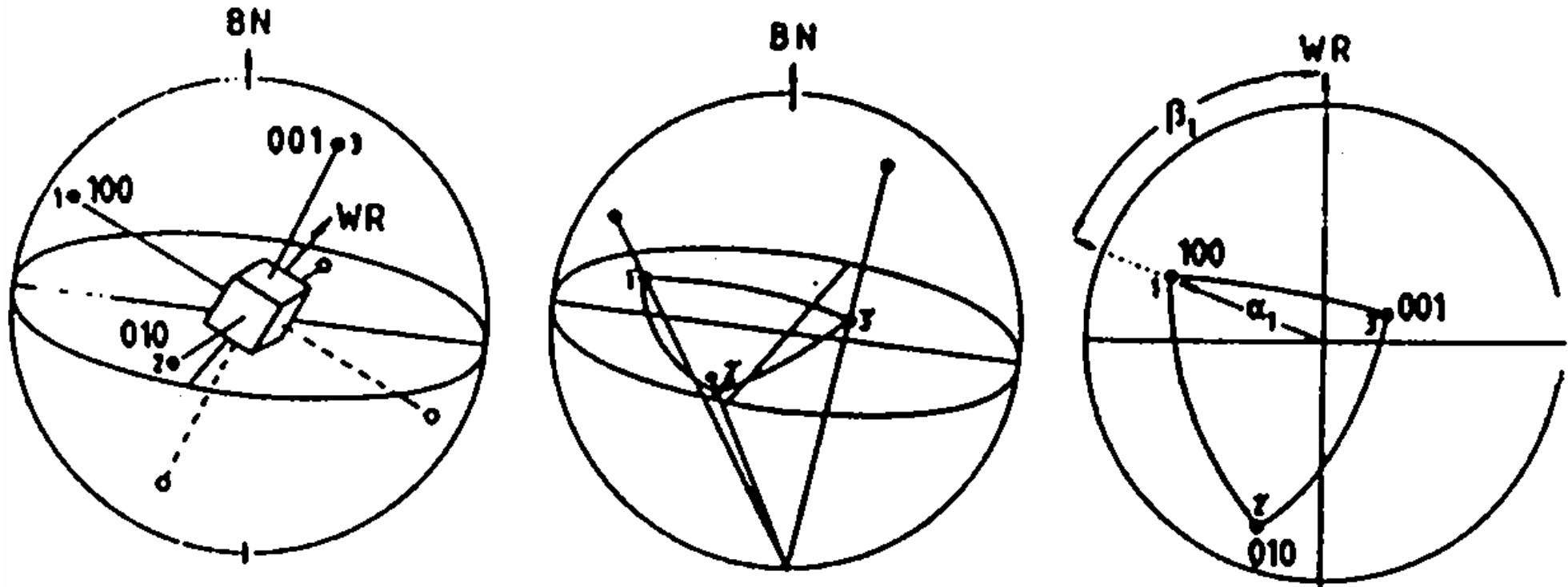
Anisotropie

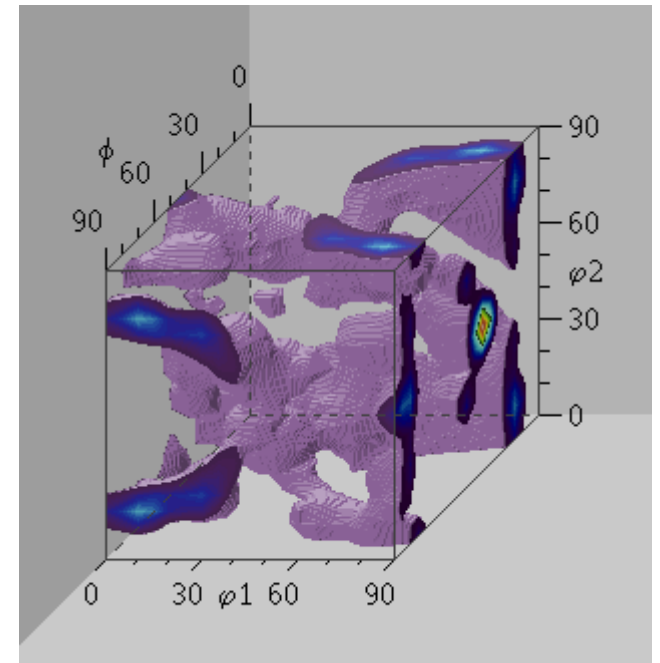
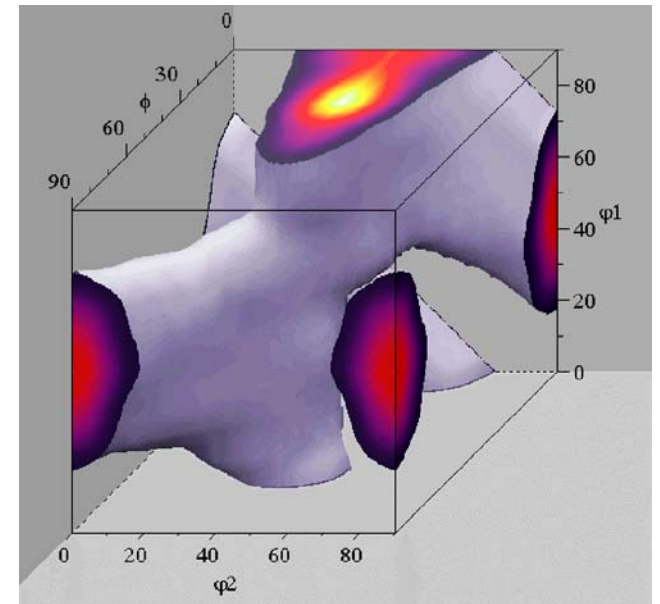
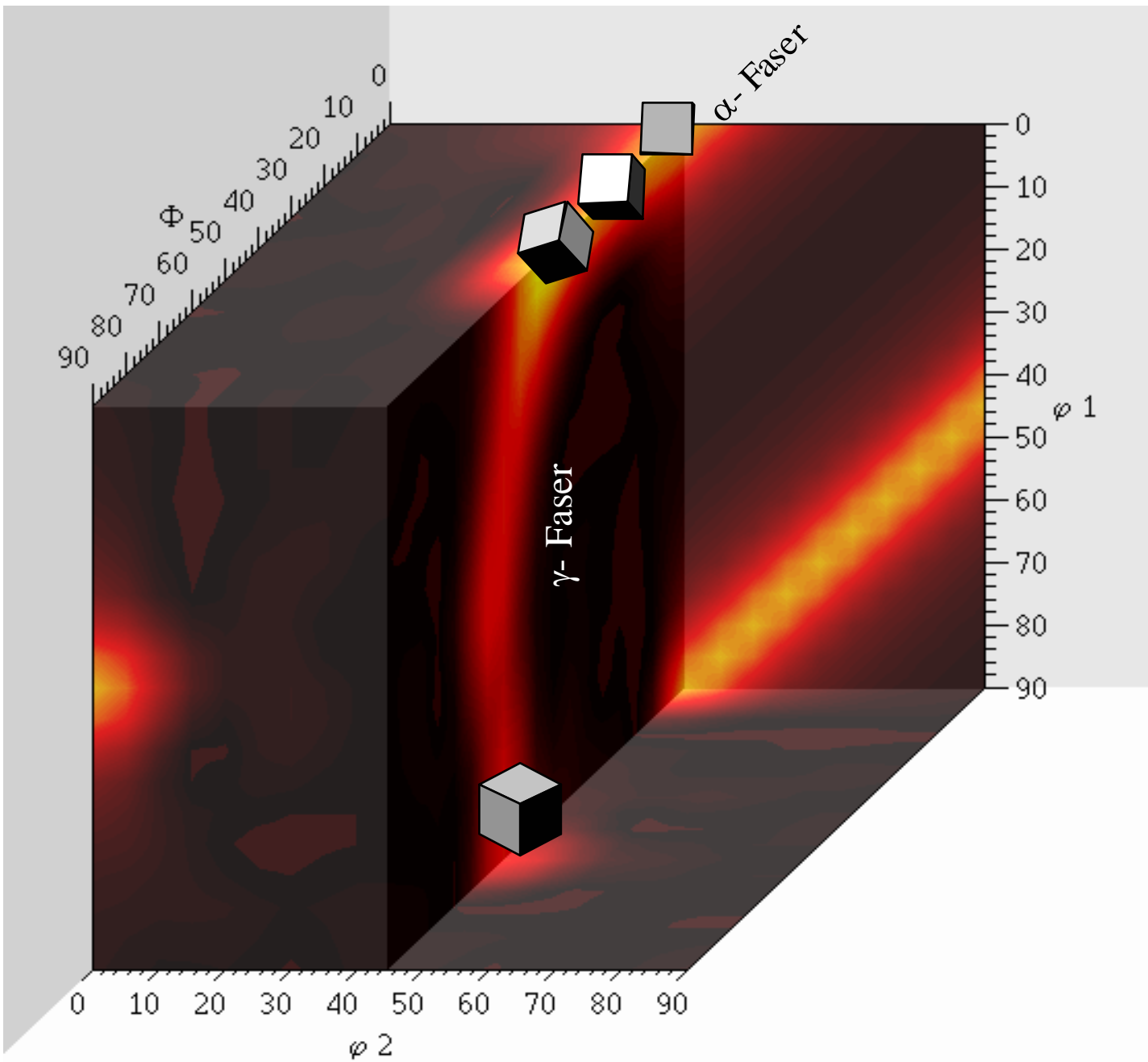
$$n \lambda = 2 d \sin \Theta$$

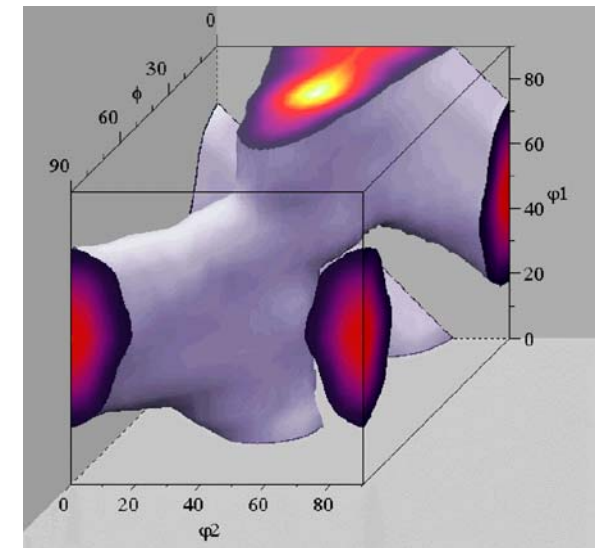
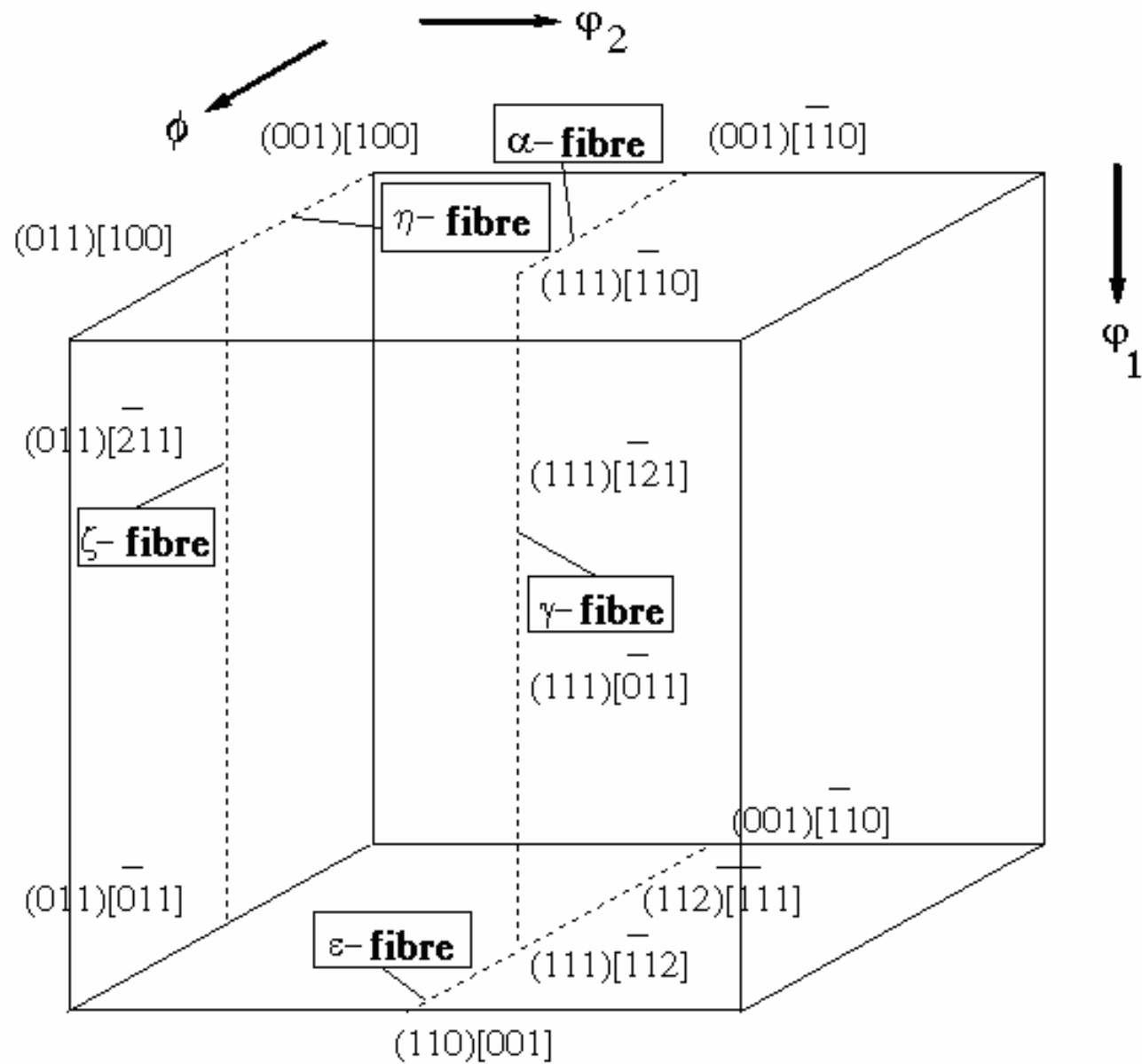
Messung



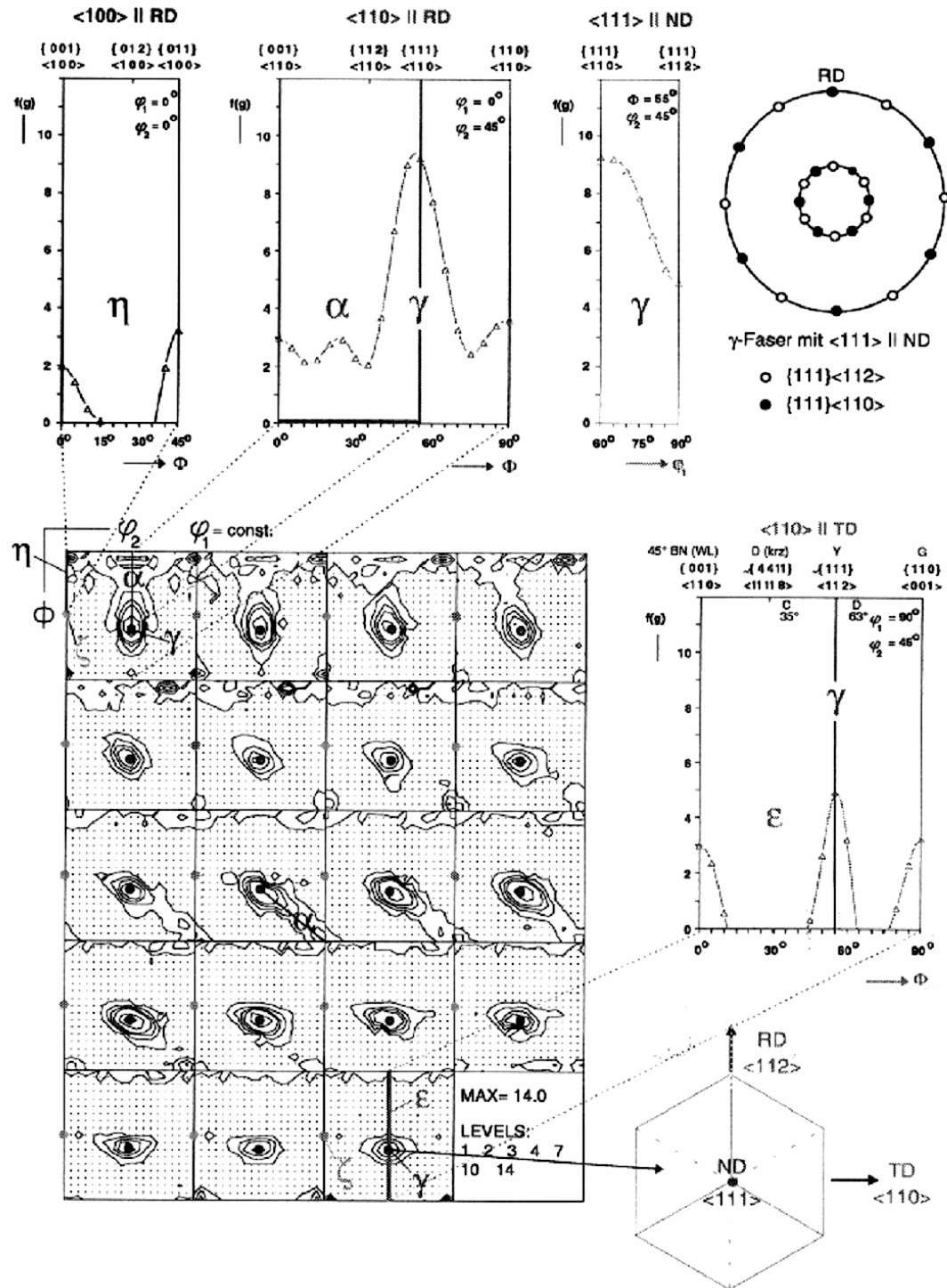
Messung und Darstellung



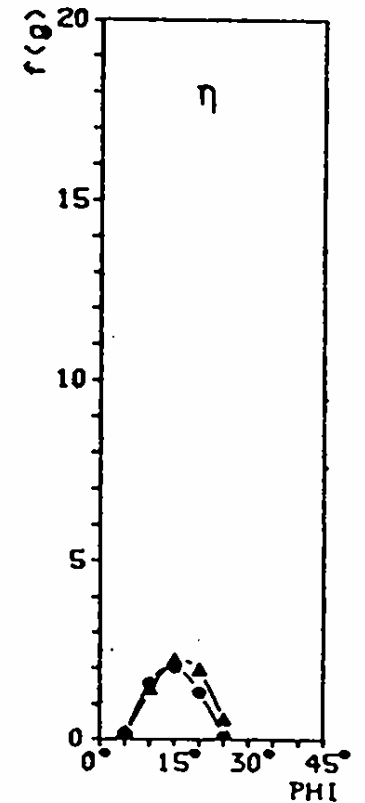
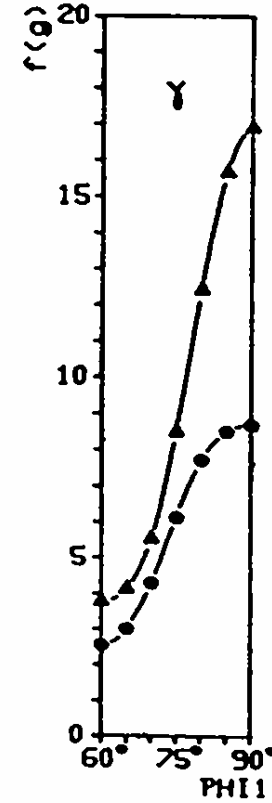
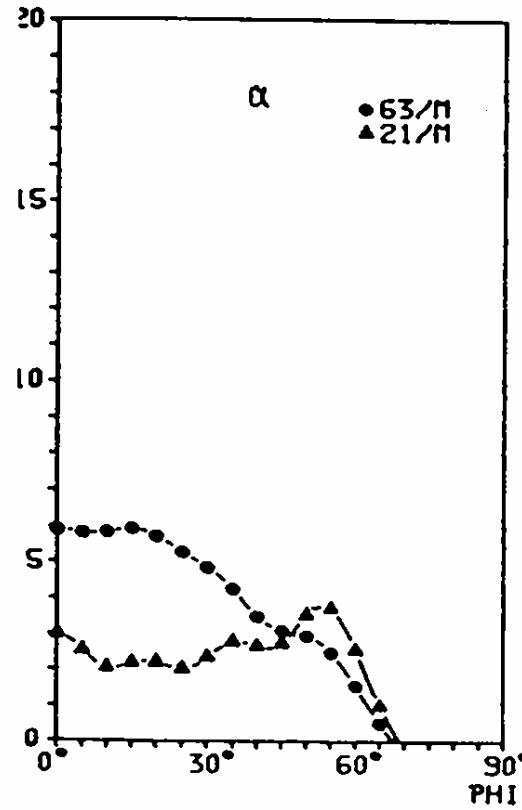
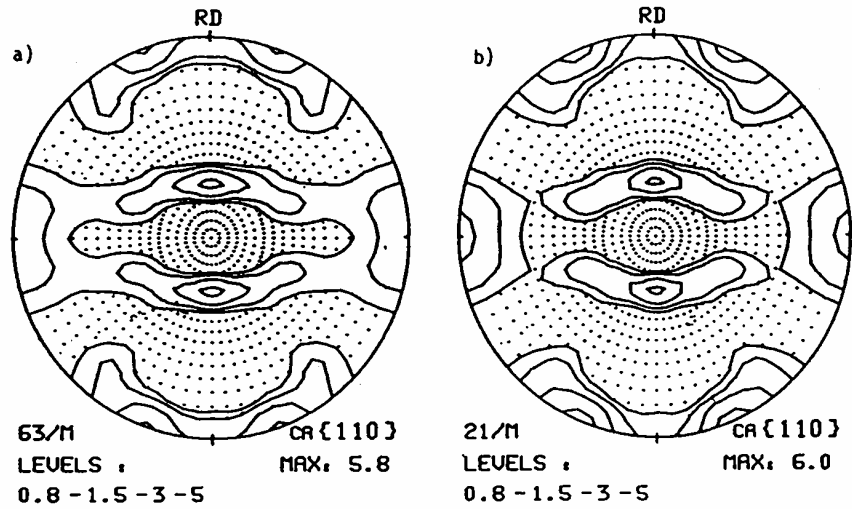




Was ist wichtig
im Eulerraum ?



Warum OVF?



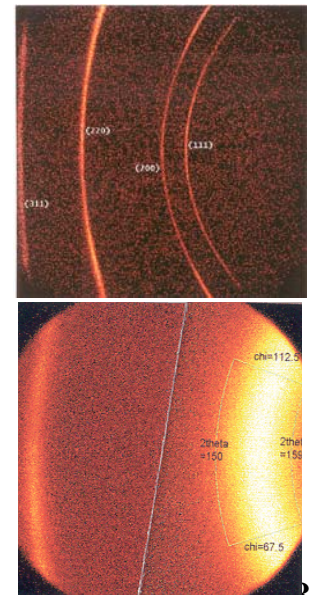
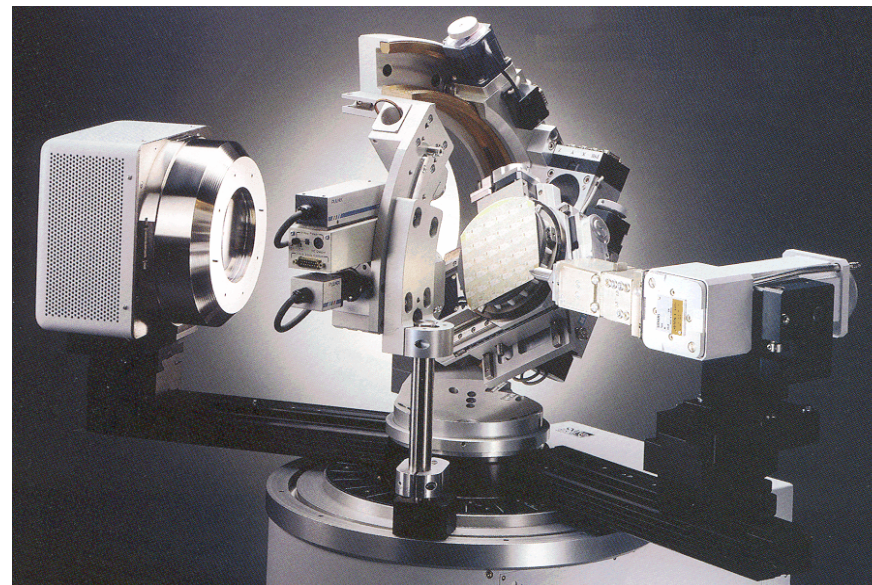
nano texture / TEM



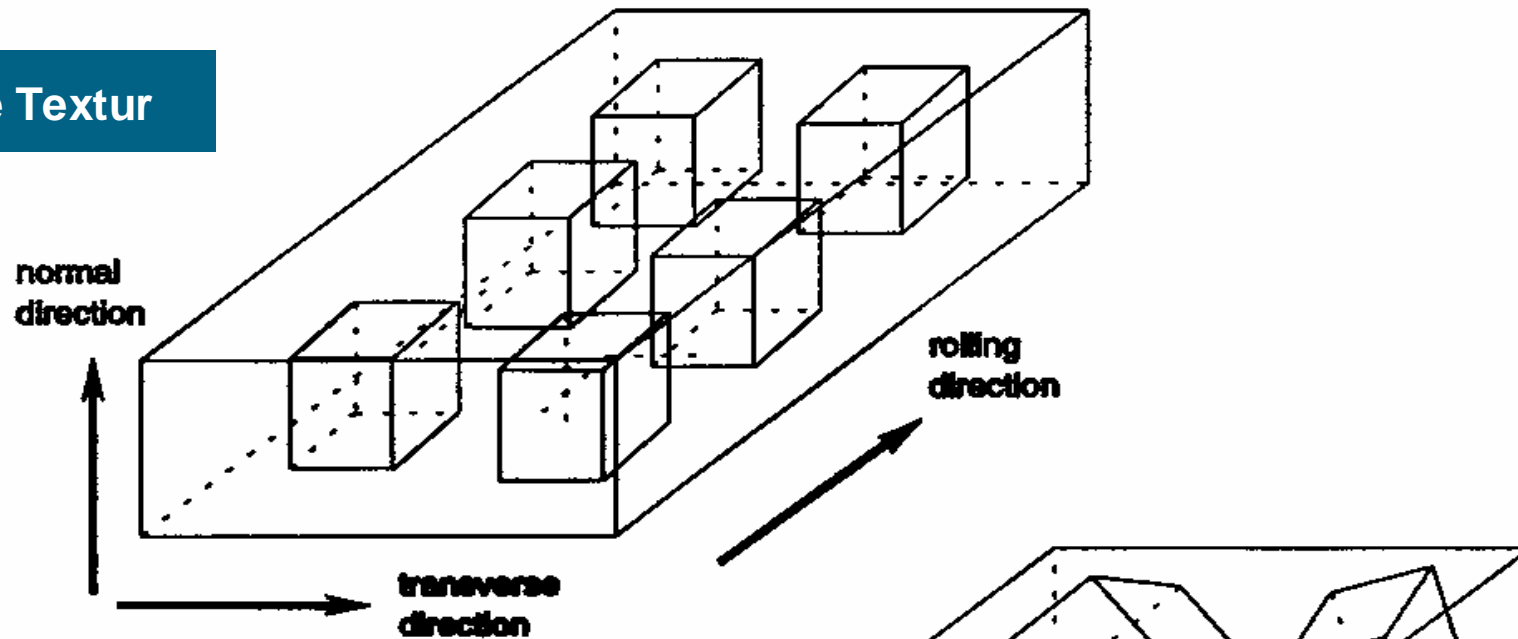
micro texture / SEM



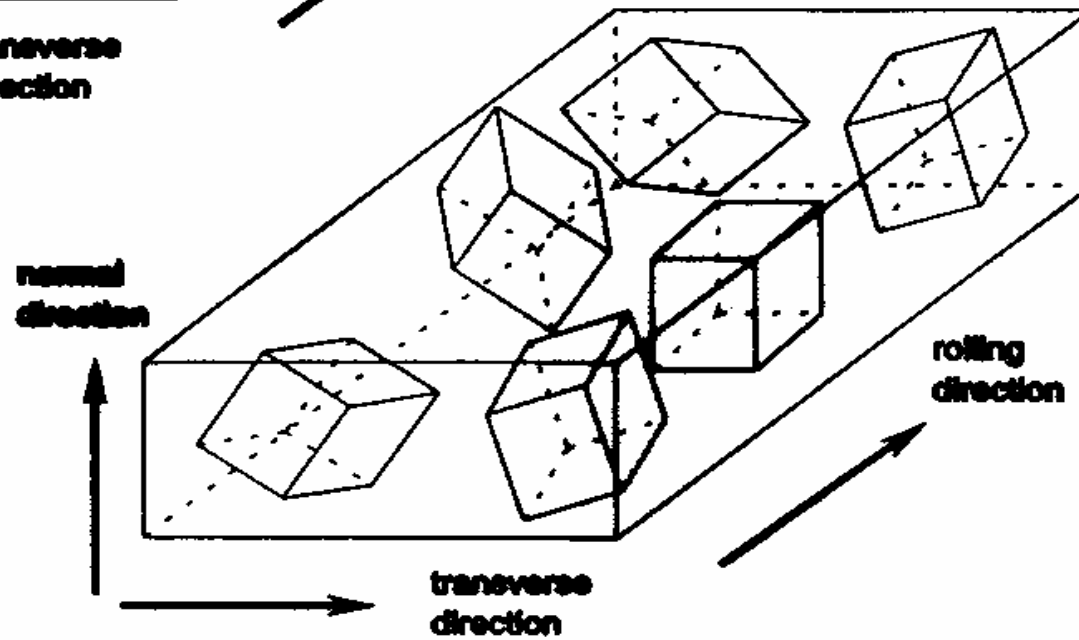
X-ray scanning microdiffraction goniometer

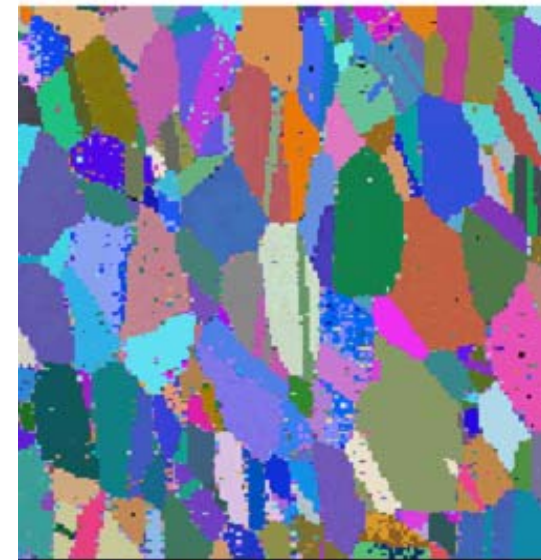
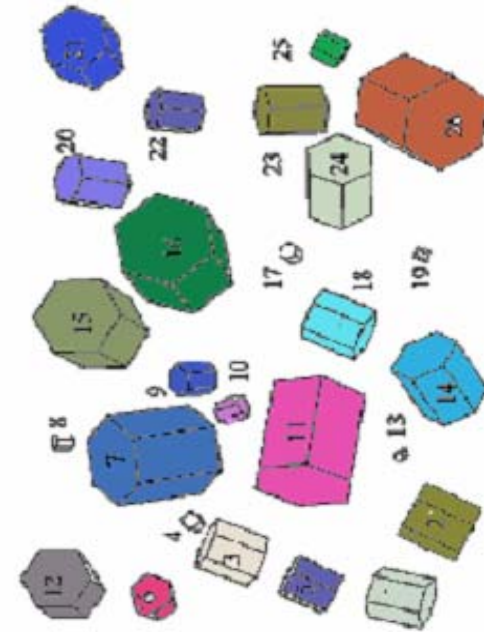
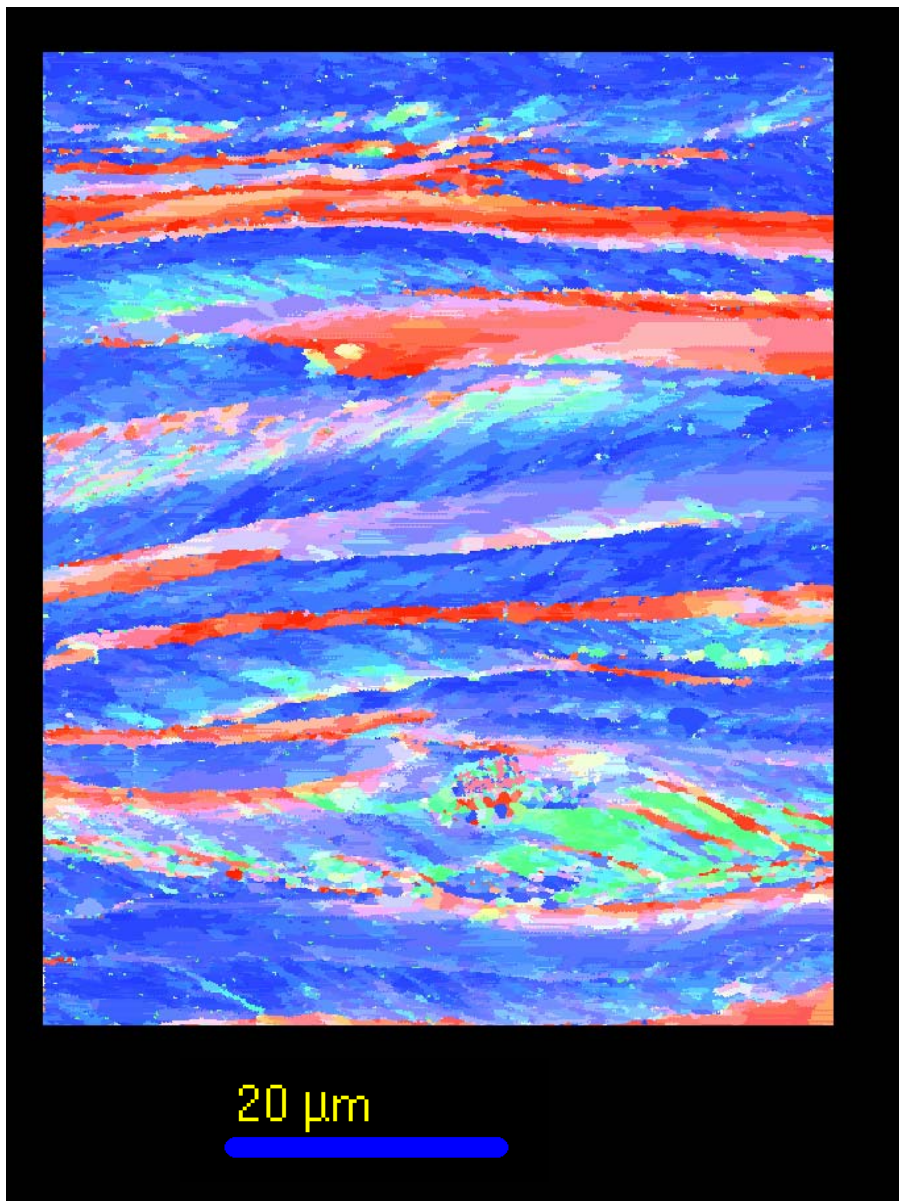


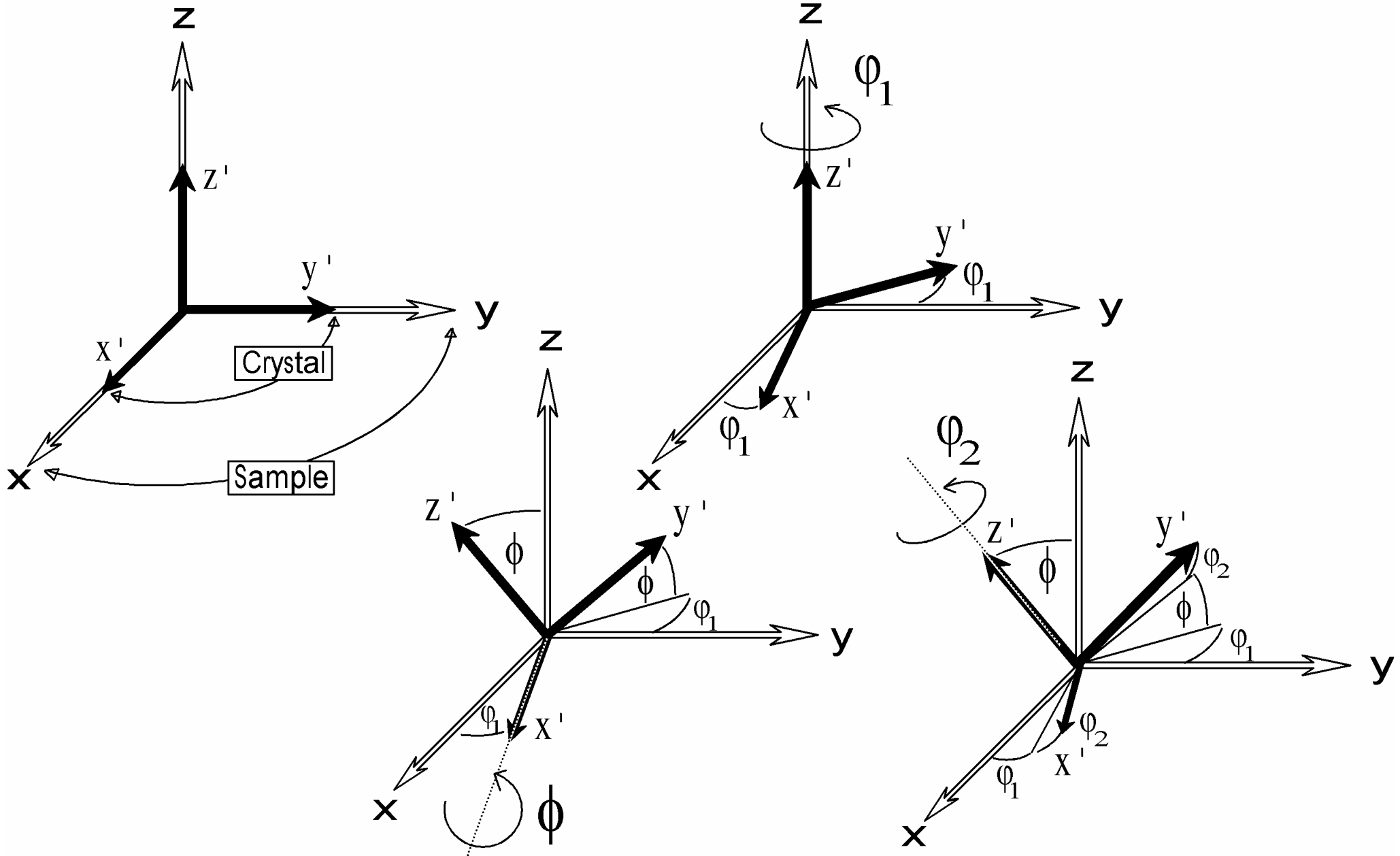
Scharfe Textur



Regellose Textur





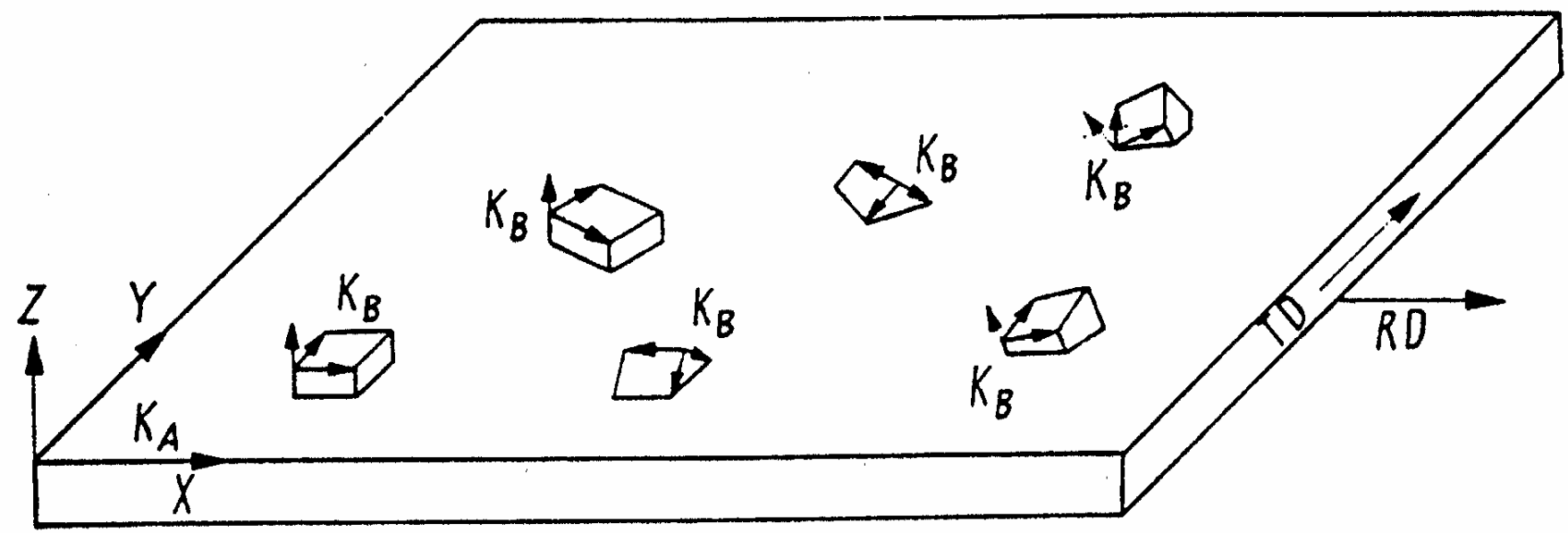
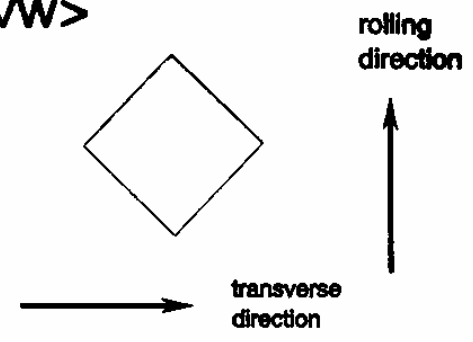


$\varphi_1 \Phi \varphi_2$

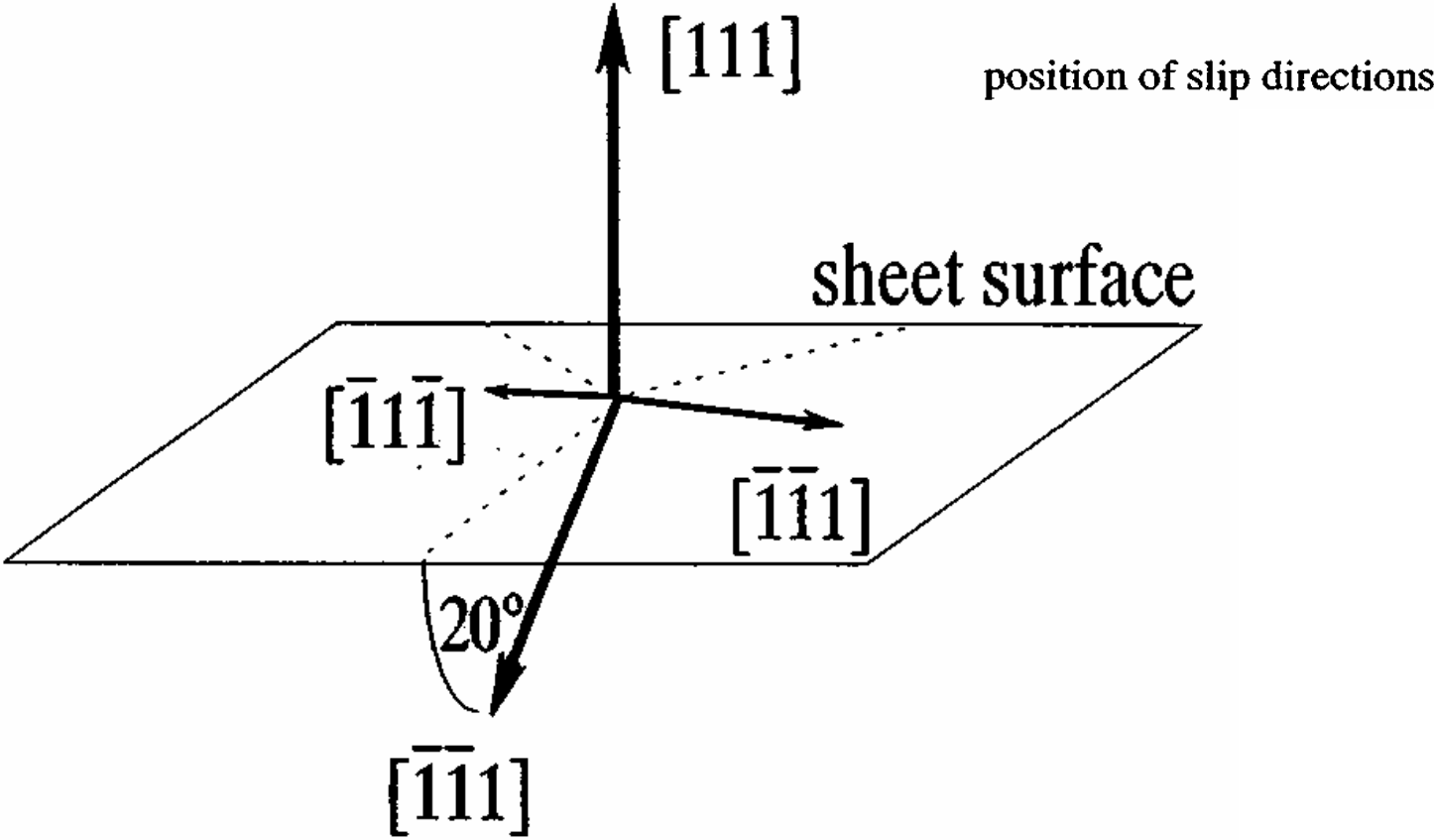
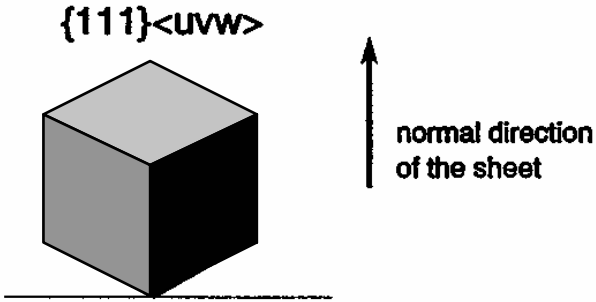
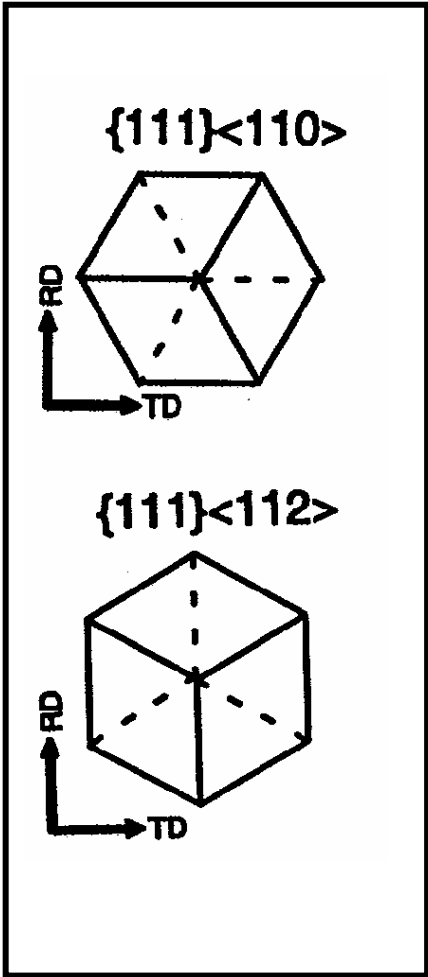
Miller Indices

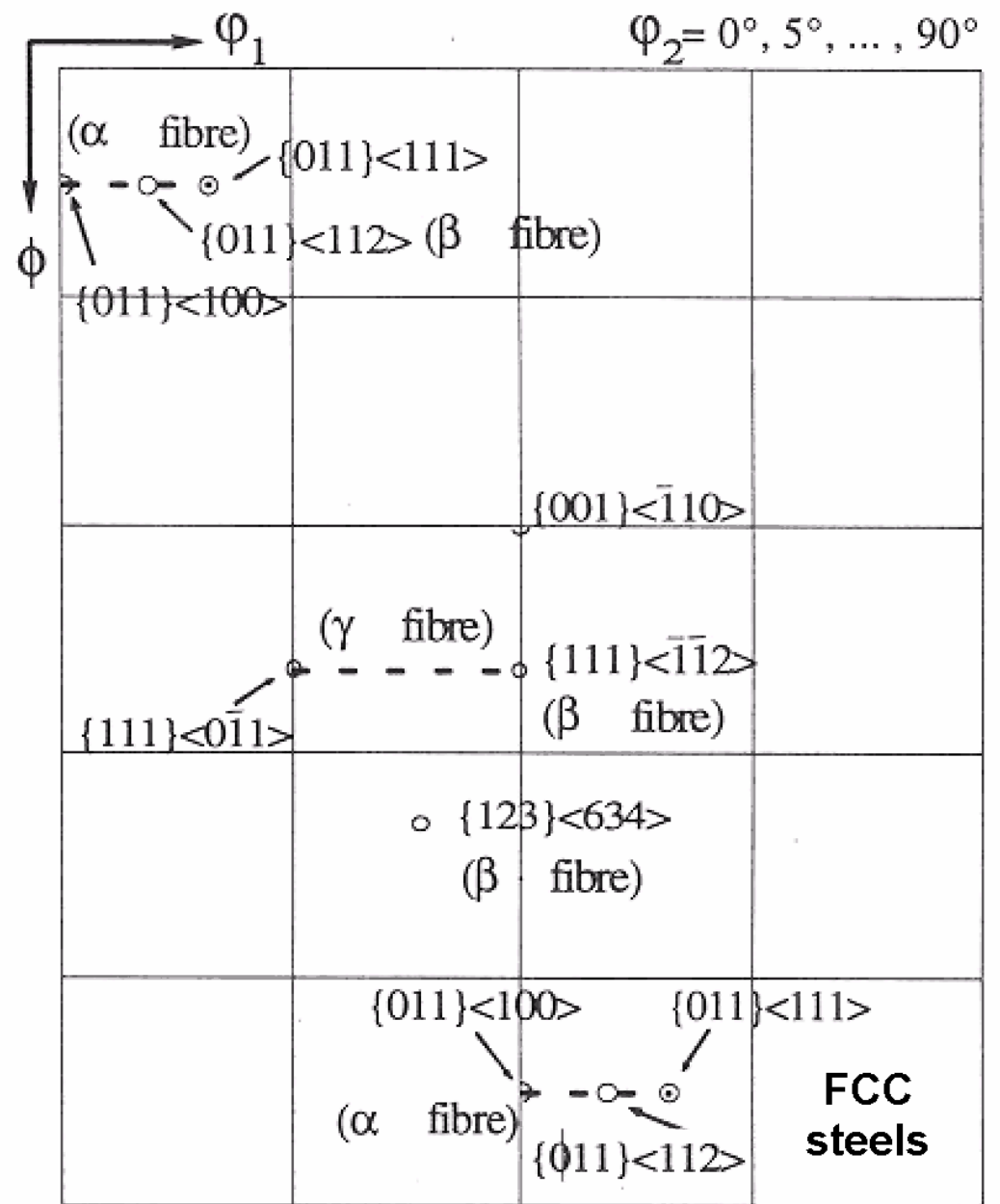
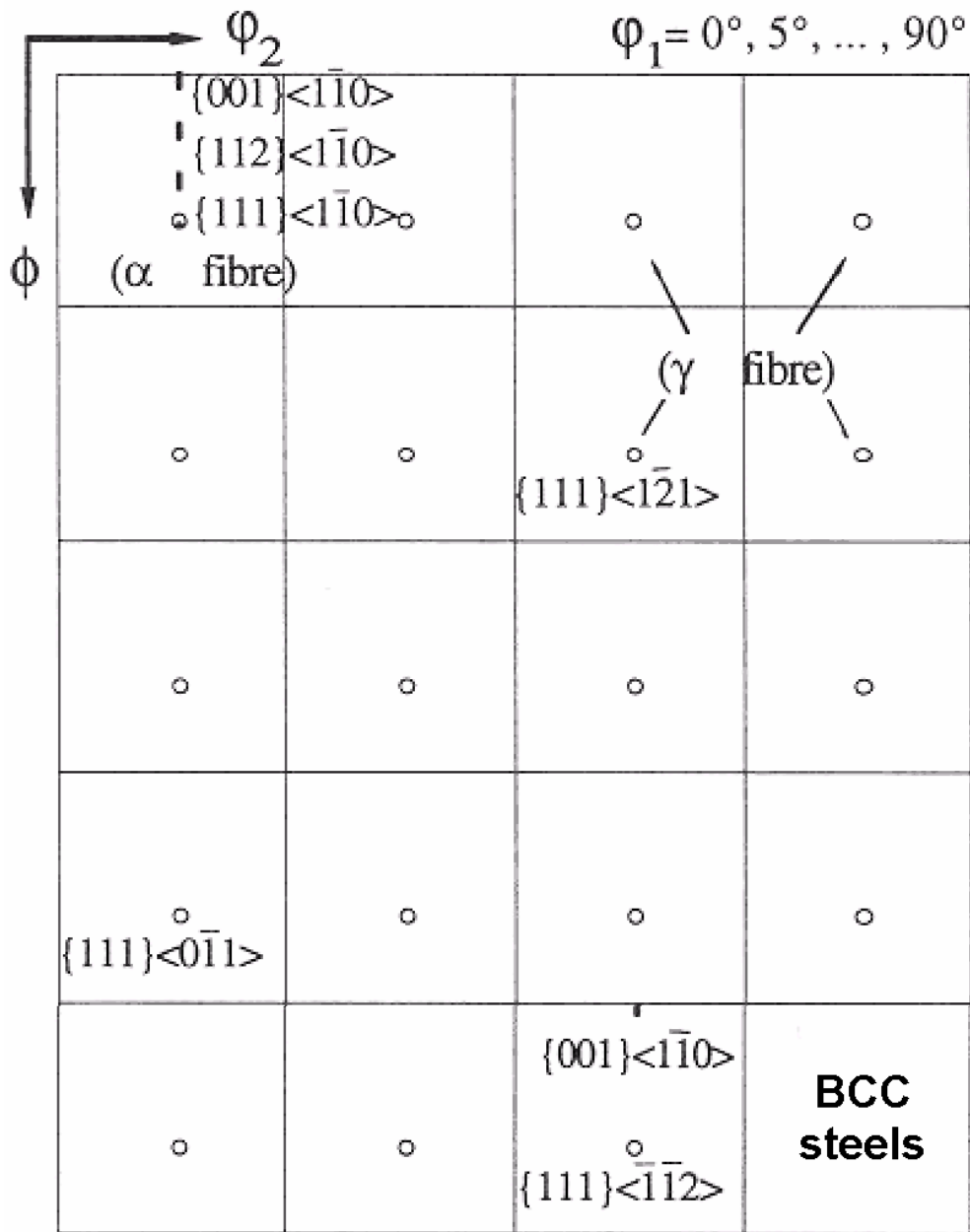
$\{hkl\}\langle uvw \rangle$

$\{001\}\langle 110 \rangle$



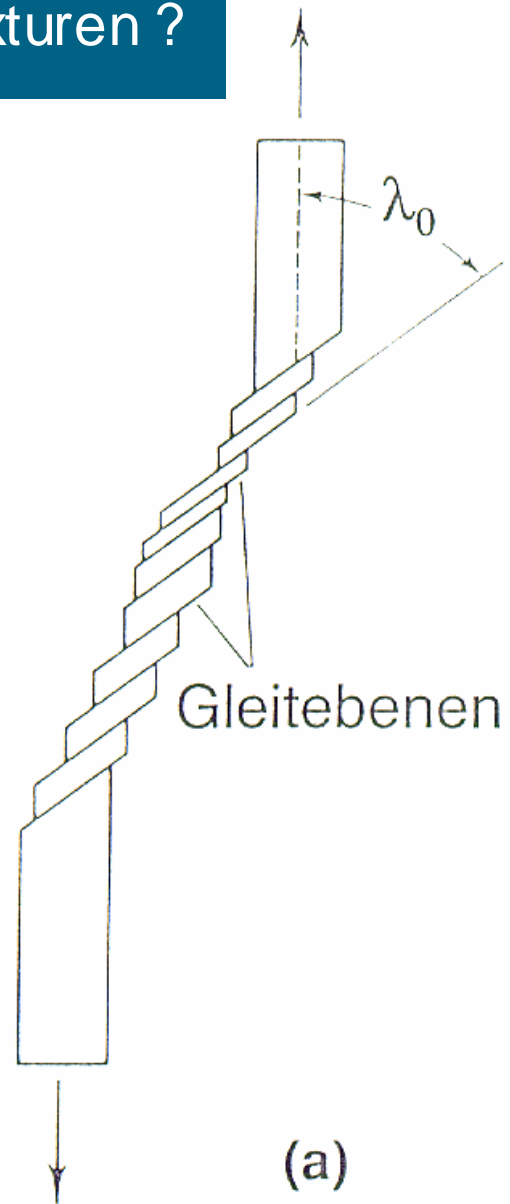
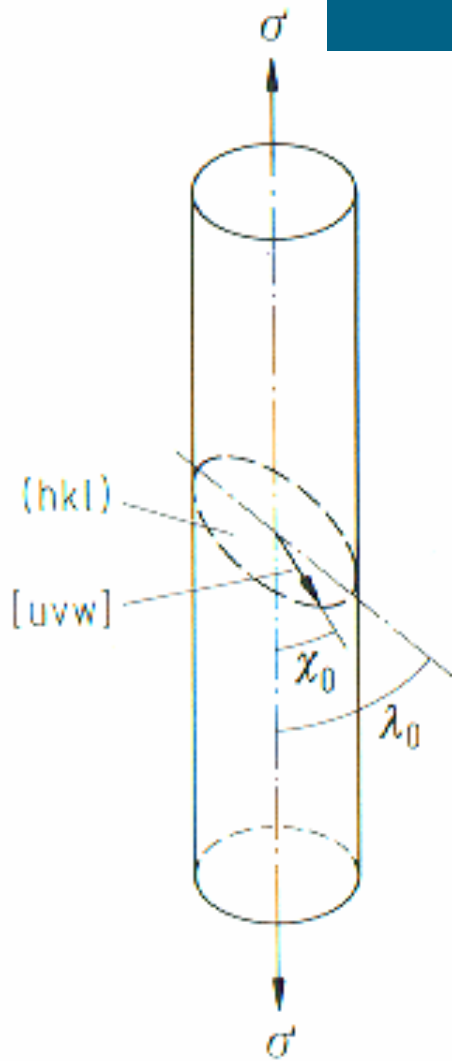
γ – Faser

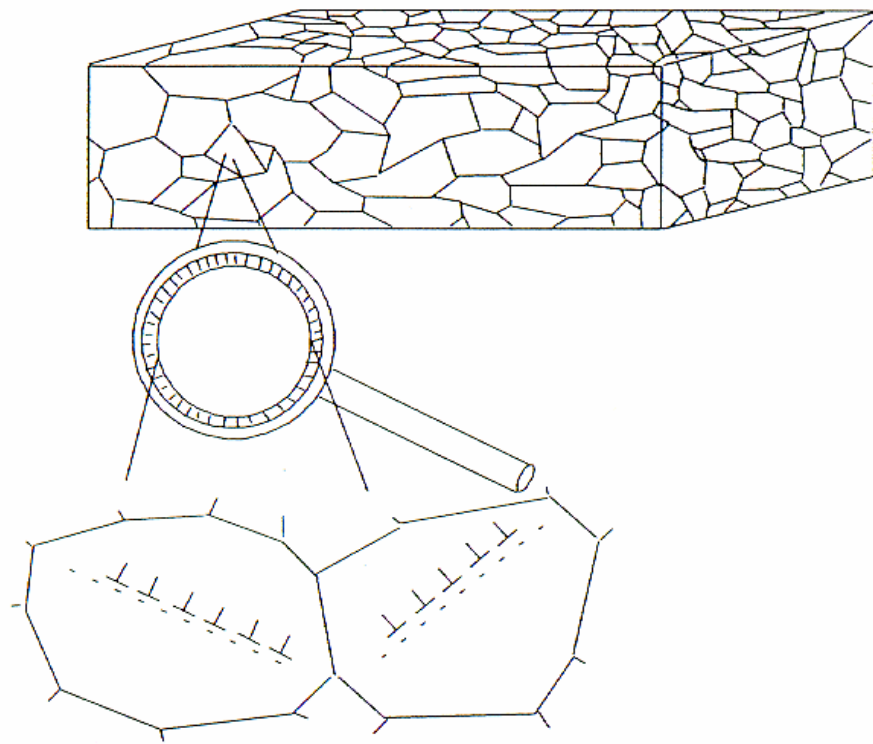




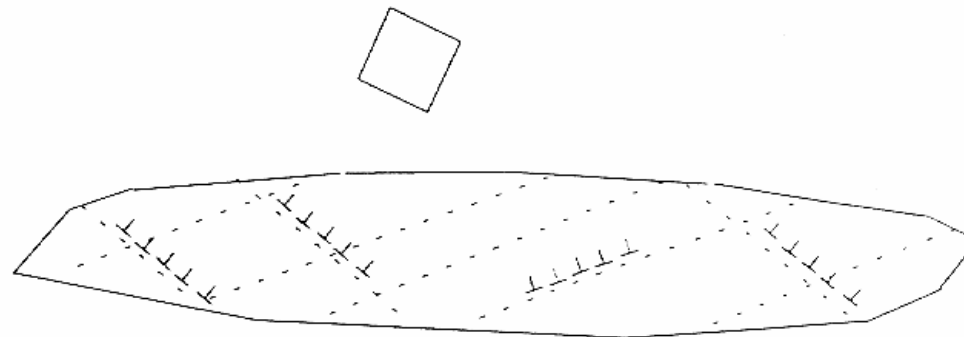
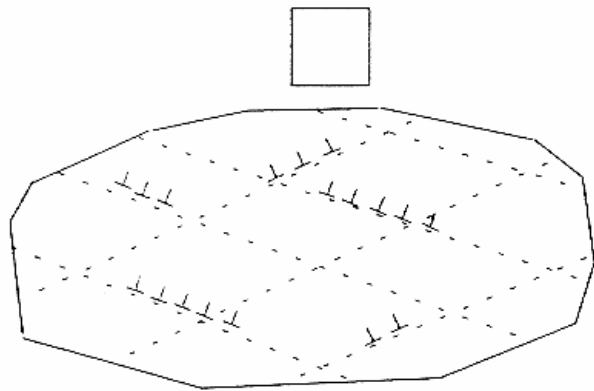
Umform-Texturen

Wie entstehen Texturen ?

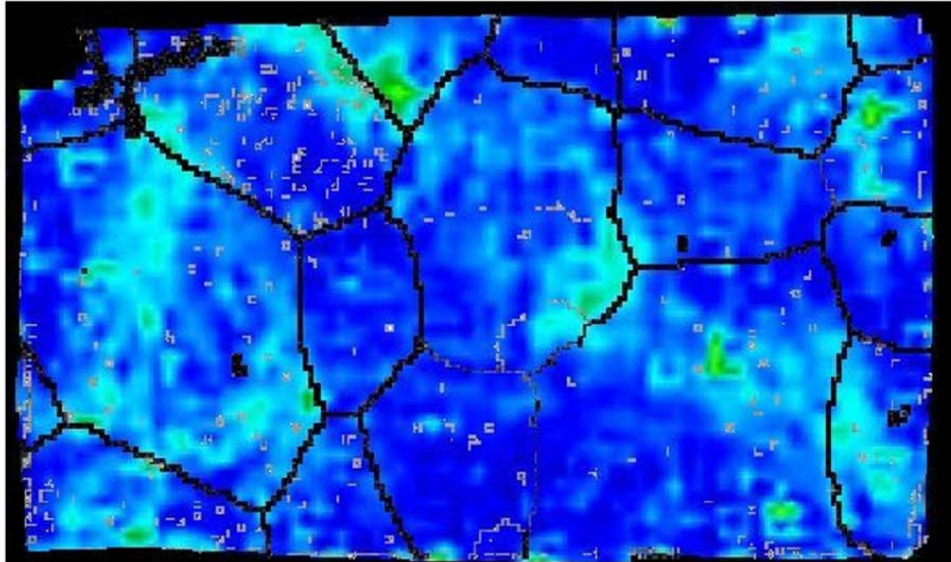




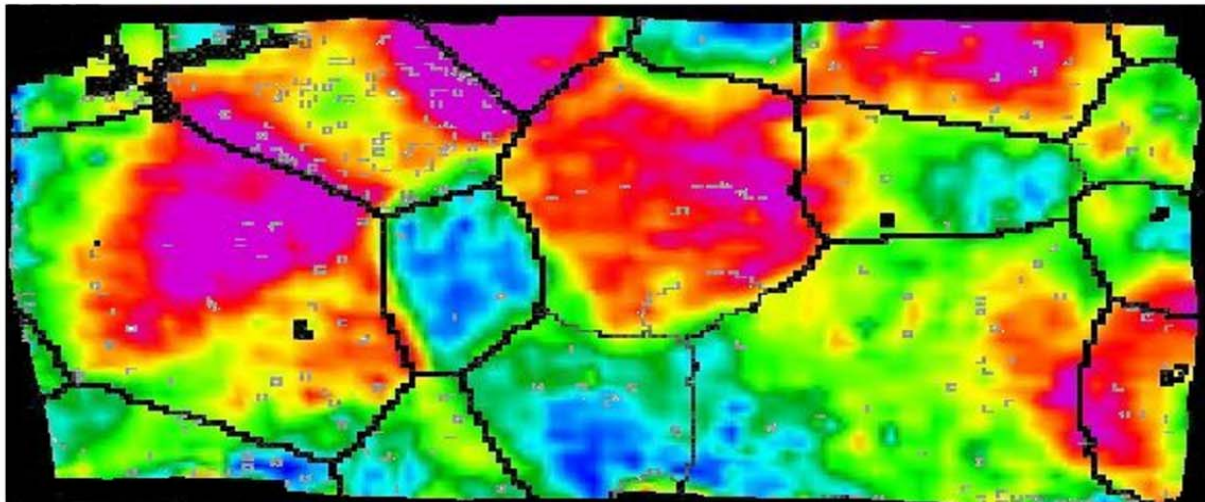
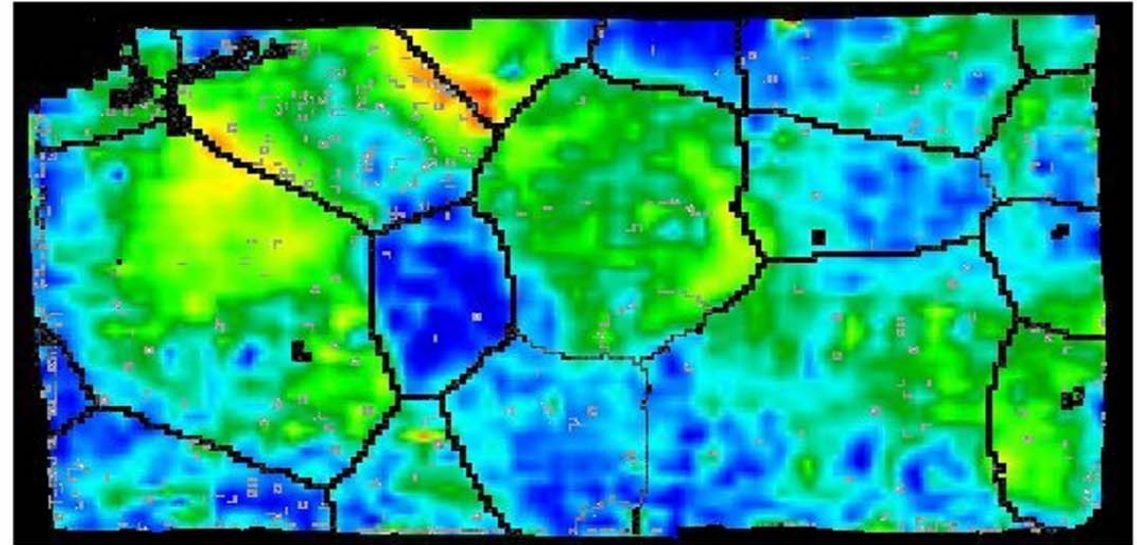
$$\epsilon_{ij} = \frac{1}{2} \sum_{s=1}^5 (n_i^s b_j^s + n_j^s b_i^s) \gamma^s$$



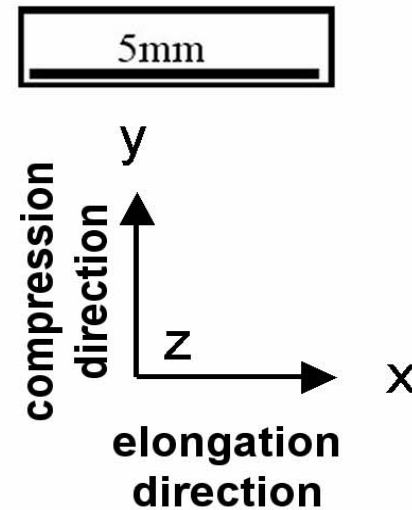
3%



8%



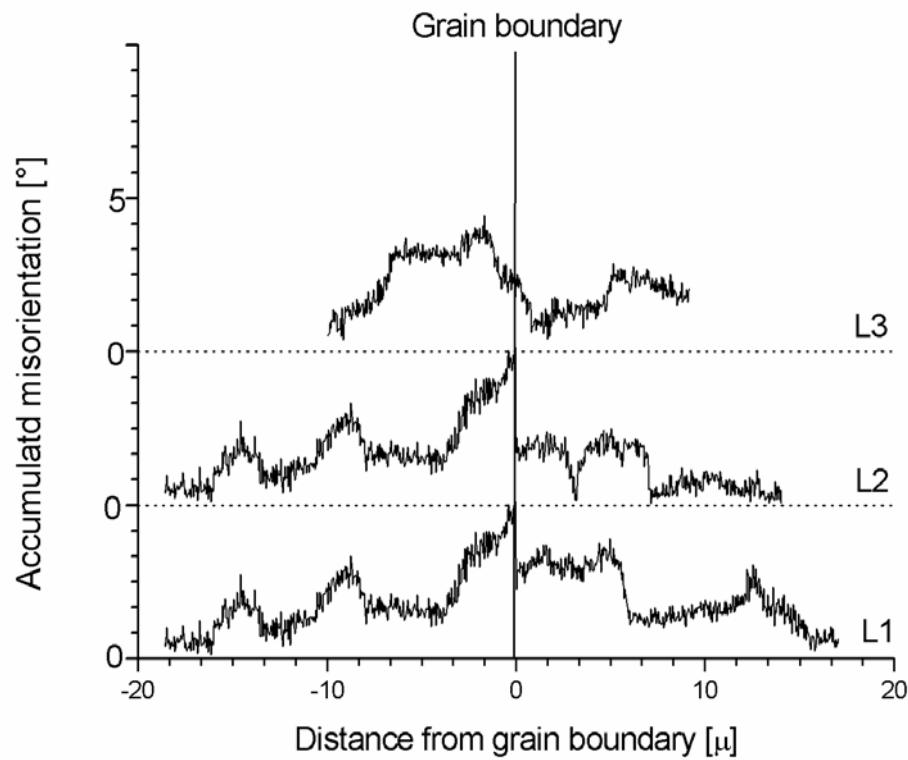
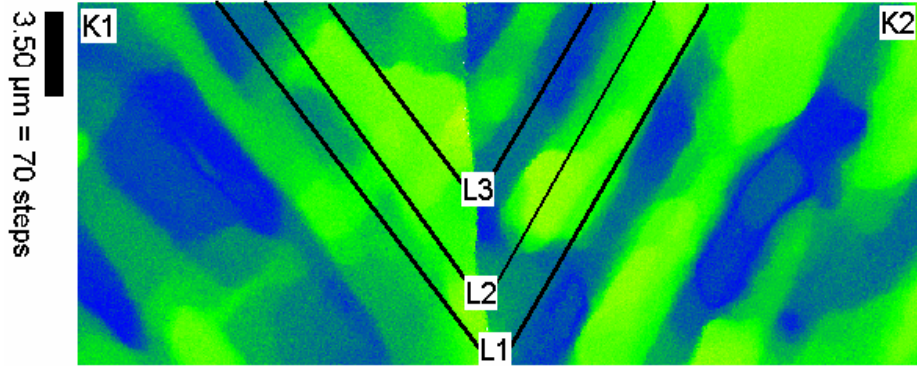
15%



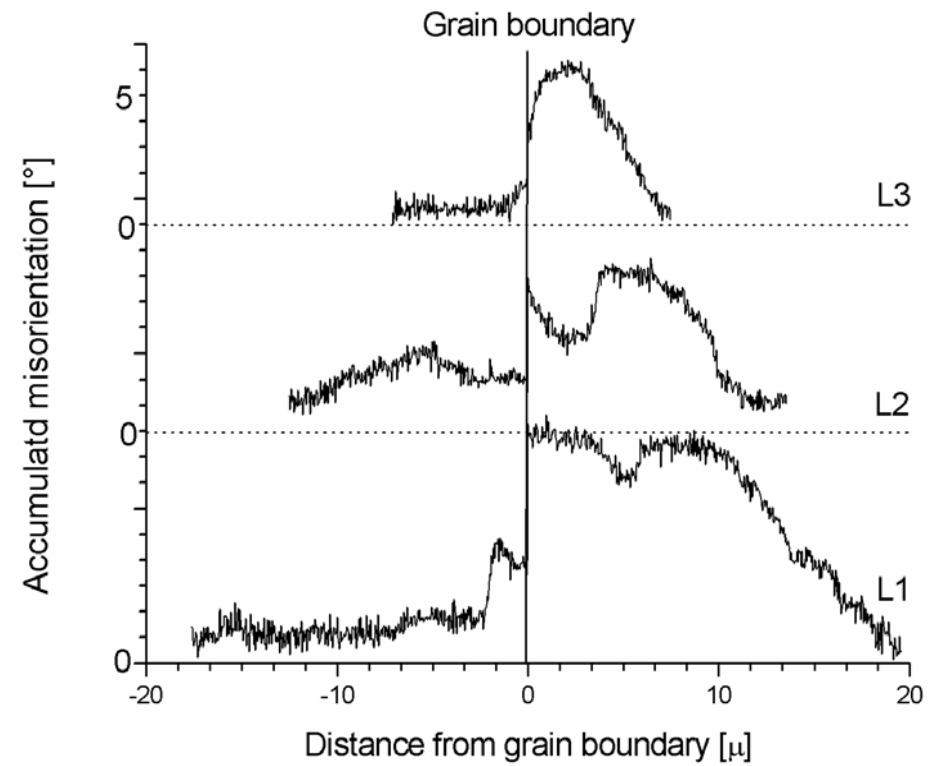
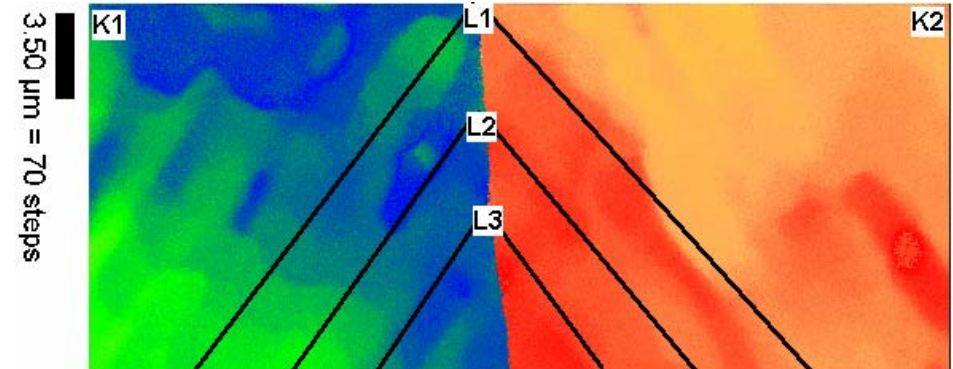
accumulated
von Mises
strain



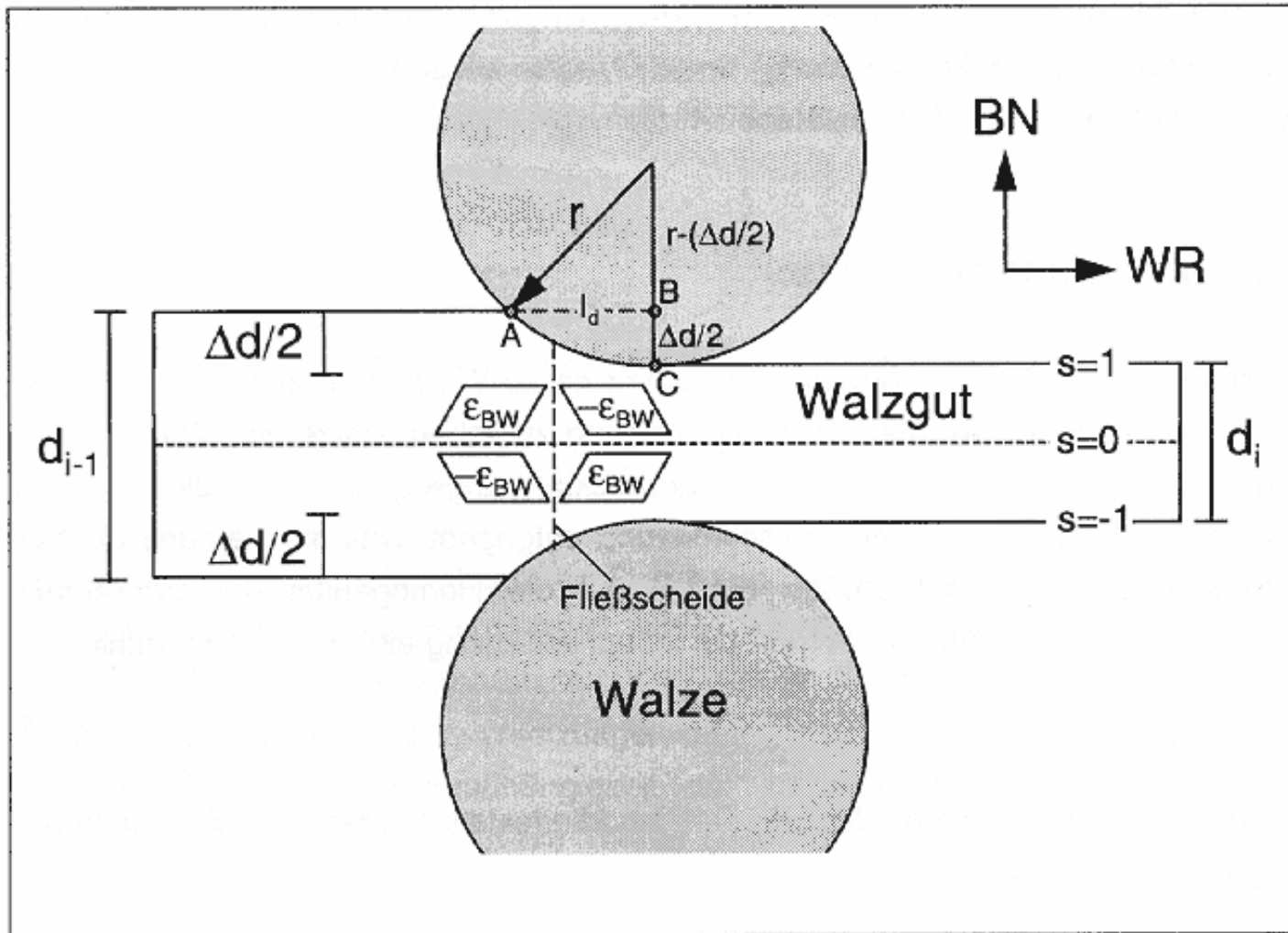
7.8°, 30% reduction



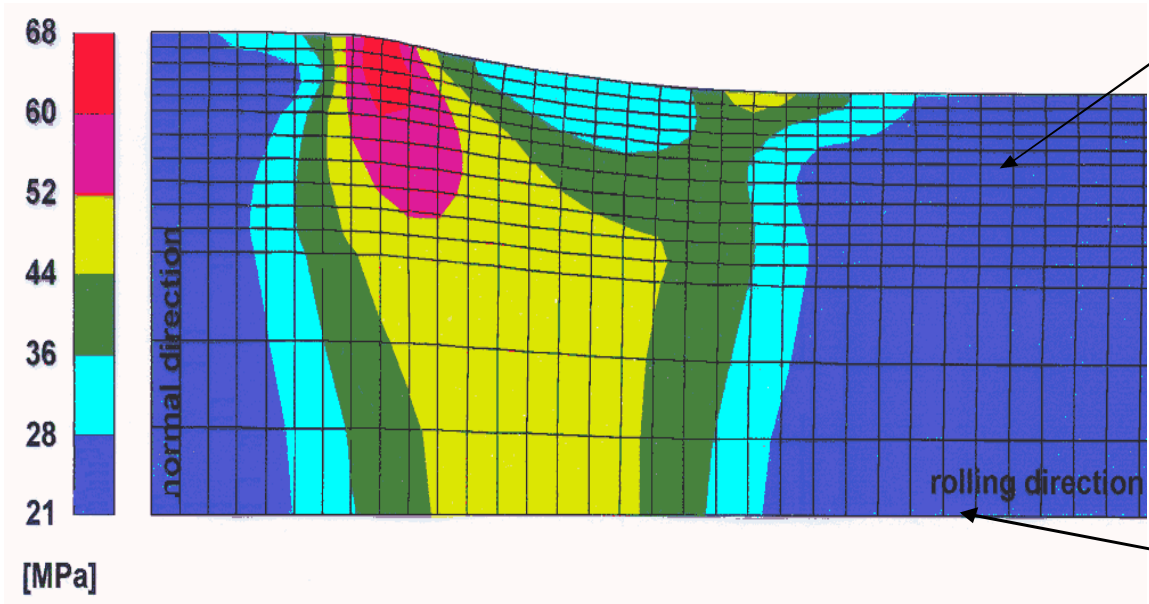
34.8°, 30% reduction



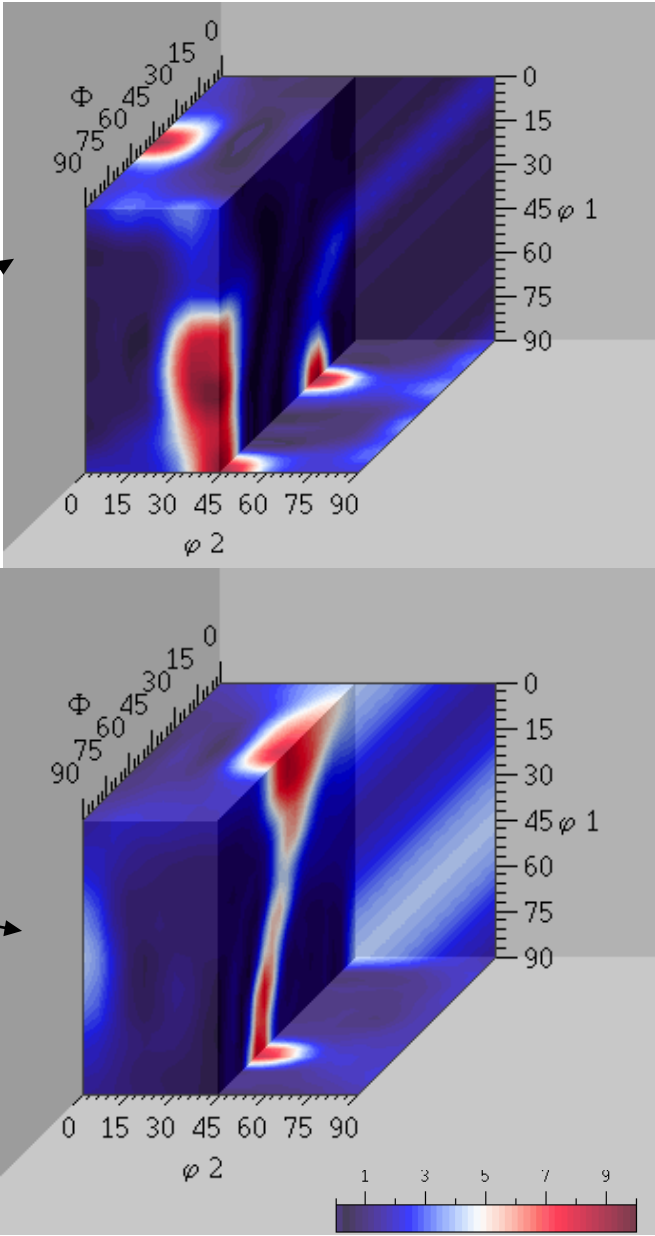
Warmwalzen

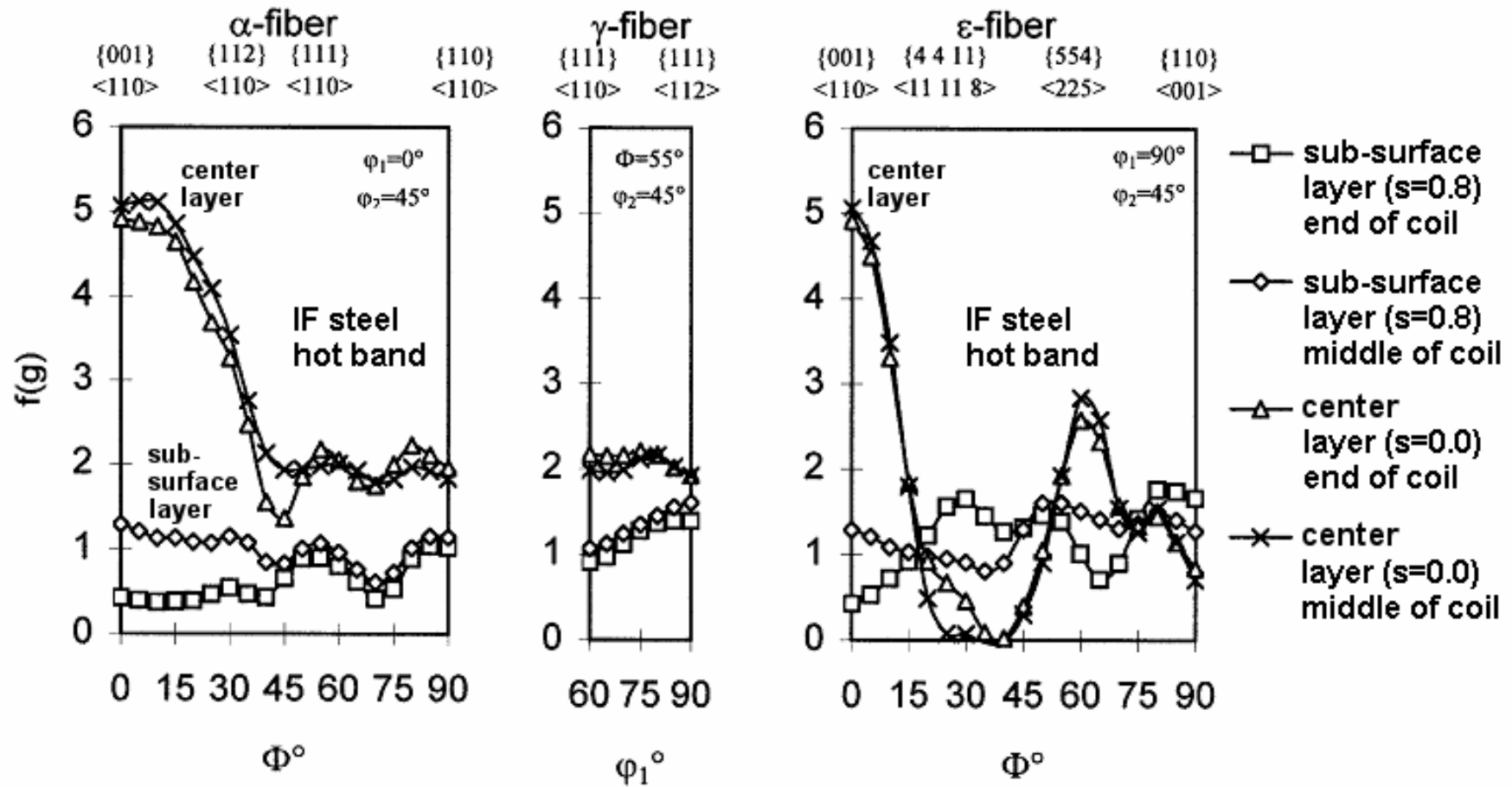


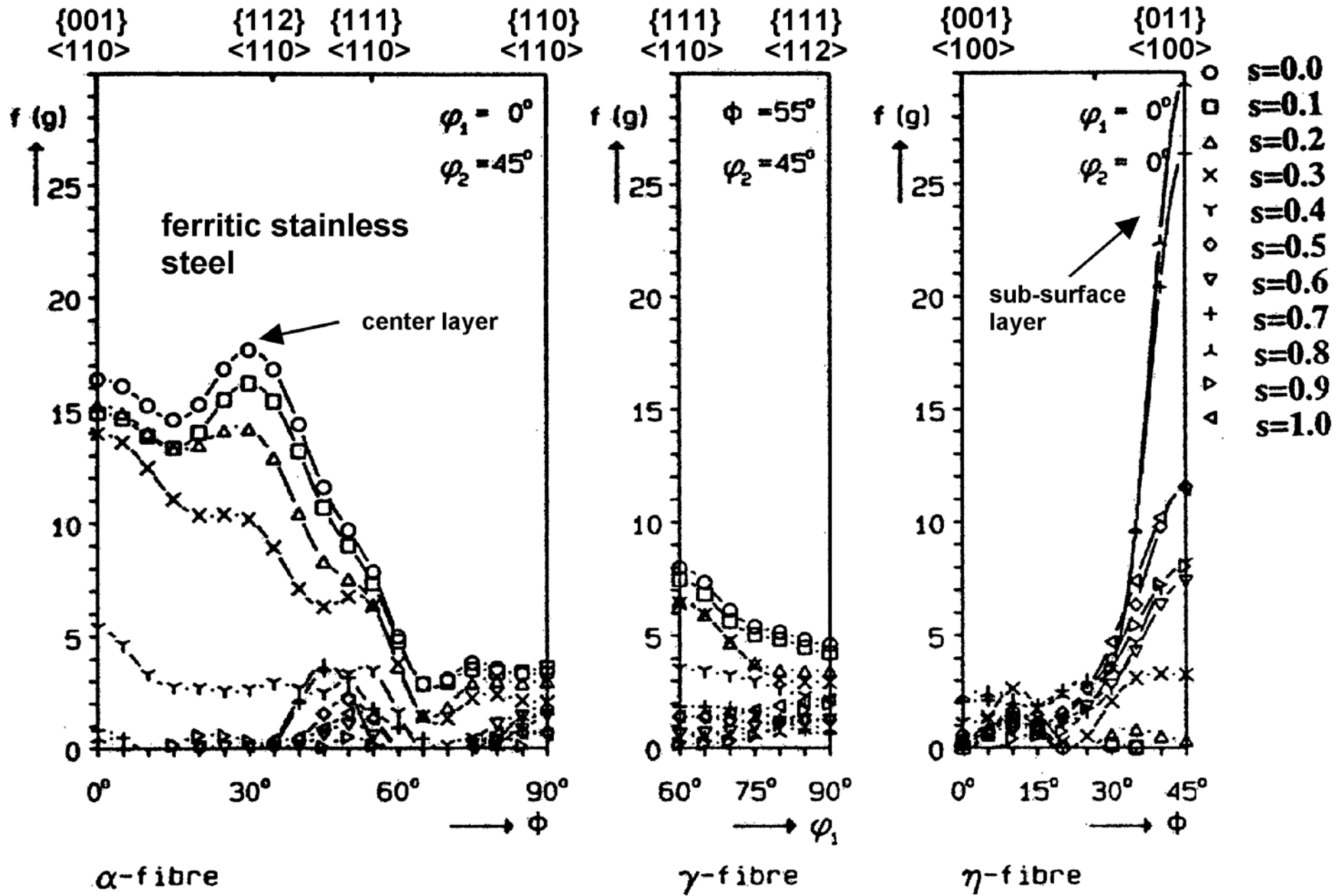
Oberfläche



Mitte

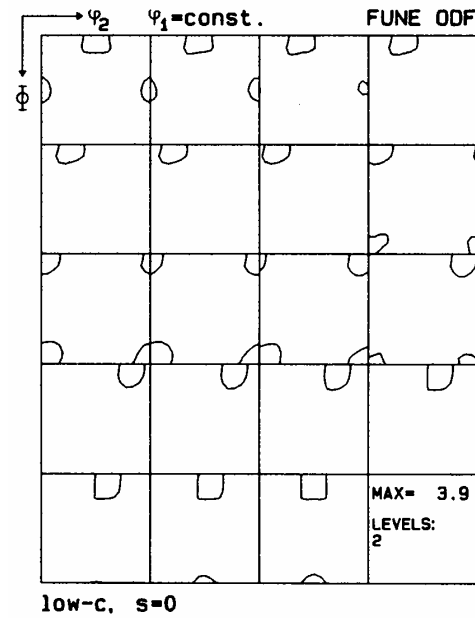






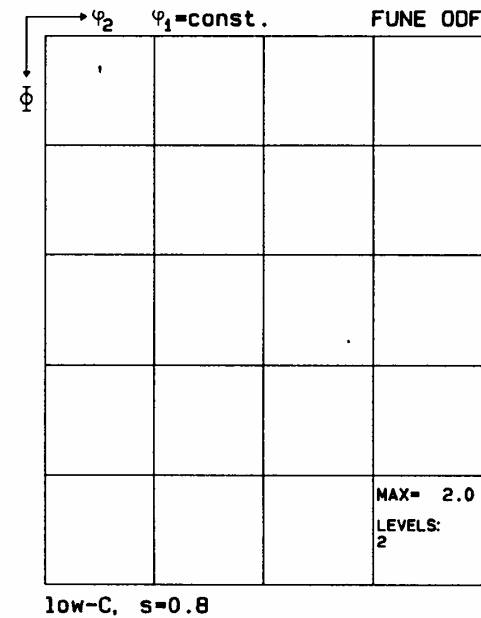
Mitte

low-C



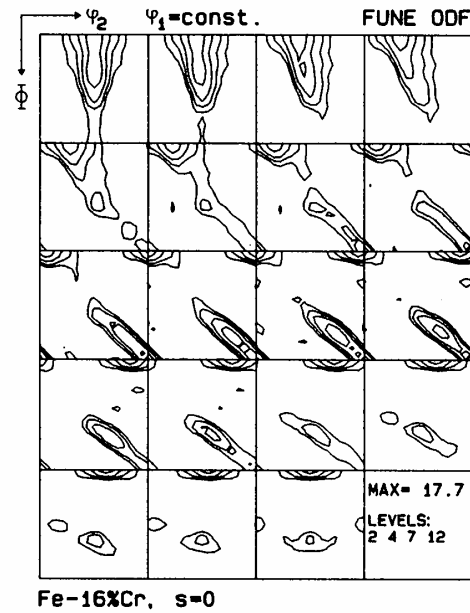
Oberfläche

low-C



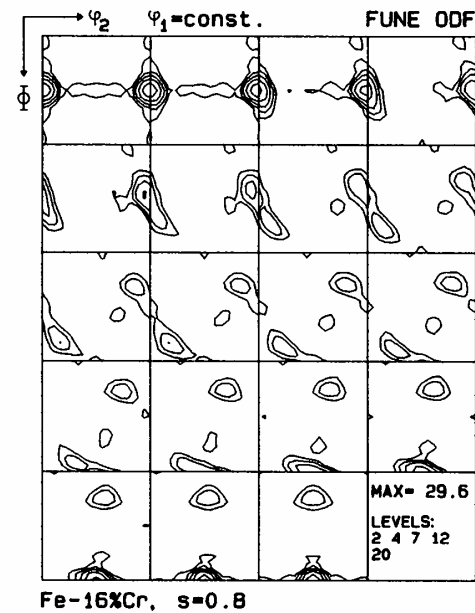
Mitte

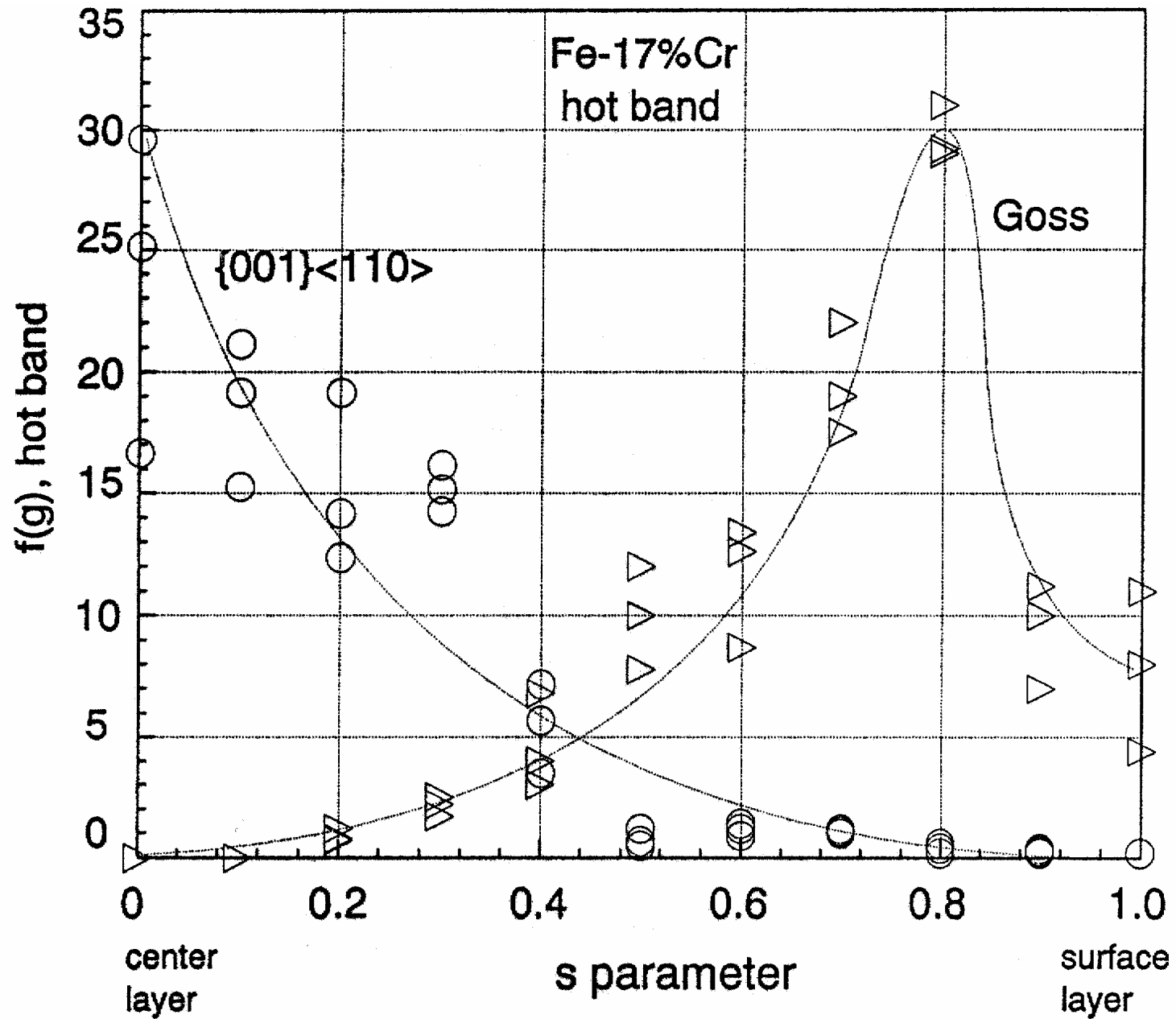
Fe-Cr

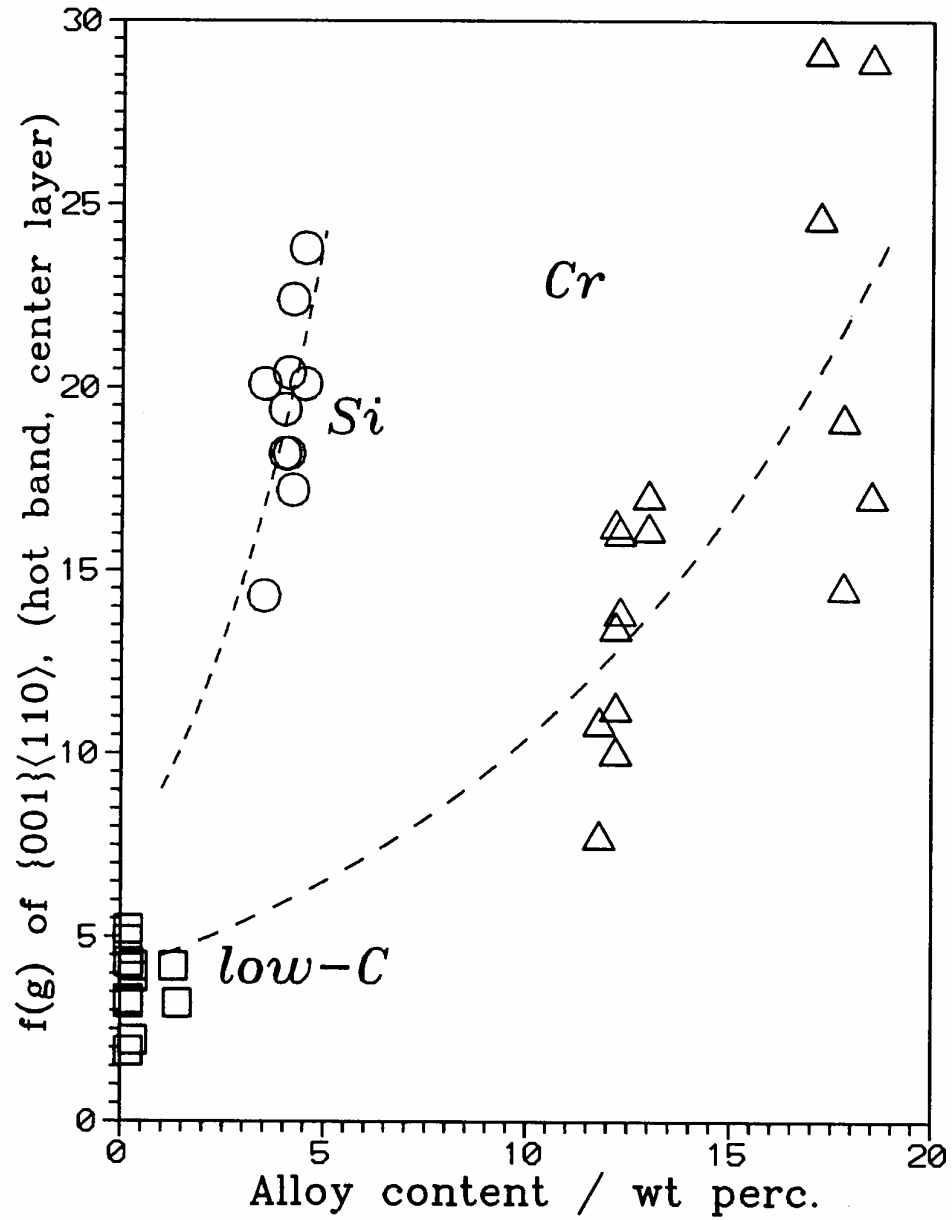


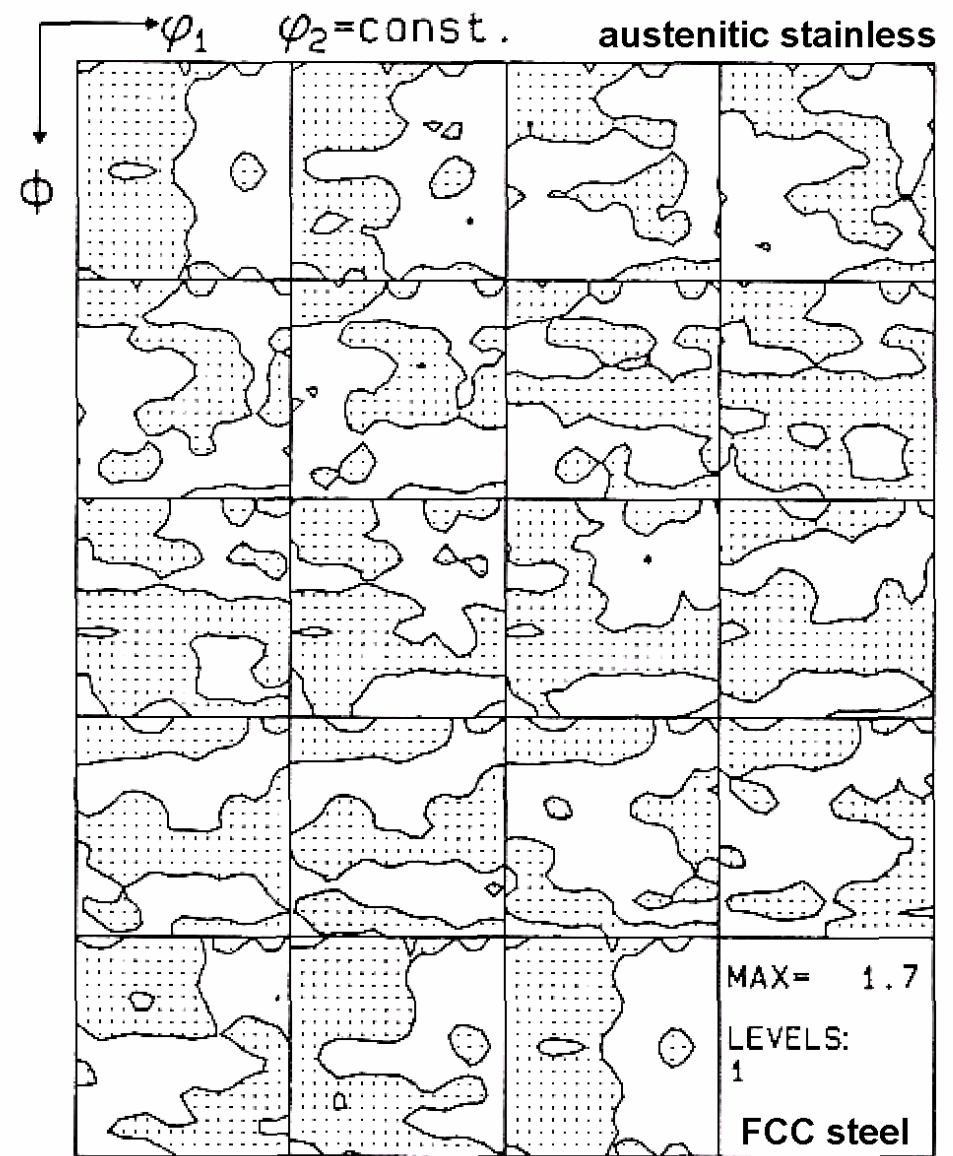
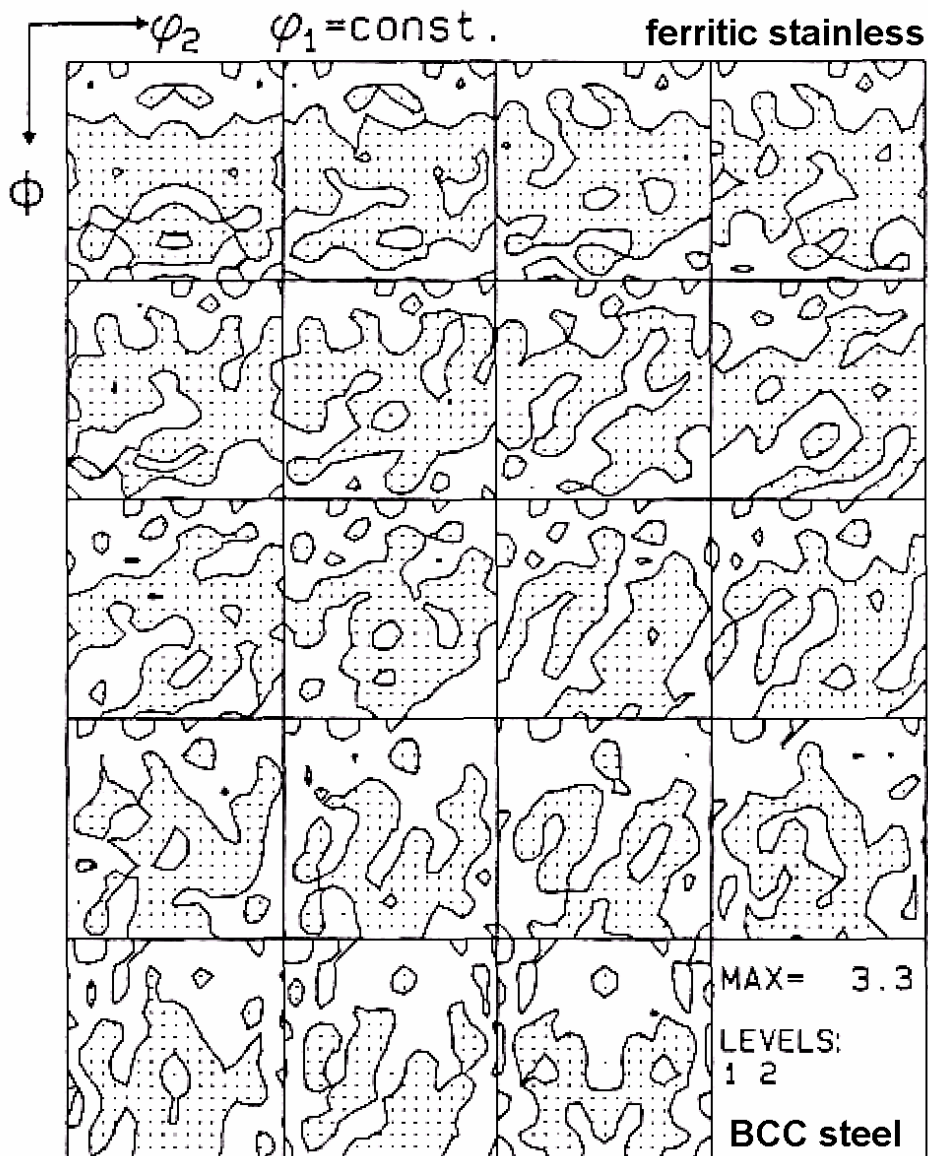
Oberfläche

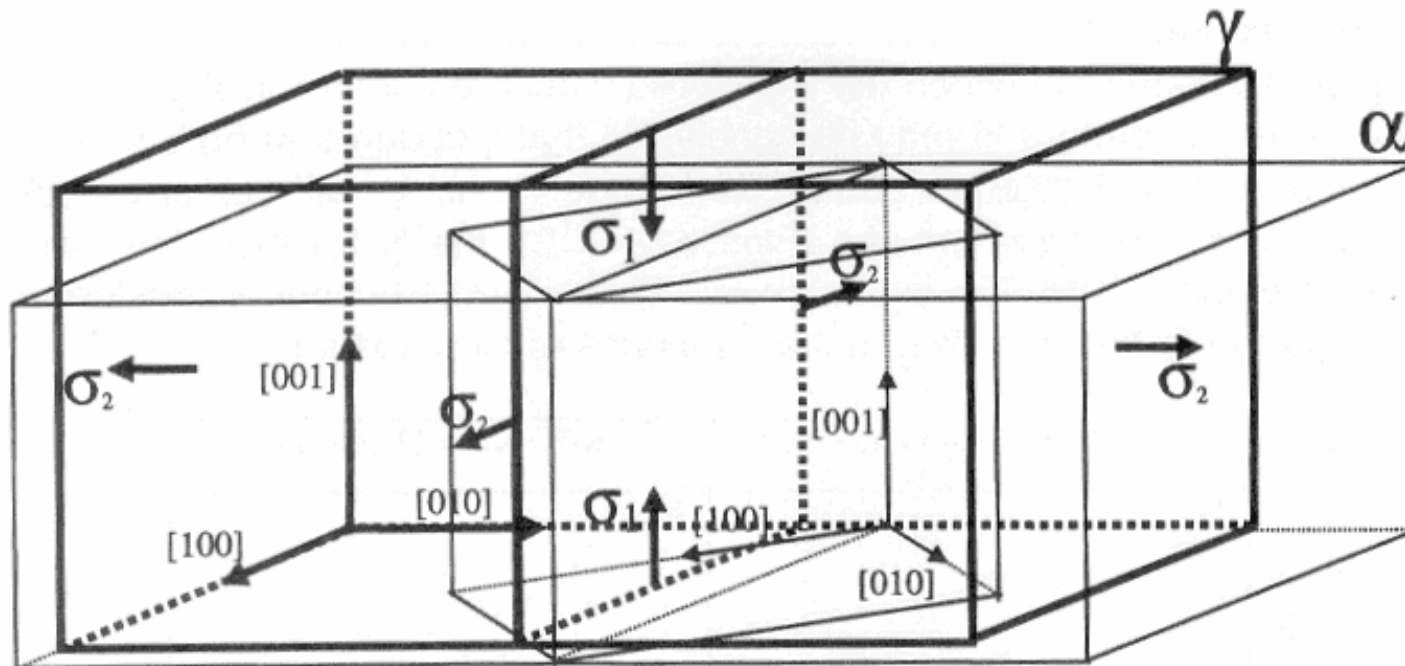
Fe-Cr





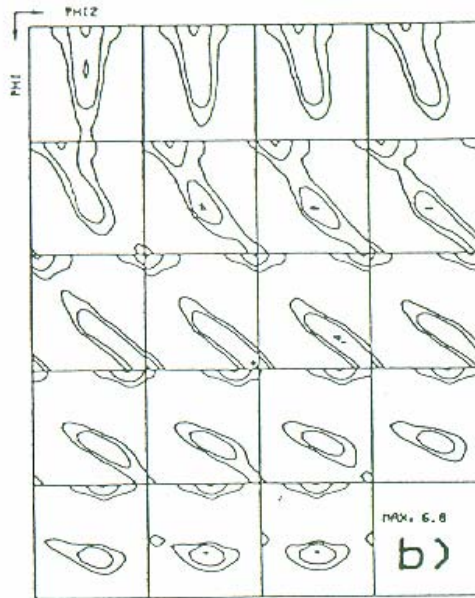
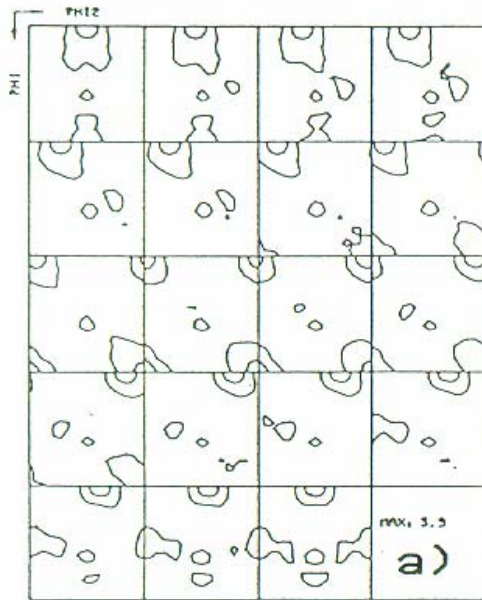






Orientierung nach Umwandlung	Orientierung im Austenit
$\{332\}\langle 113\rangle_{\alpha}$	$\{110\}\langle 112\rangle_{\gamma}$ rolled γ texture component (brass component)
$\{113\}\langle 110\rangle_{\alpha}$	$\{11\bar{2}\}\langle 1\bar{1}1\rangle_{\gamma}$ rolled γ texture component (copper component)
$\{100\}\langle 011\rangle_{\alpha}$	$\{100\}\langle 001\rangle_{\gamma}$ recrystallised γ texture component (cube component)

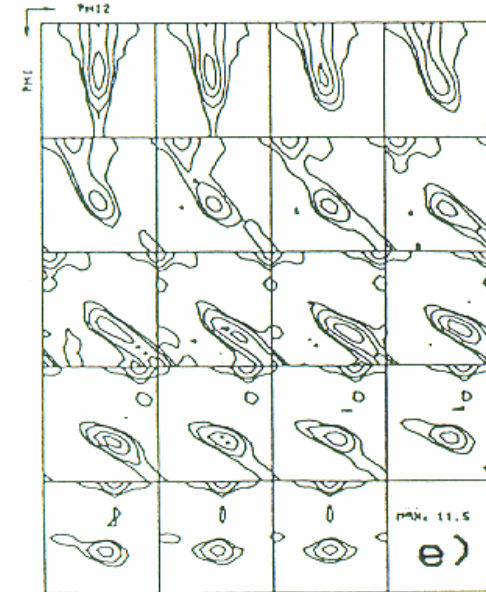
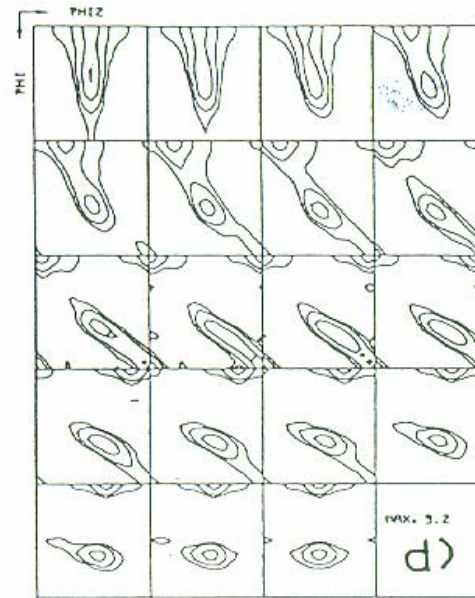
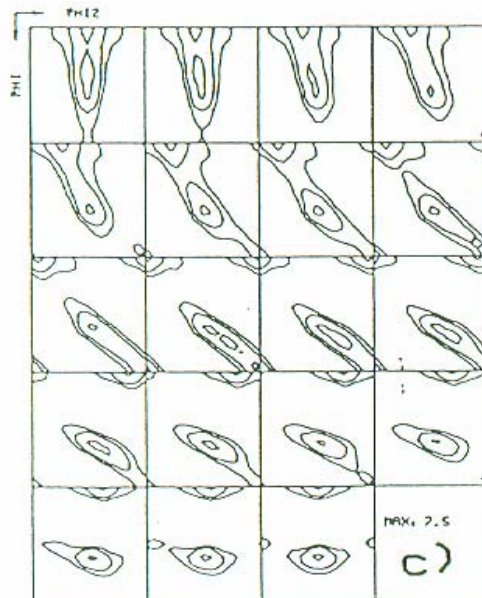




Levels: 1-5-3-6-9
PHI1 = CONST

Kaltwalzen

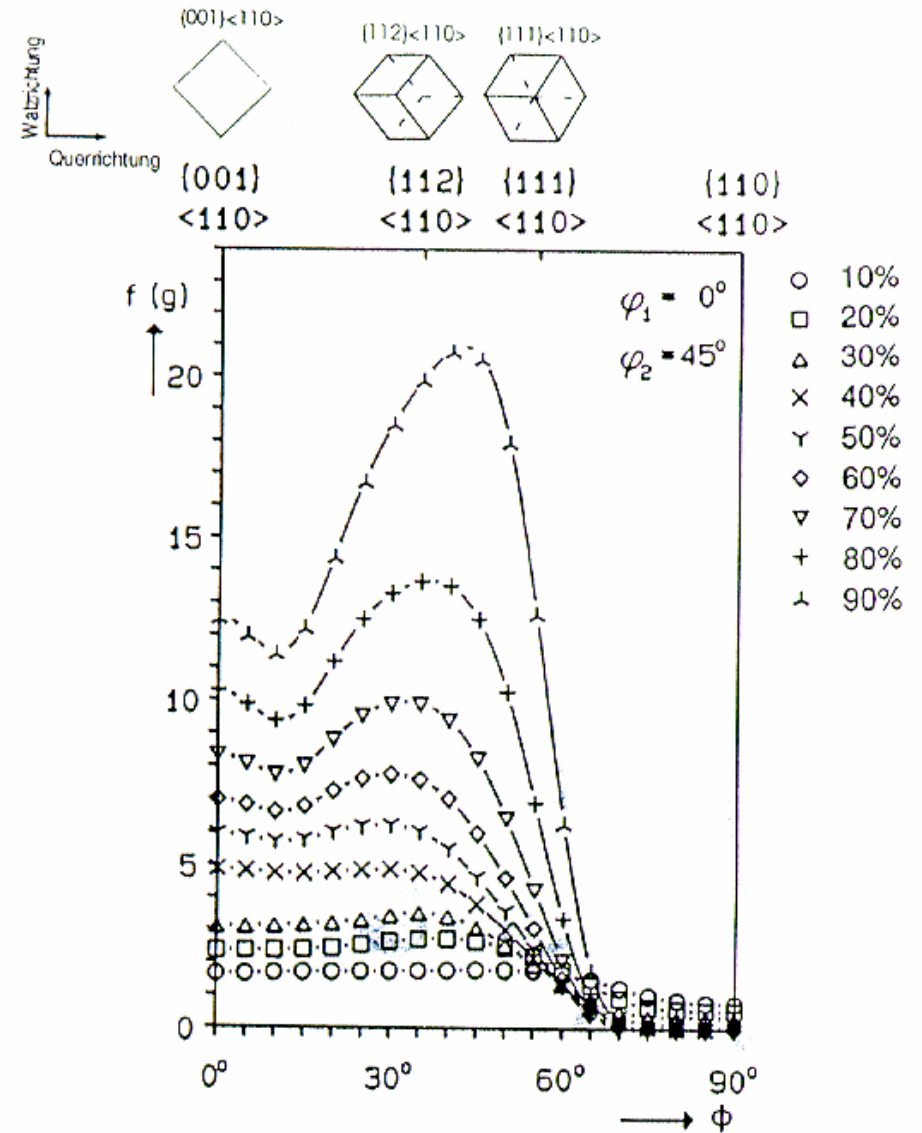
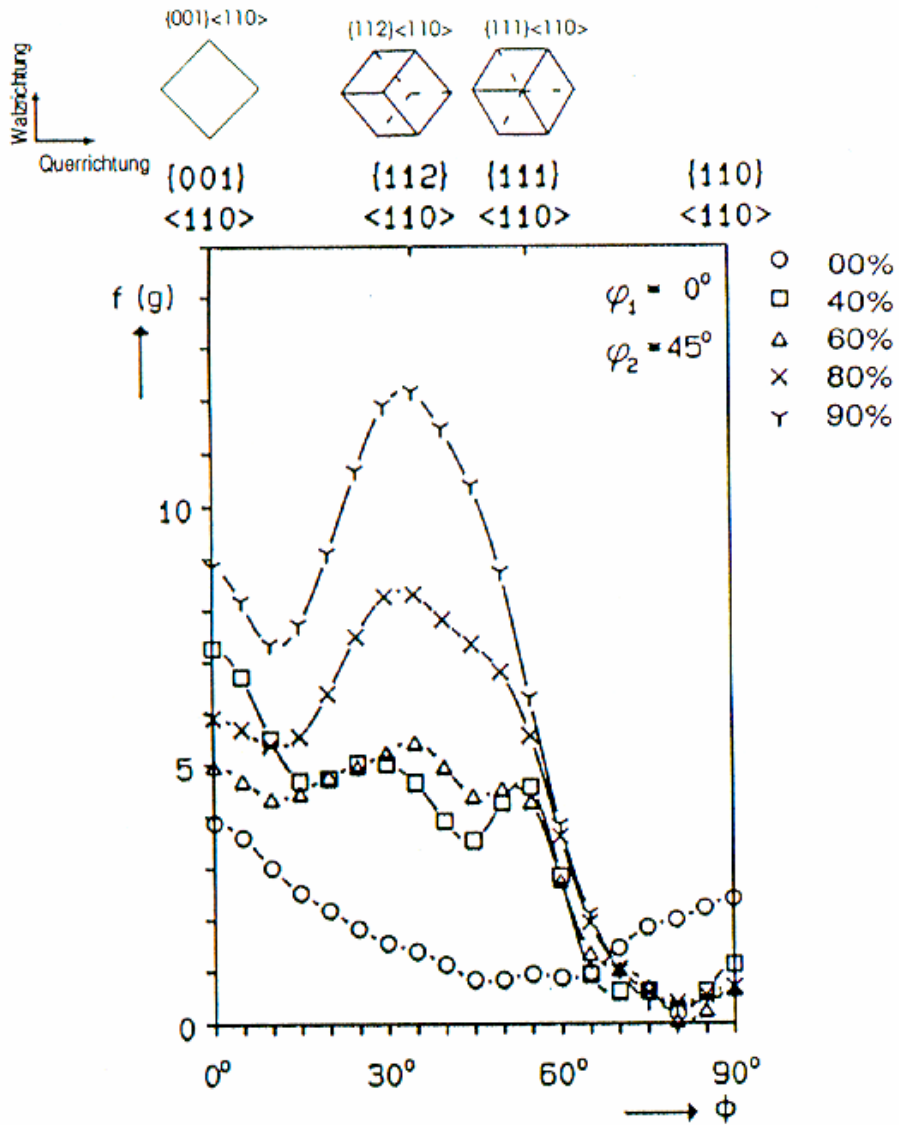
- a) H. B.
- b) 60% C.R.
- c) 70% C.R.
- d) 80% C.R.
- e) 90% C.R.



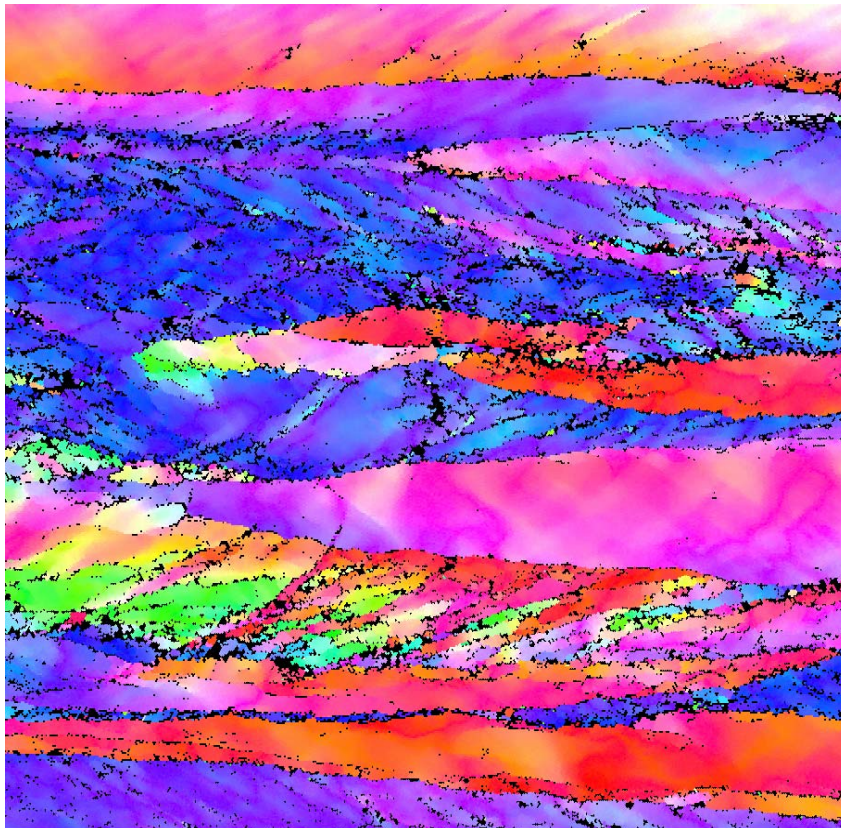
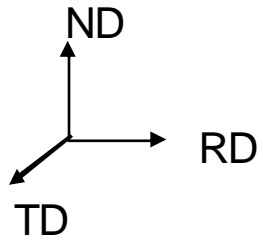
Experiment

Kaltwalzen

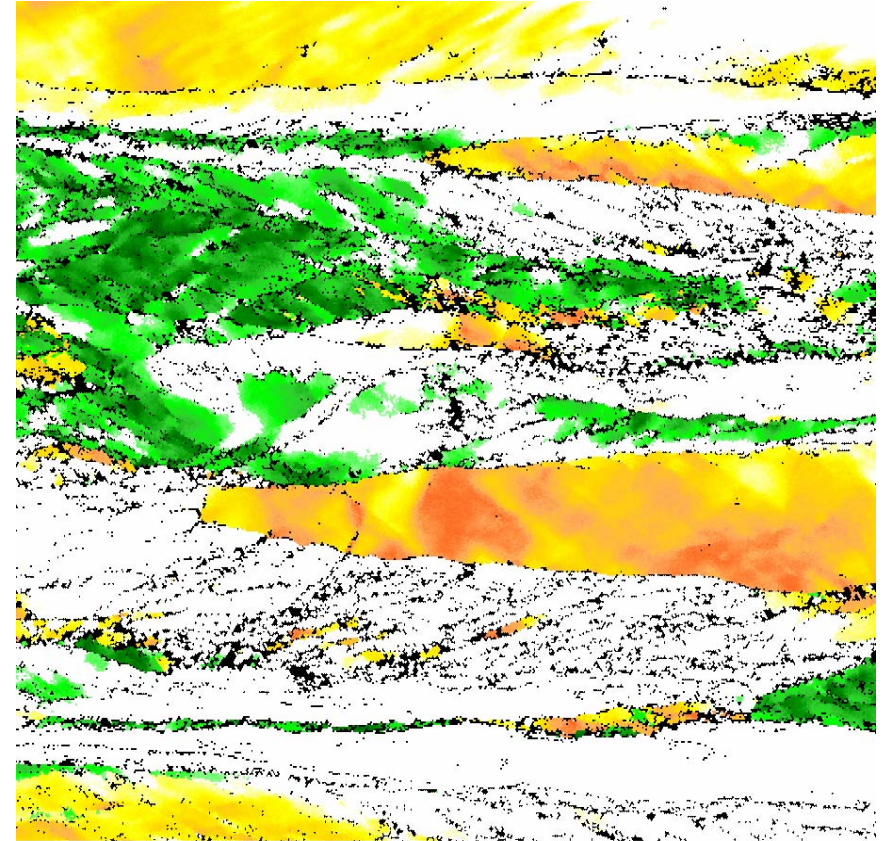
Simulation



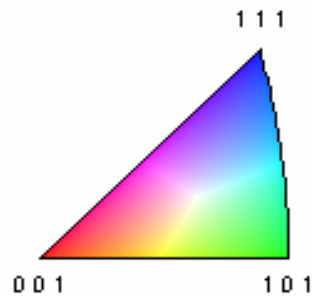
walzhart



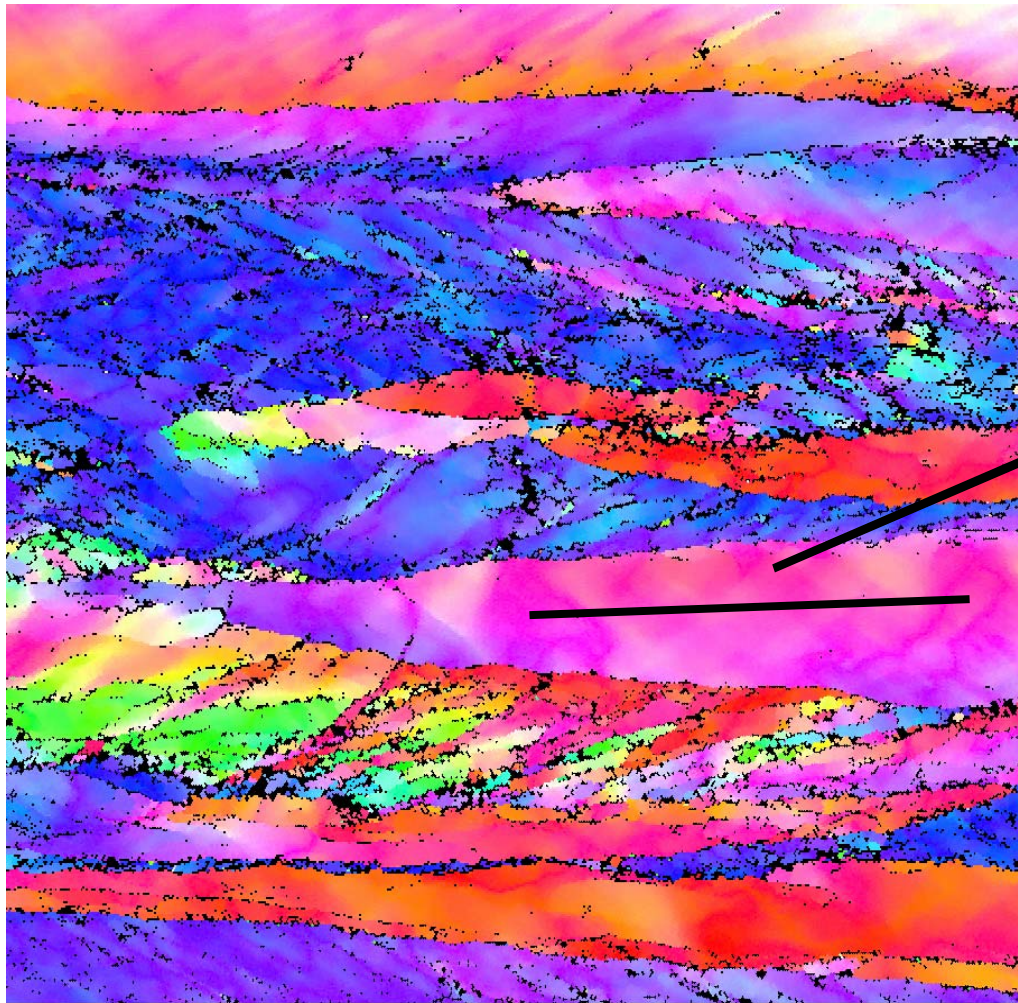
9.00 μm = 90 steps IPF [001]



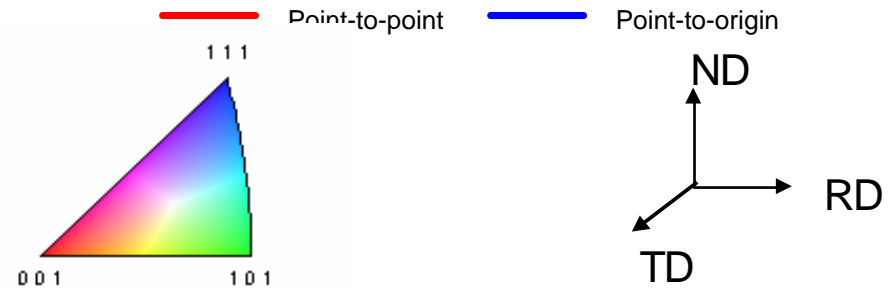
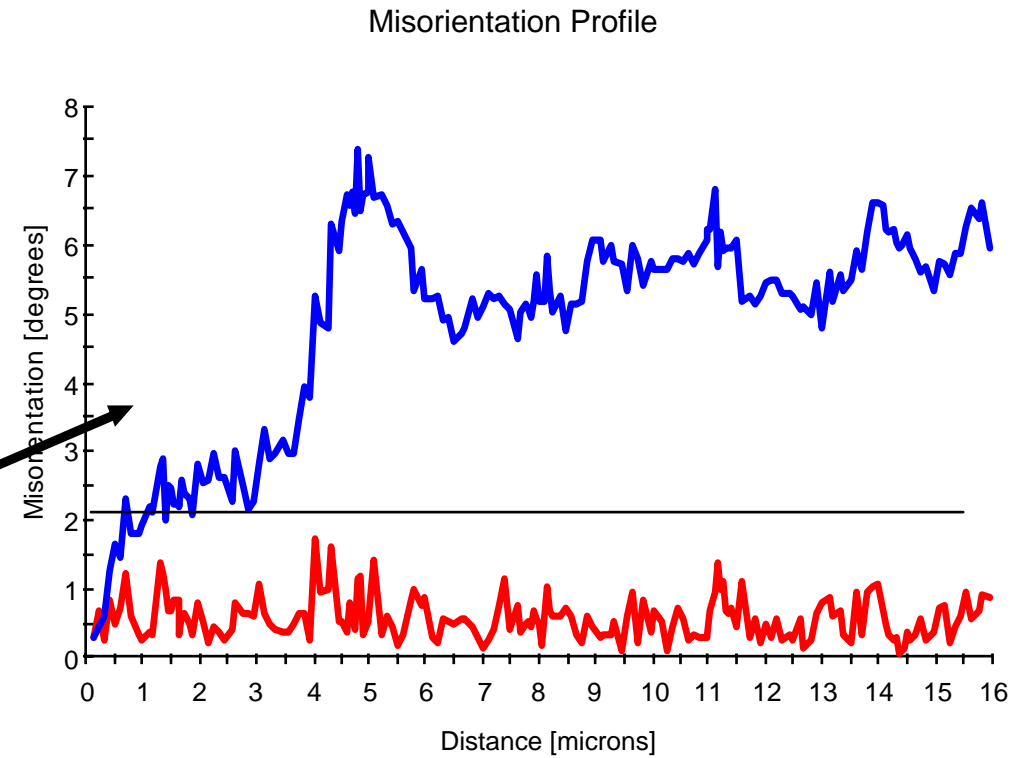
9.00 μm = 90 steps Direction



Direction	Min	Max	Total Fraction	Partition Fraction
$\langle 1\ 1\ 0 \rangle \parallel [1\ 0\ 0]$	0°	10°	0.276	0.276
$\langle 1\ 1\ 1 \rangle \parallel [0\ 0\ 1]$	0°	10°	0.183	0.183



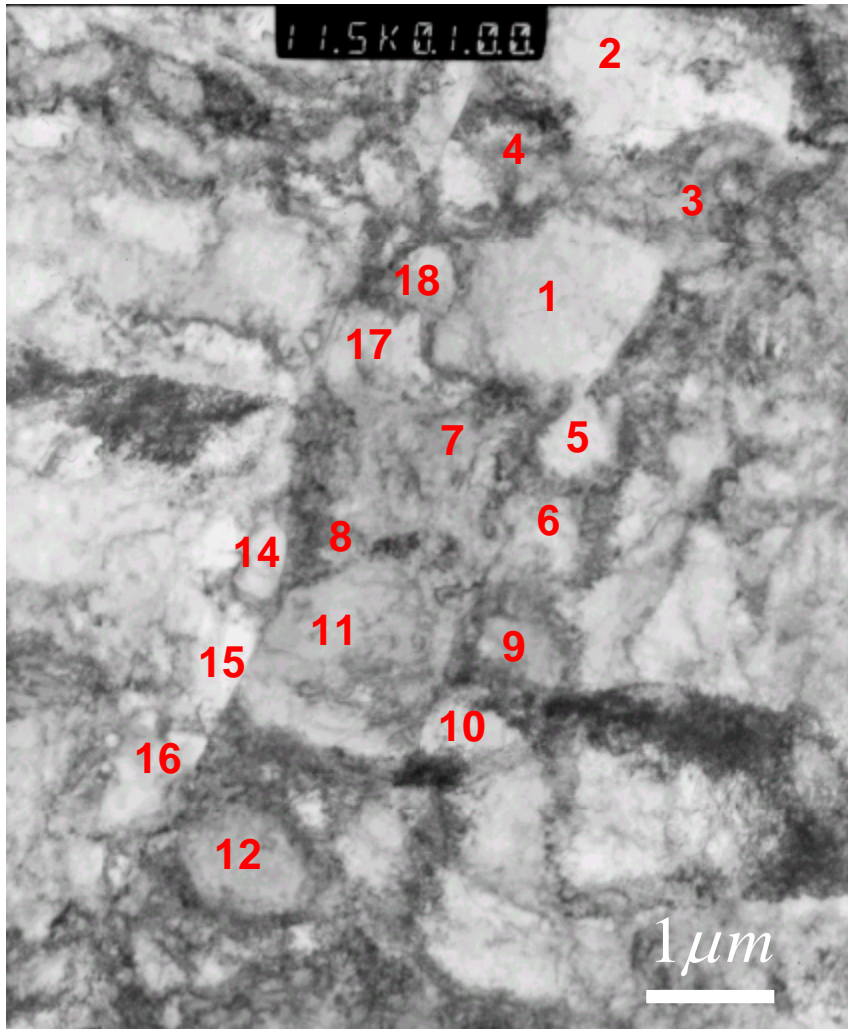
9.00 μm = 90 steps IPF [001]



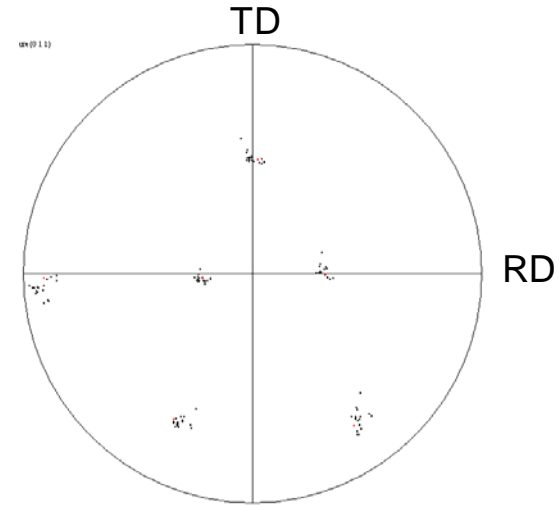
walzhart

- Alpha-Faser zeigt kontinuierlichen Orientierungsgradienten

RD



alpha-fiber, cold rolled



pole figure (011)

misorientations of adjacent subgrains:

2/3 : 2.8°

3/1 : 1.2°

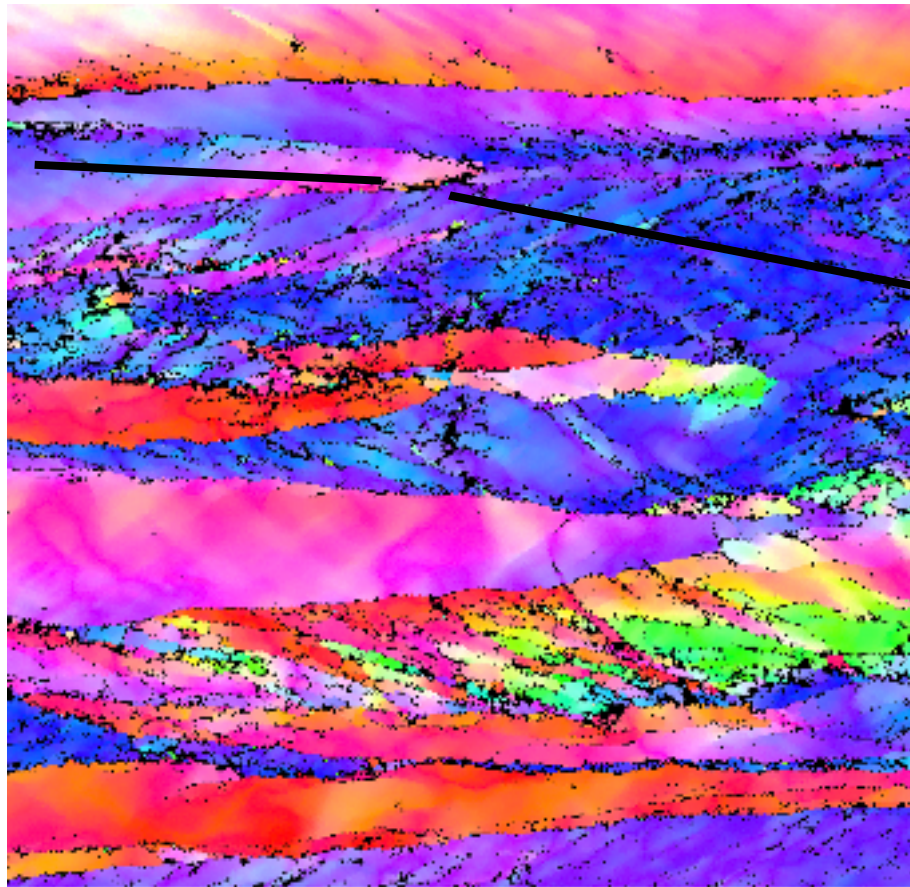
1/5 : 4.4°

5/6 : 1.9°

9/10: 1.5°

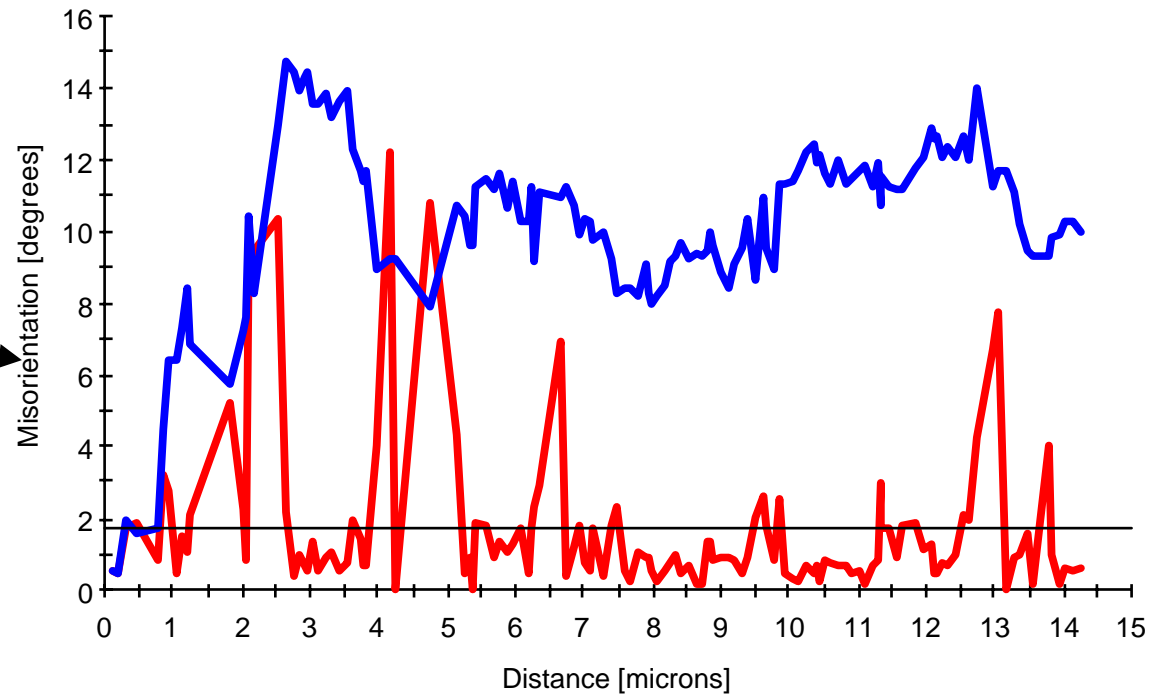
14/15: 1.3°

walzhart

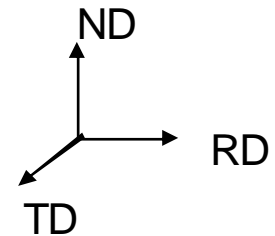


0.00 μm = 20 steps [100] 191

Misorientation Profile

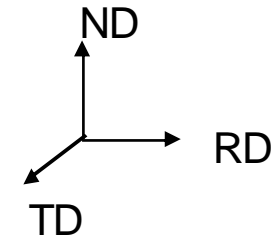
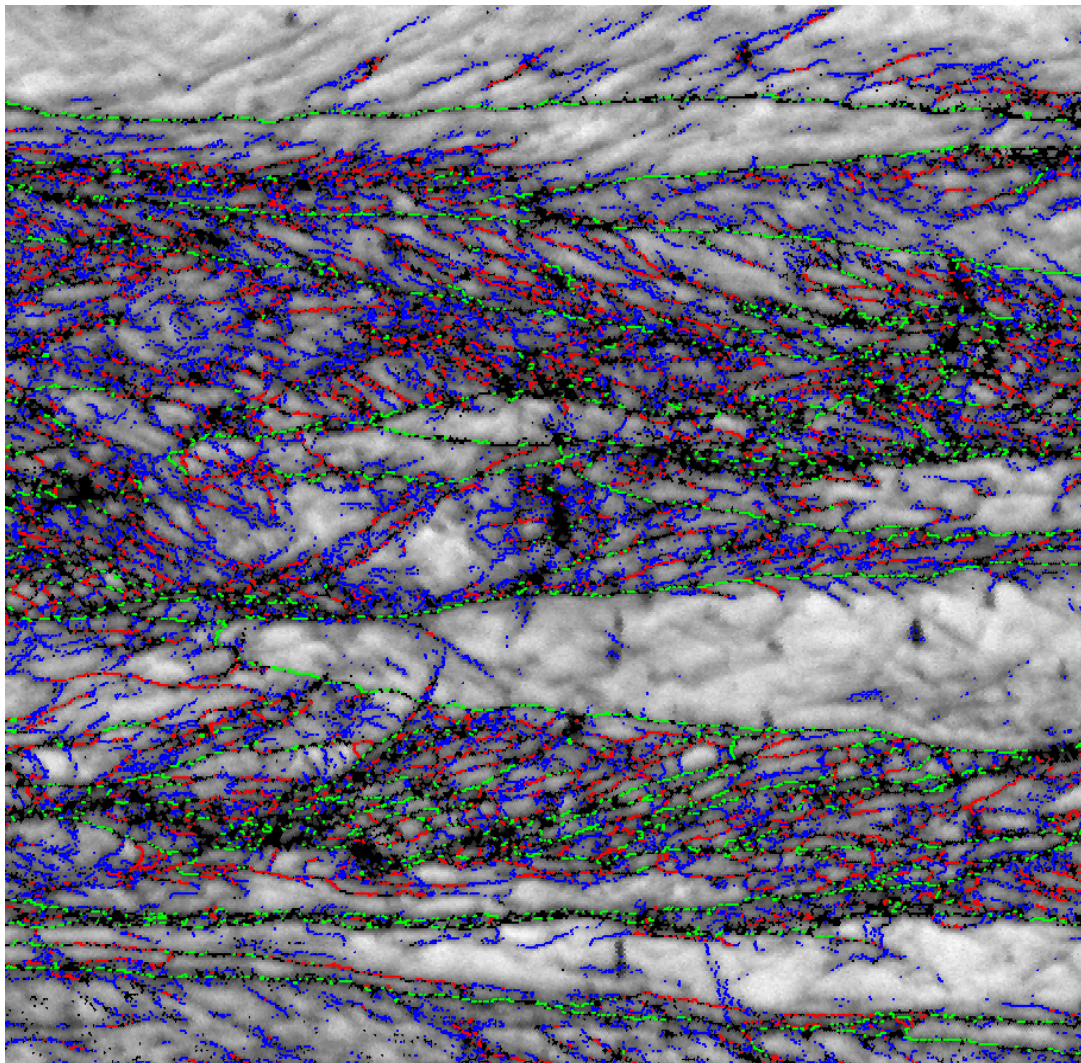


— Point-to-point — Point-to-origin



- in der Gamma-Faser zeigt die Orientierung diskrete Sprünge



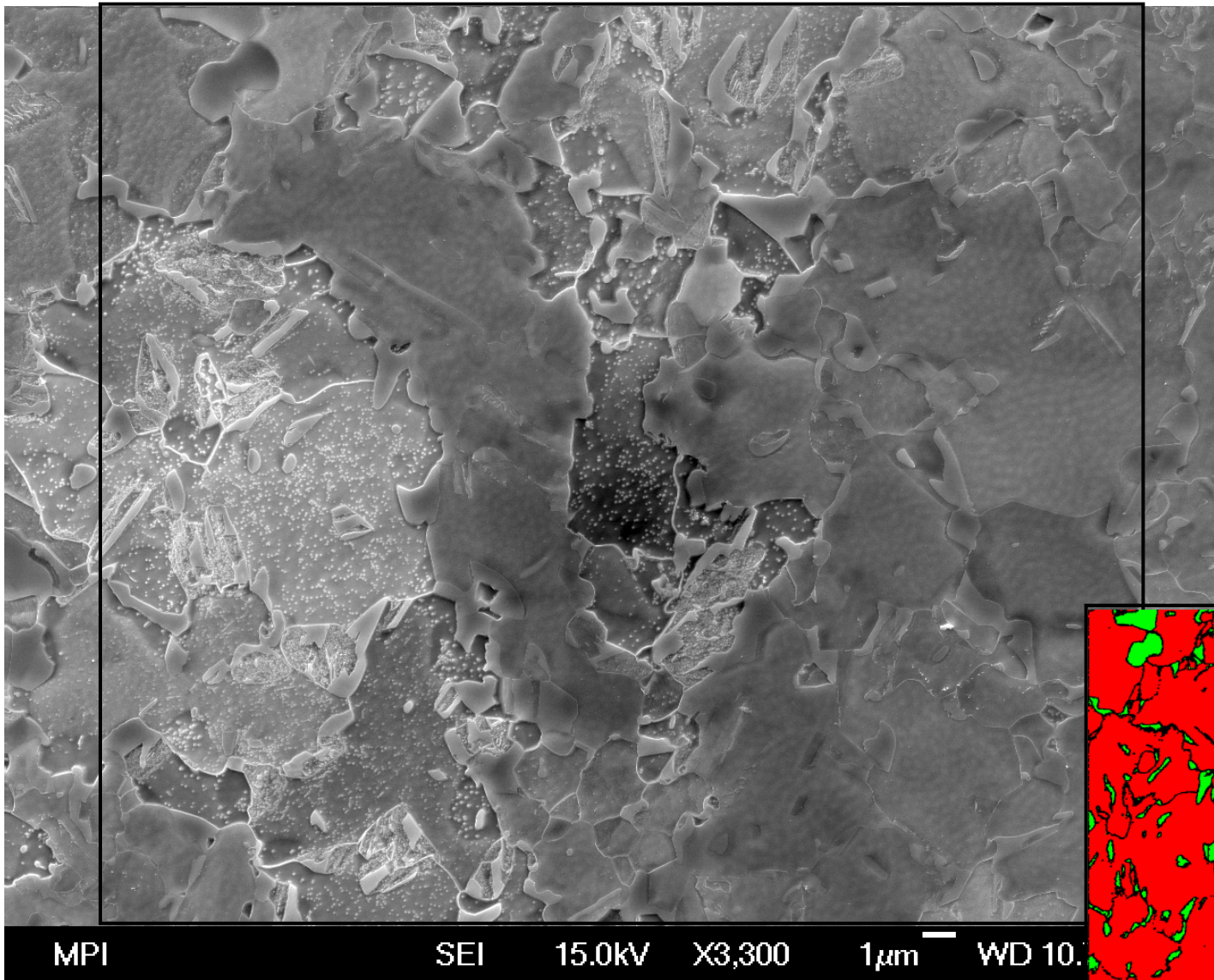


Boundaries: Rotation Angle

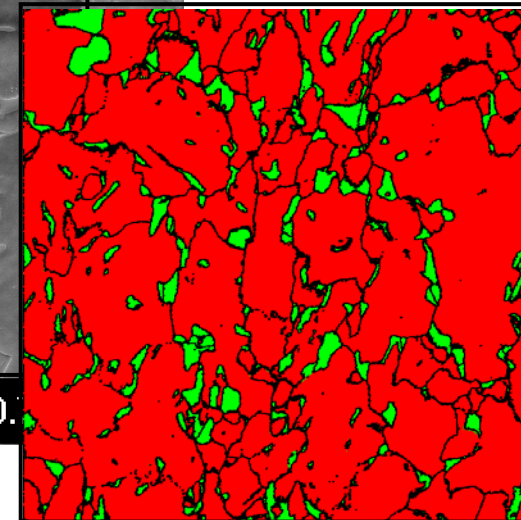
	Min	Max	Fraction
—	2°	5°	0.487
—	5°	15°	0.248
—	15°	180°	0.265

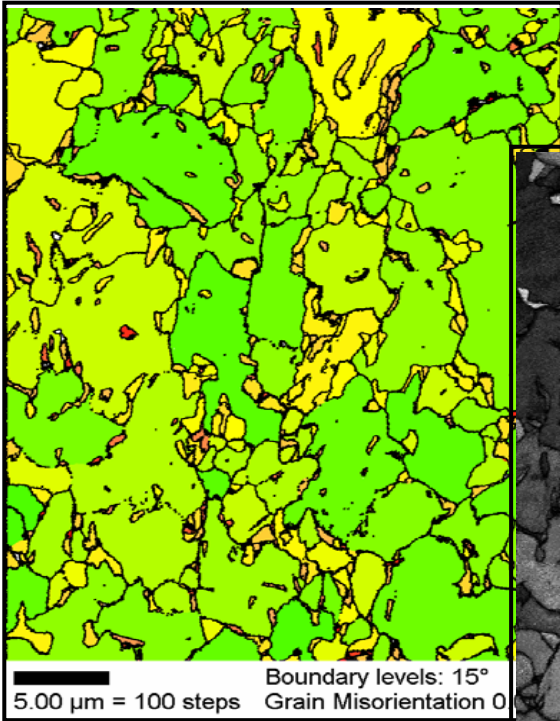
9.00 μm = 90 steps Boundary levels: 2° 5° 15° IQ 18...167.9

- Subkörner bilden teilweise Großwinkelkorngrenzen

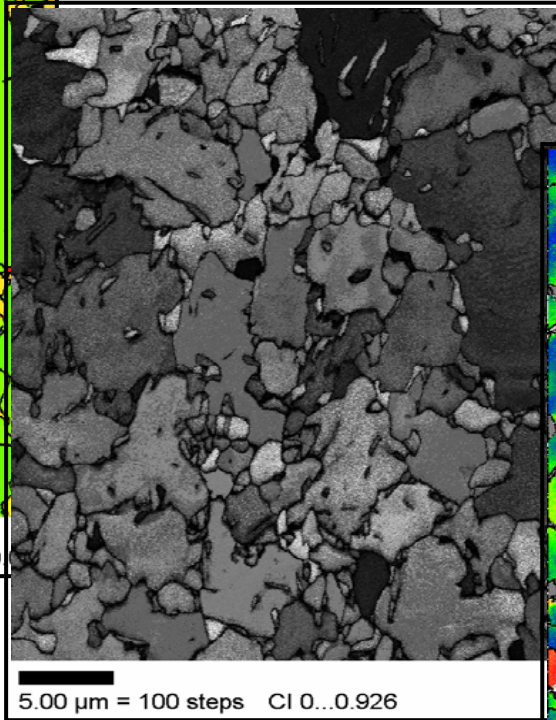


Phase
distribution
(from ACOM)



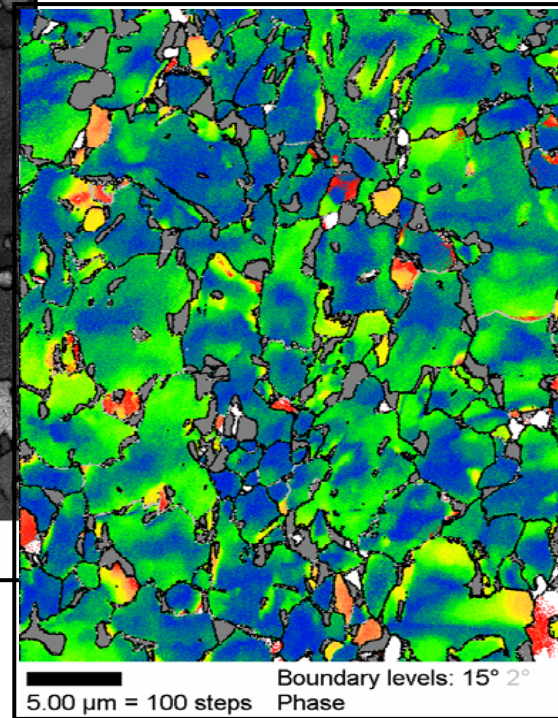


grain average
misorientation



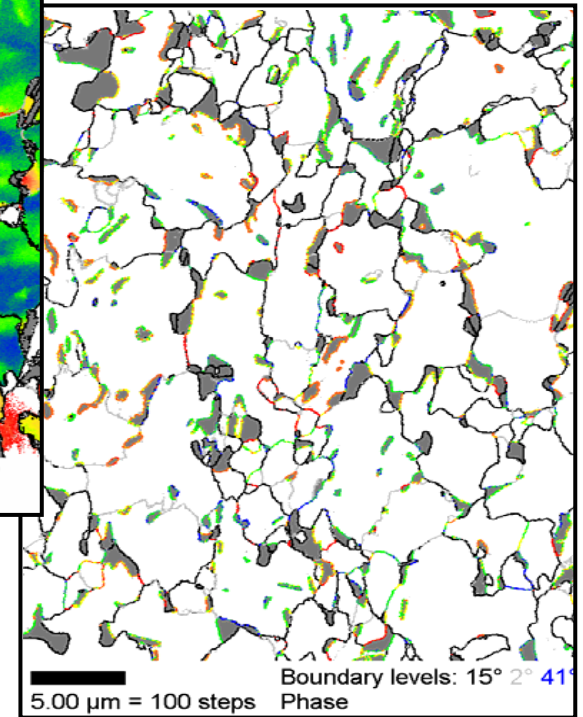
confidence index

grain internal
misorientations



grain boundary
character

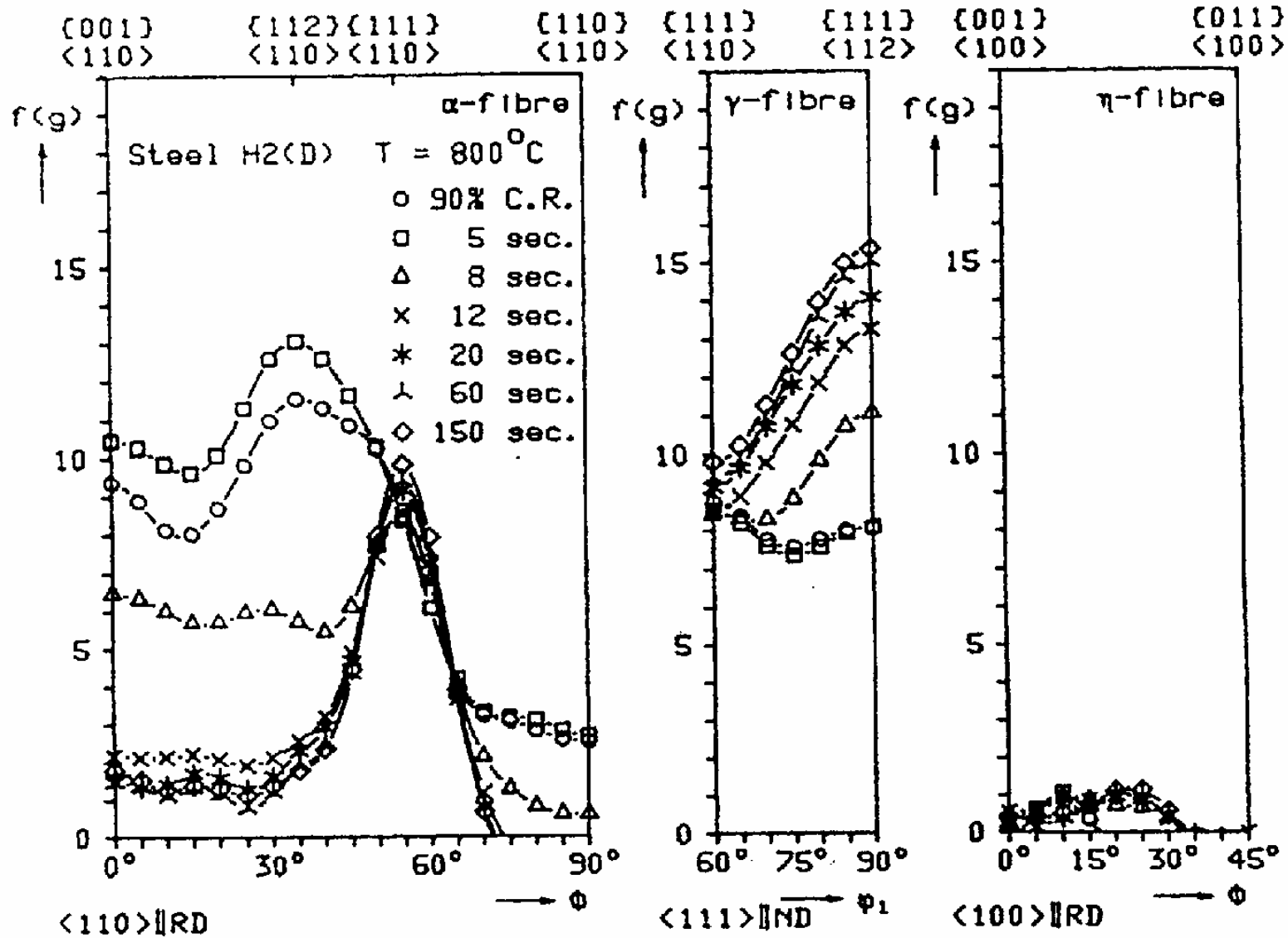
Phase	Min	Max	Fraction
—	15°	180°	0.428
—	2°	15°	0.079
—	41°	42°	0.020
—	42°	43°	0.042
—	43°	44°	0.051
—	44°	45°	0.046
—	45°	46°	0.034
—	46°	47°	0.010

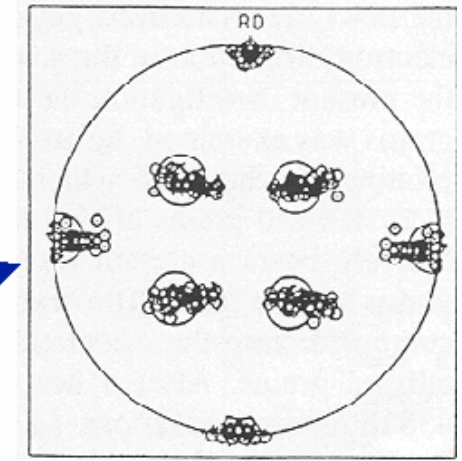
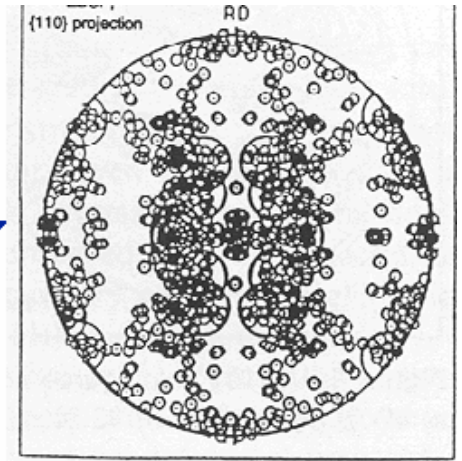
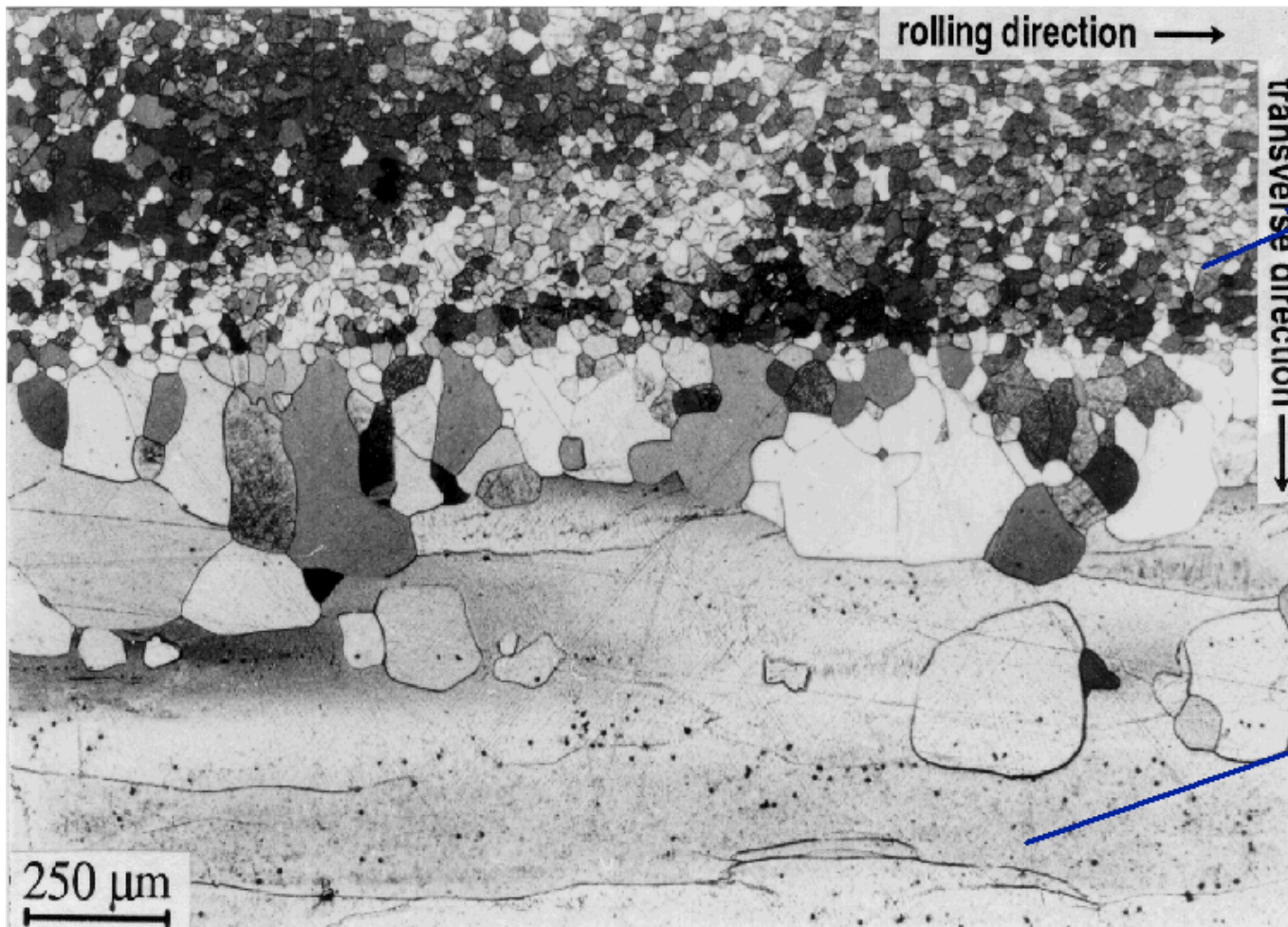


Glüh textures

Glühung

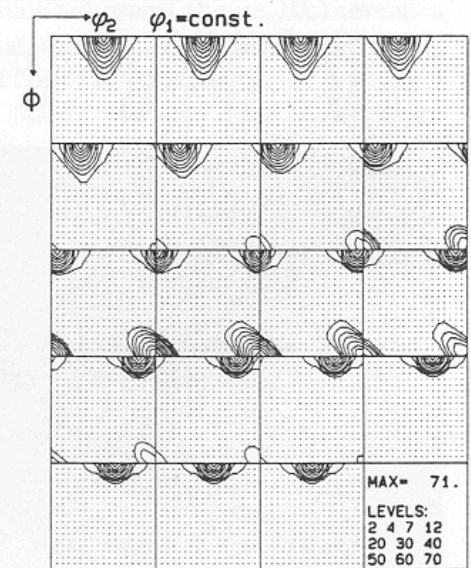
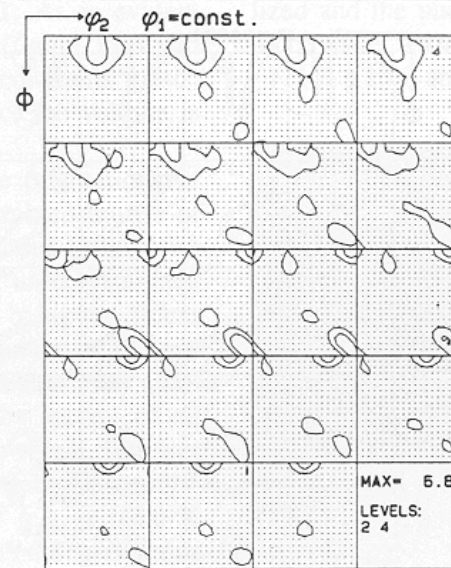
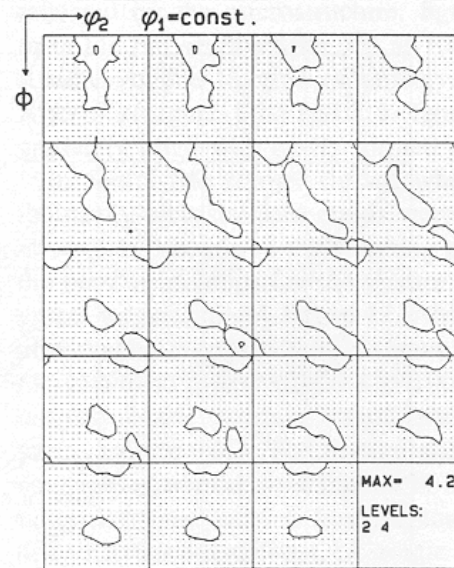
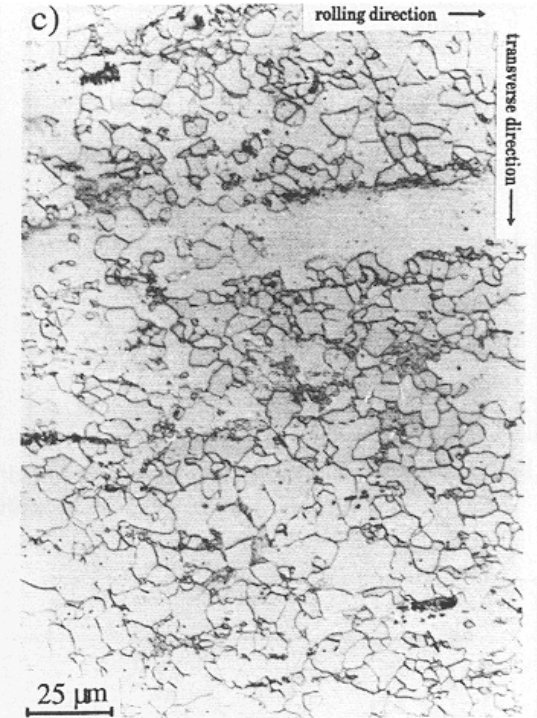
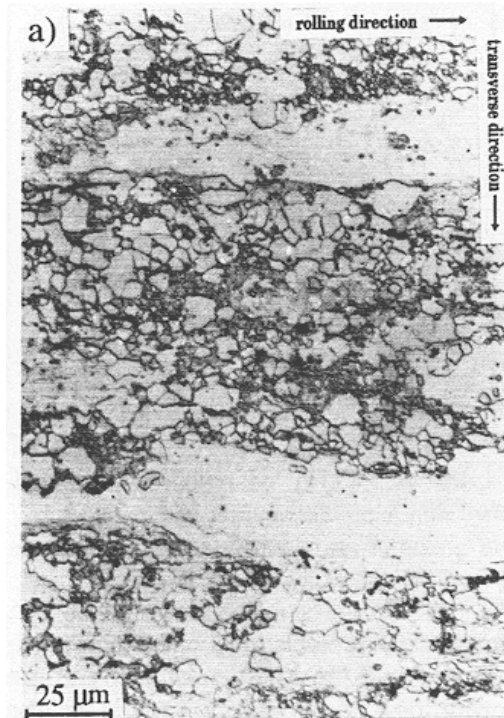
low C, kein IF





Glühung

low C, kein IF

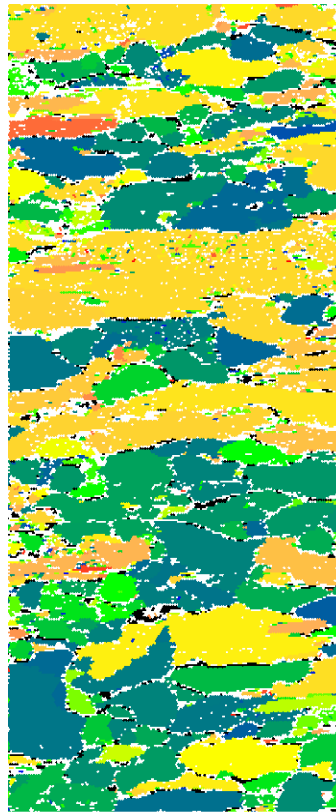


Gefügevergleich

verformt/erholt

teilrekristallisiert

Misorientierung
innerhalb der einzelnen
Körner

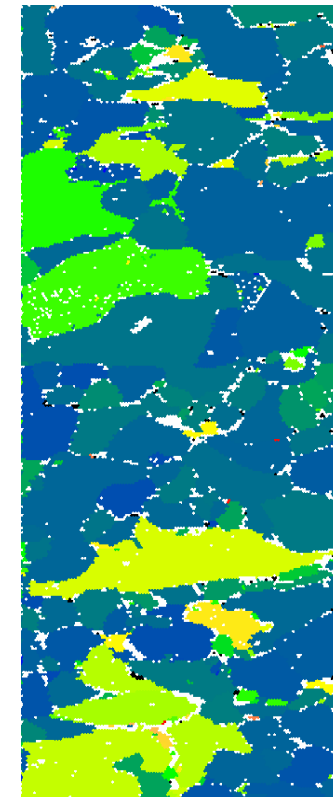
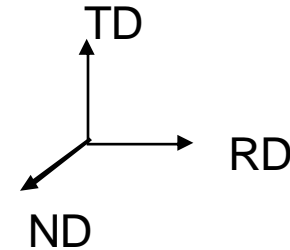


35.00 µm = 35 steps

Gray Scale Map Type: <none>

Color Coded Map Type: Grain Average Misorientation

	Min	Max	Total Fraction	Partition Fraction
	0.068528	4.98609	0.838	0.838



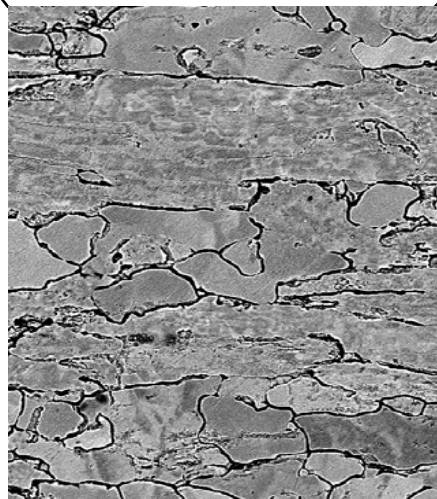
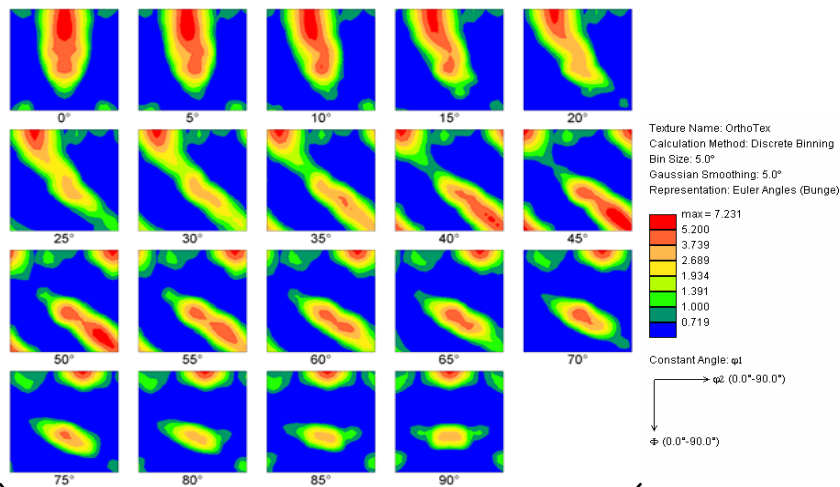
25.00 µm = 25 steps

Gray Scale Map Type: <none>

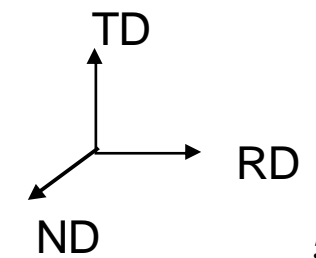
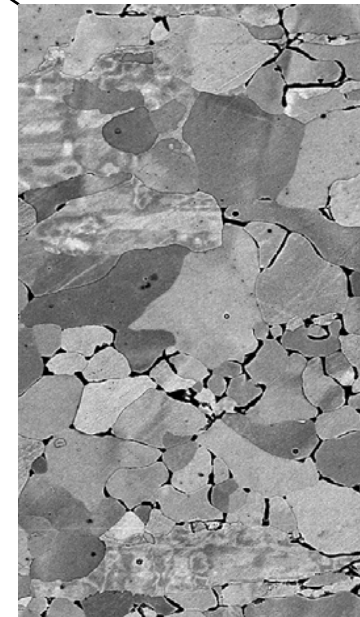
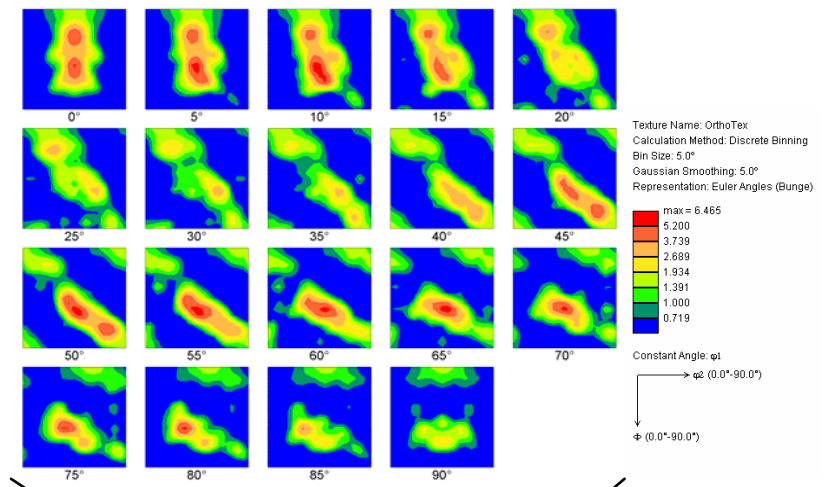
Color Coded Map Type: Grain Average Misorientation

	Min	Max	Total Fraction	Partition Fraction
	0.0791294	4.83229	0.938	0.938

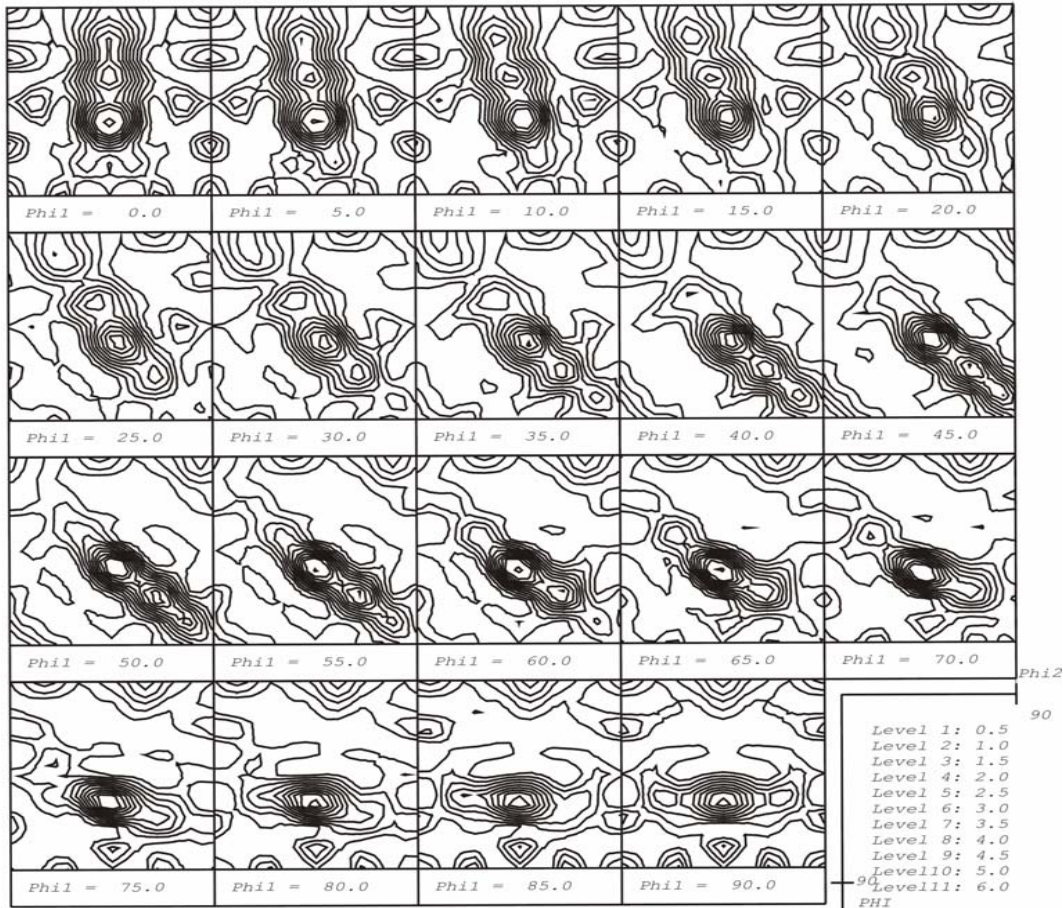
verformter/erholter Gefügebereich



teilkristallisierter Gefügebereich

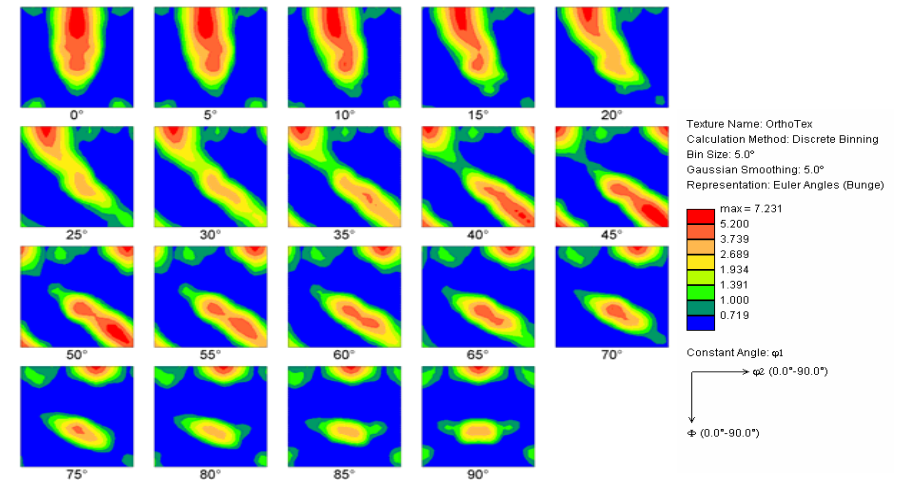


Makrotextur

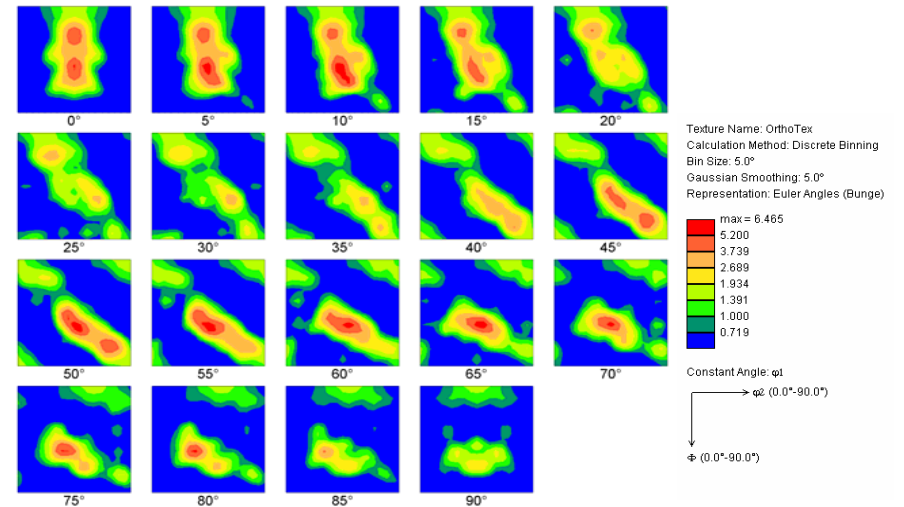


Mikrotextur

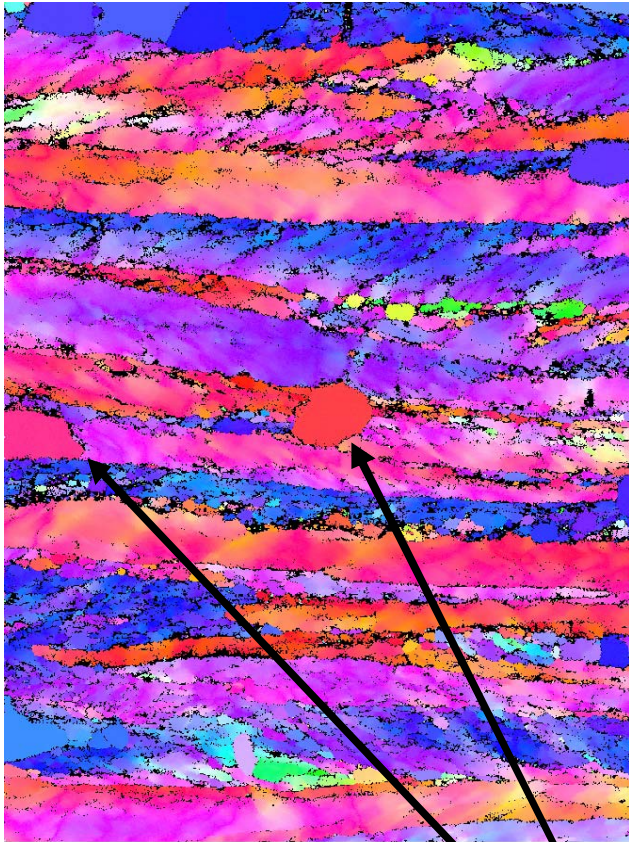
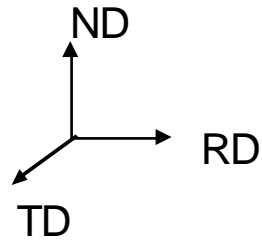
verformter/erholter Gefügebereich



teilkristallisierter Gefügebereich



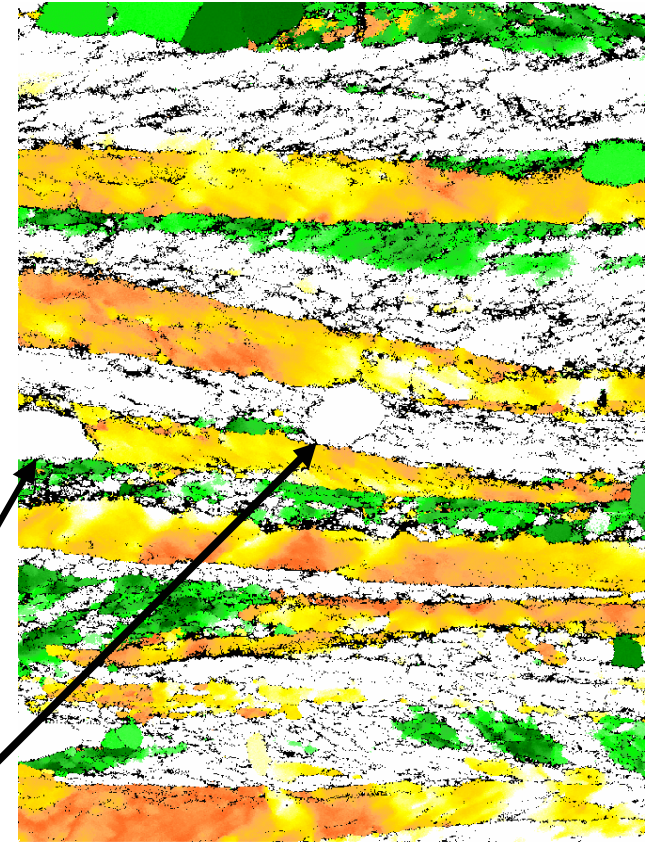
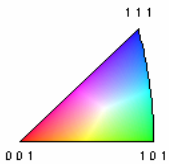
680°C; 3min



10.00 μm = 100 steps IPF [001]

Color Coded Map Type: Inverse Pole Figure [001]

Iron (Alpha)

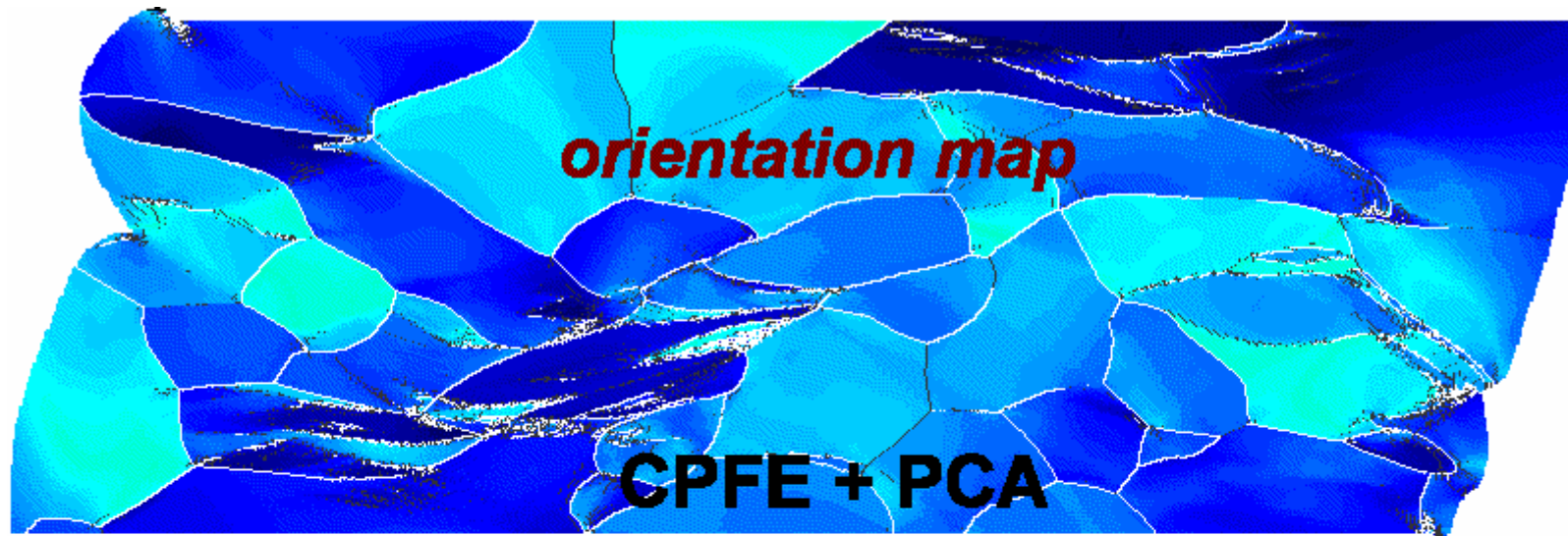


10.00 μm = 100 steps Direction

Color Coded Map Type: Crystal Direction

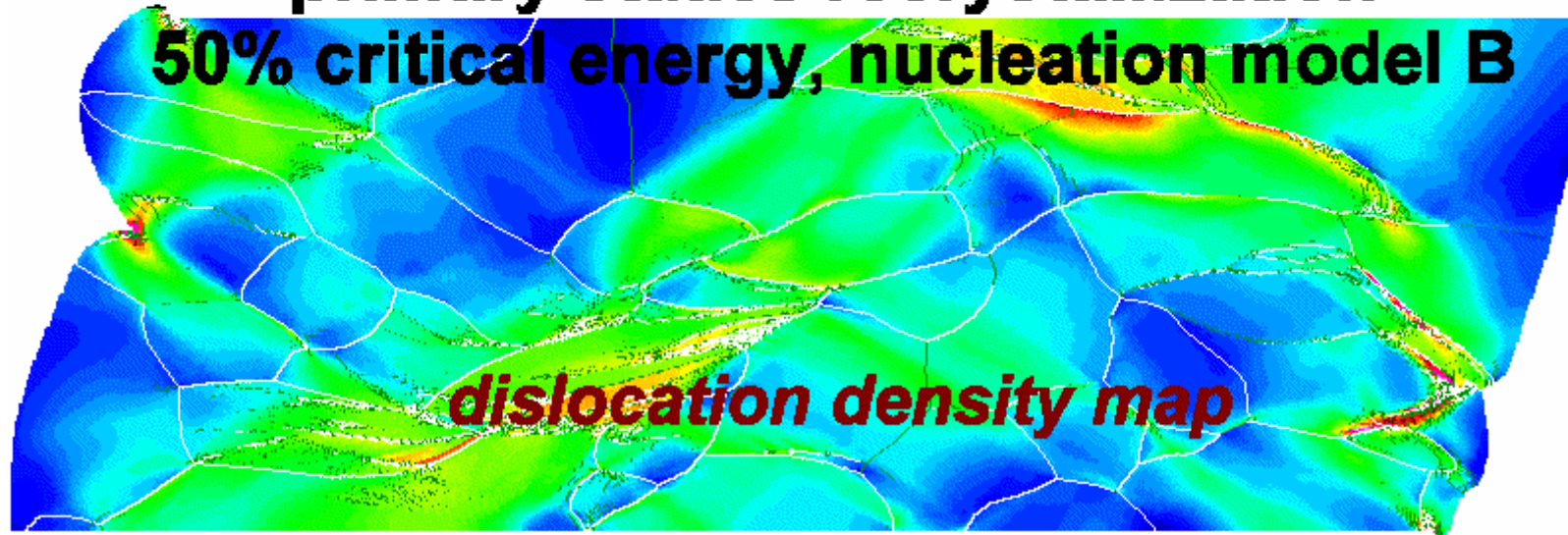
Direction	Min	Max	Total Fraction	Partition Fraction
<1 1 0> [1 0 0]	0°	10°	0.367	0.367
<1 1 1> [0 0 1]	0°	10°	0.154	0.154

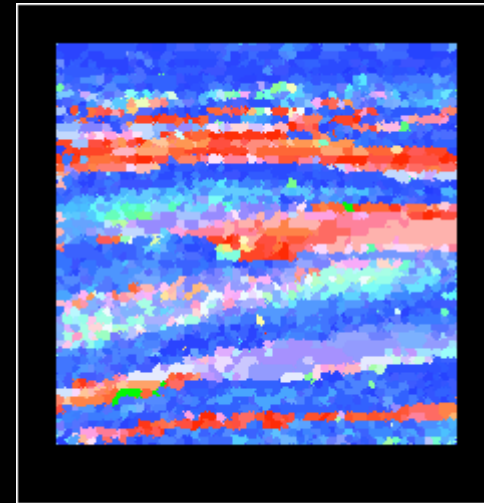
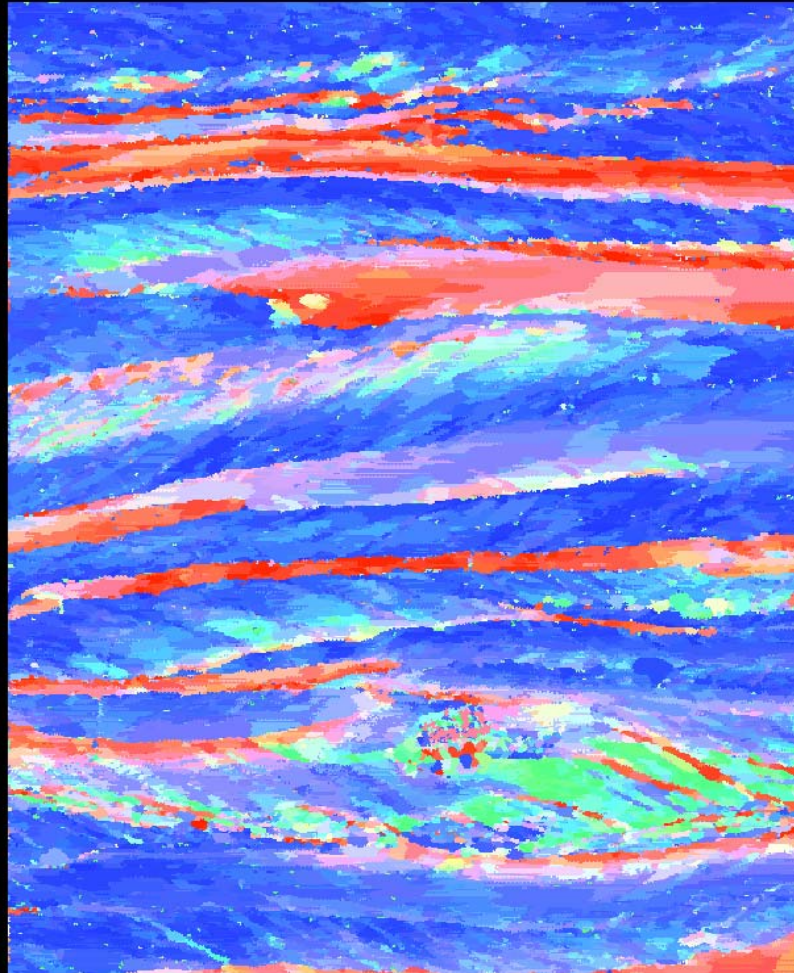
• beginnende Rekristallisation



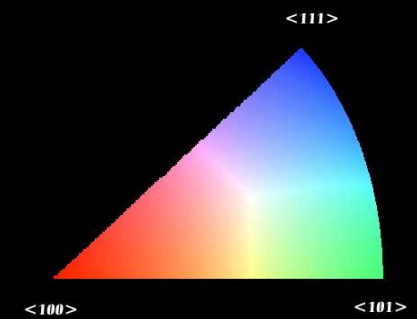
primary statics recrystallization

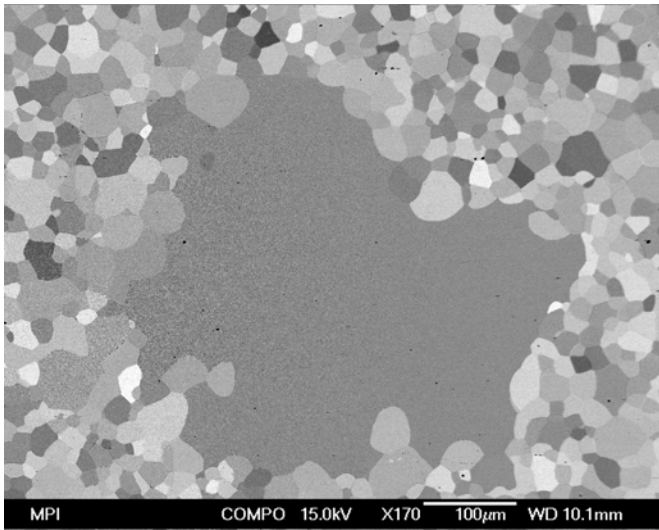
50% critical energy, nucleation model B



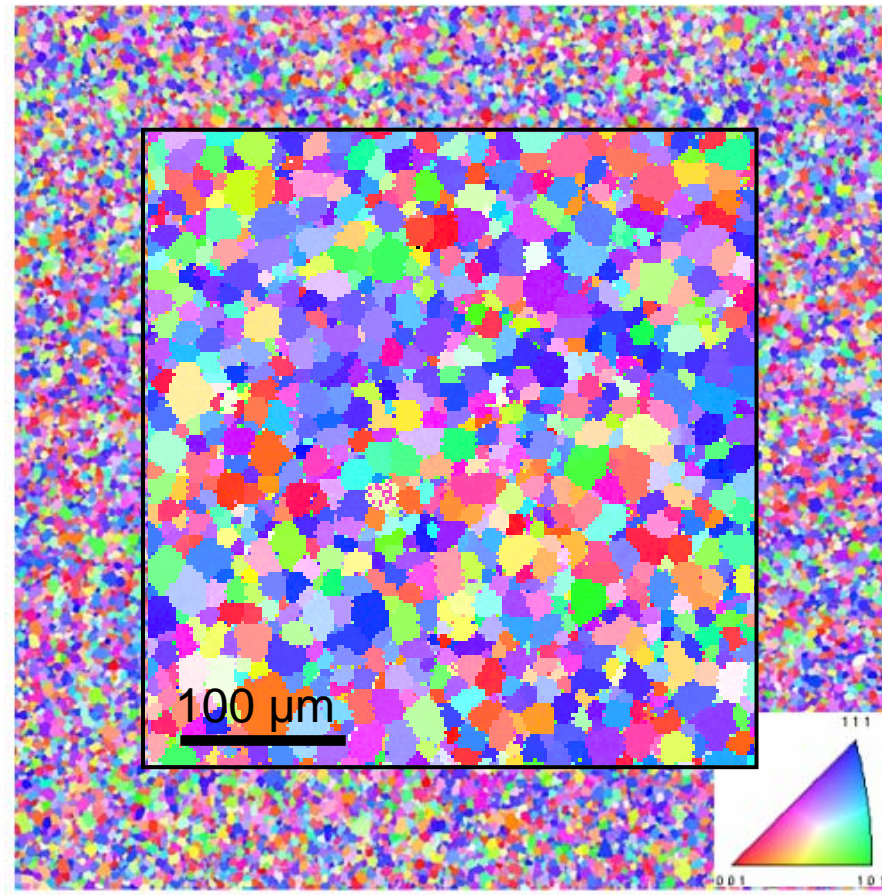


20 μm





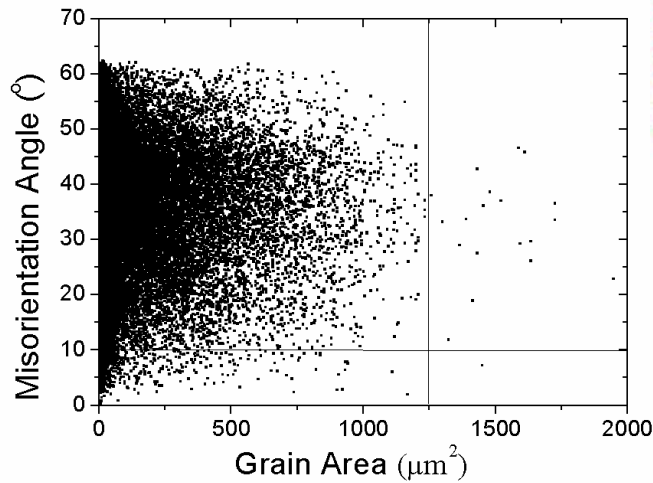
Example of abnormally growing Goss grain during 2nd recrystallization



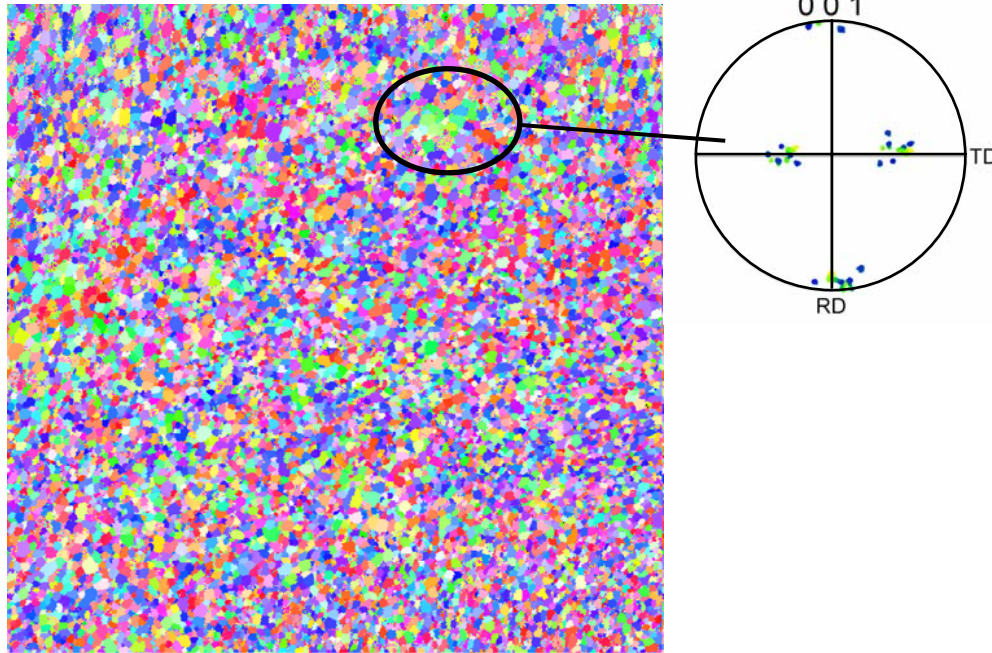
200.0 µm = 100 steps IPF [001]

large crystal orientation map of primary recrystallized material:
1 grain out 10^6 will grow!!

Goss-
misorientation
vs. grain size
distribution

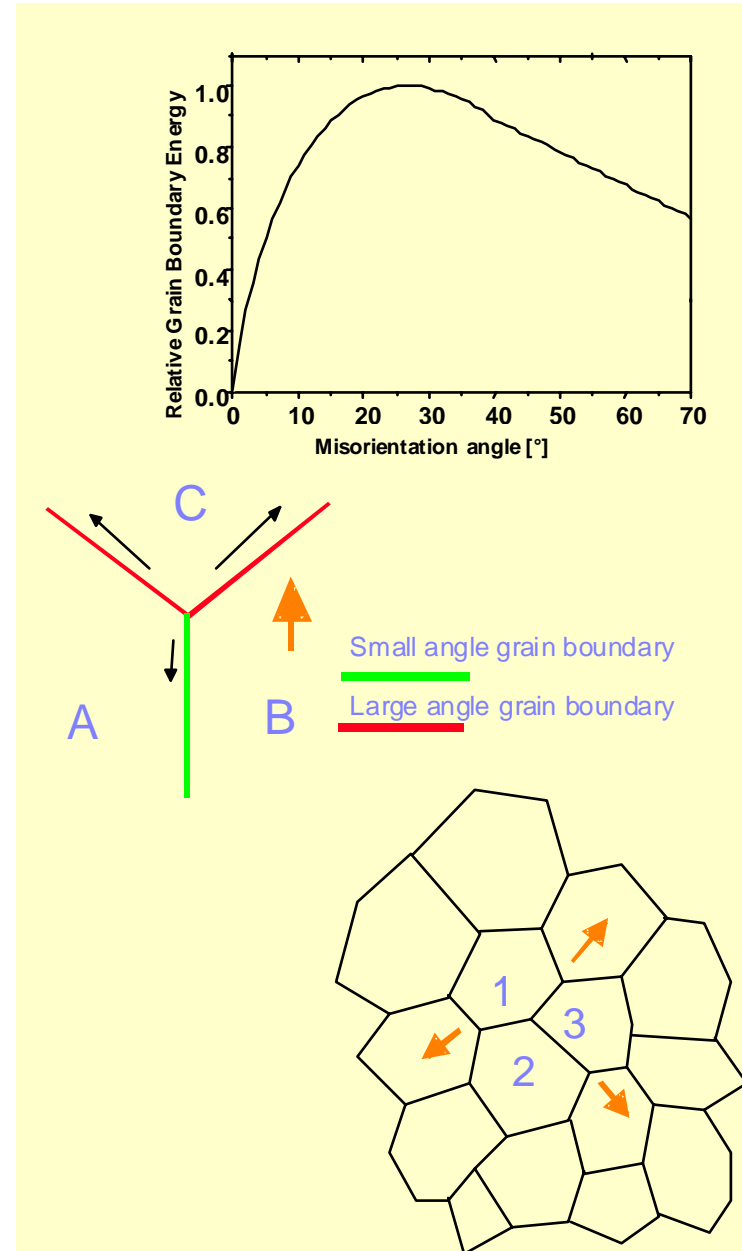


Role of Goss-grain clusters



400.0 μm = 100 steps IPF [001]

Clusters of Goss-oriented grains act like one large grain \Rightarrow
Nucleation for secondary recrystallization?



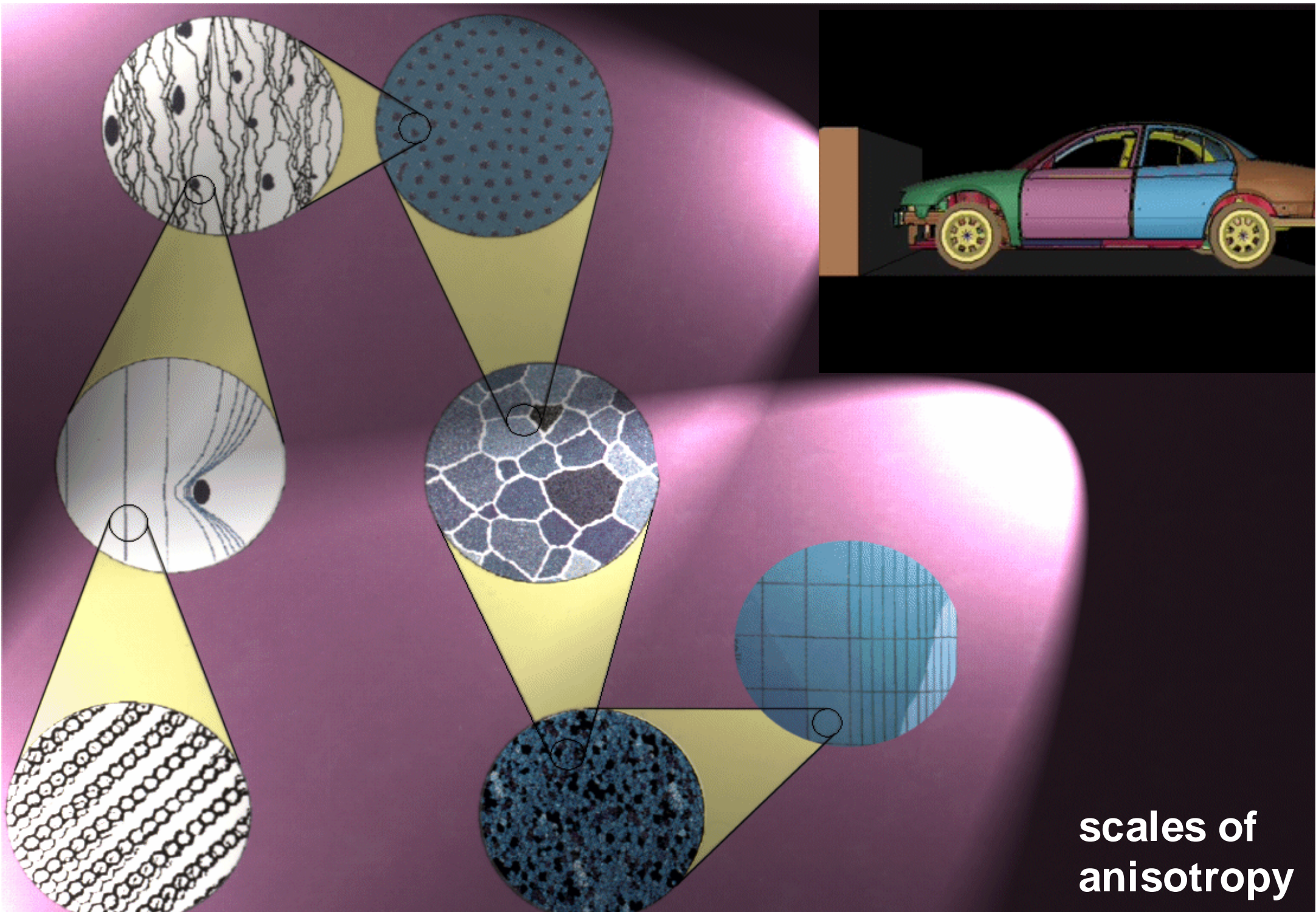
Grundbegriffe

Kristallographie

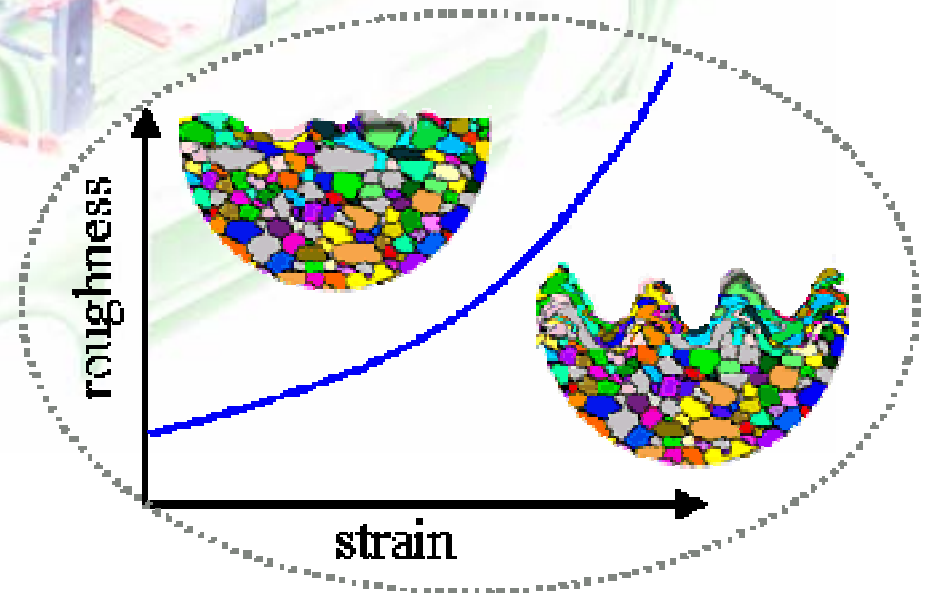
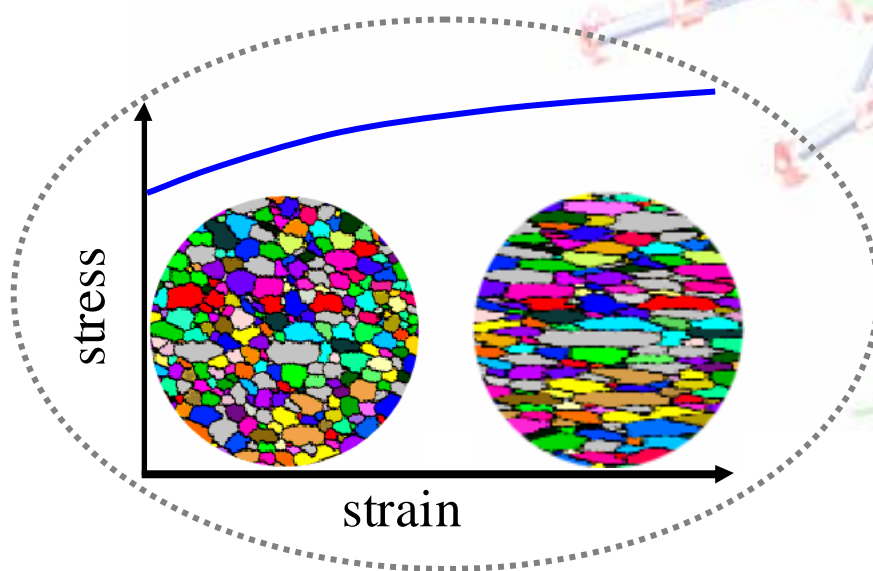
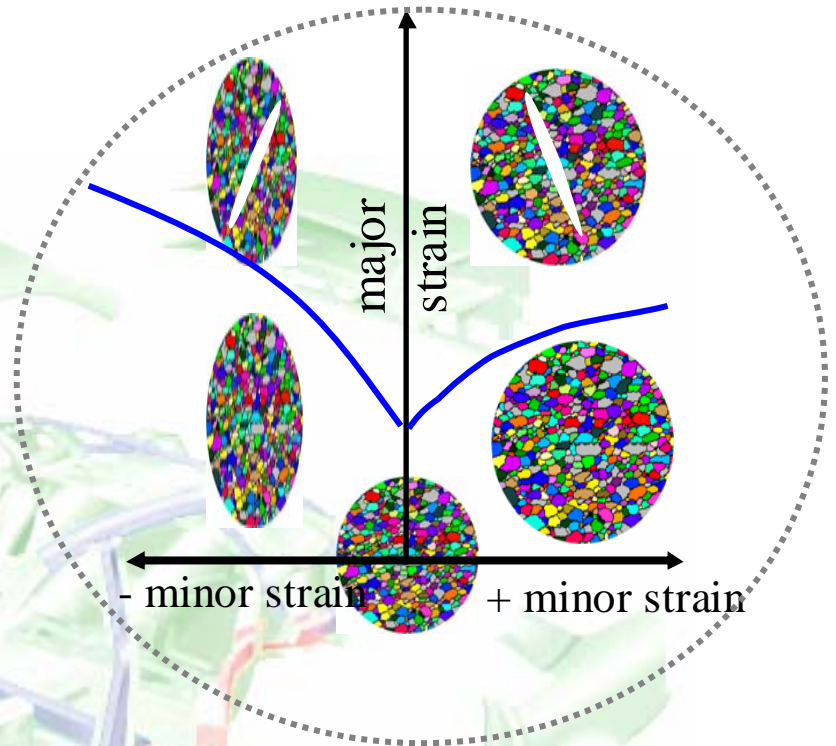
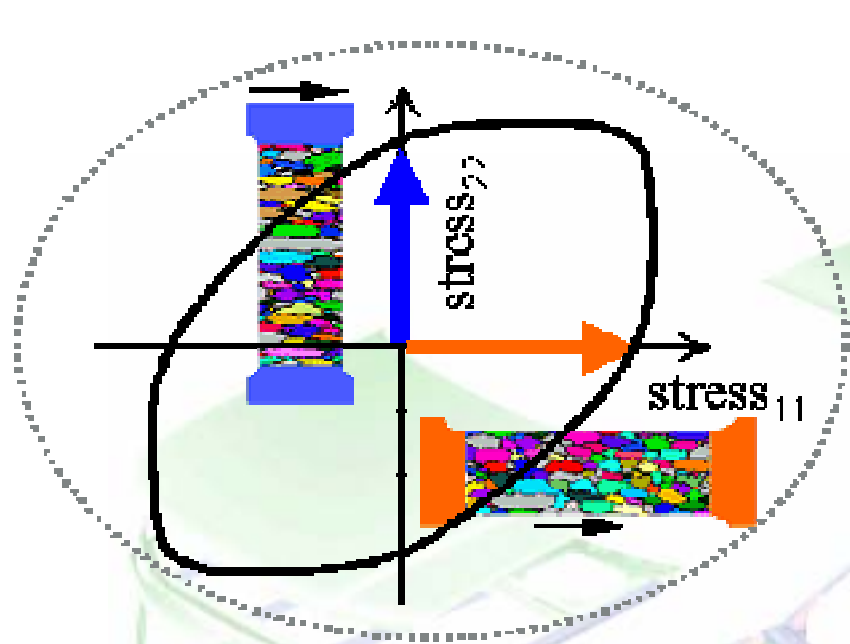
Textur

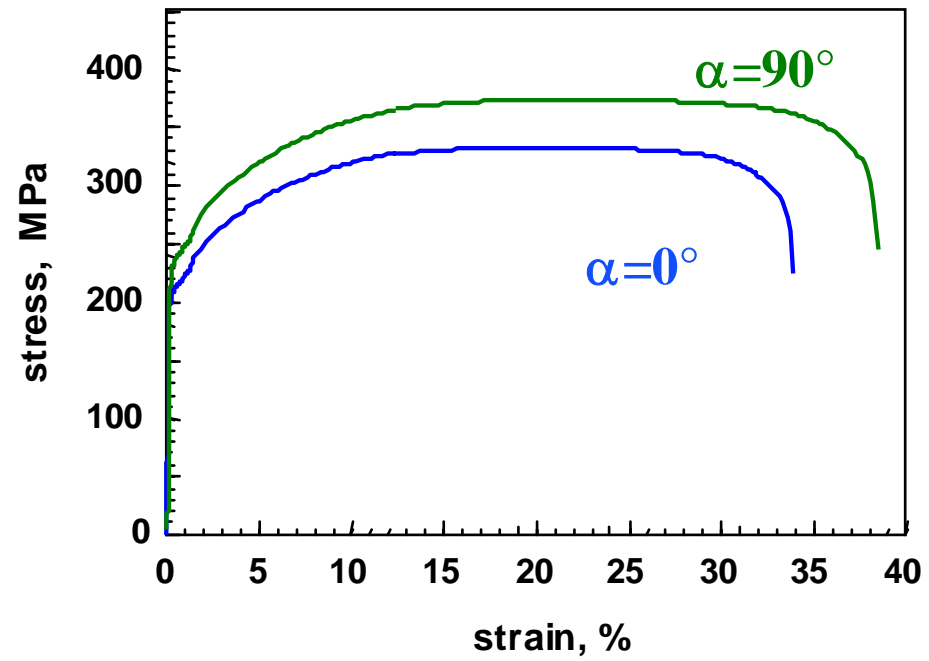
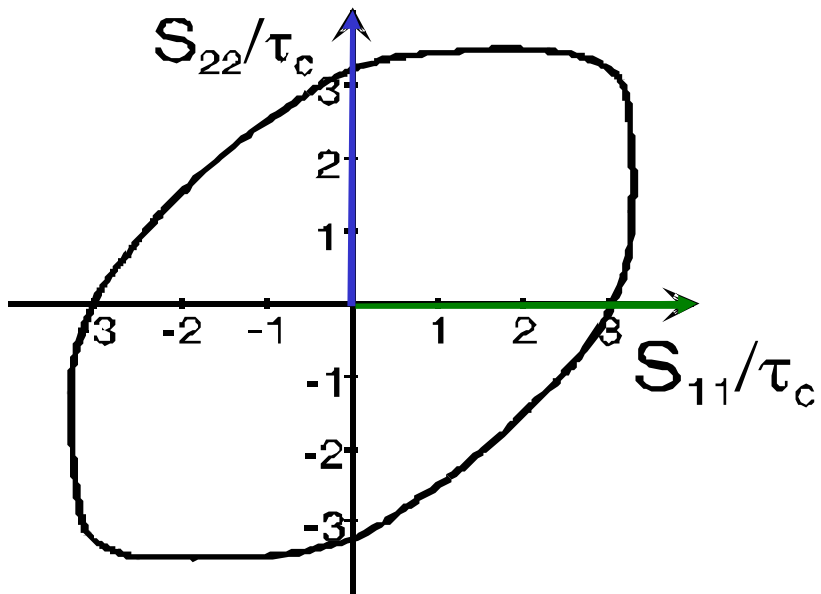
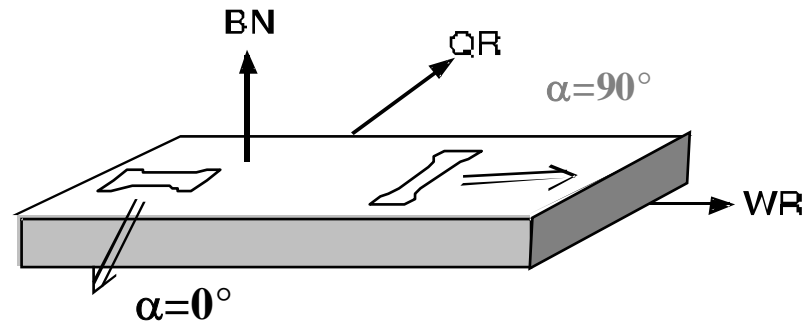
Anisotropie

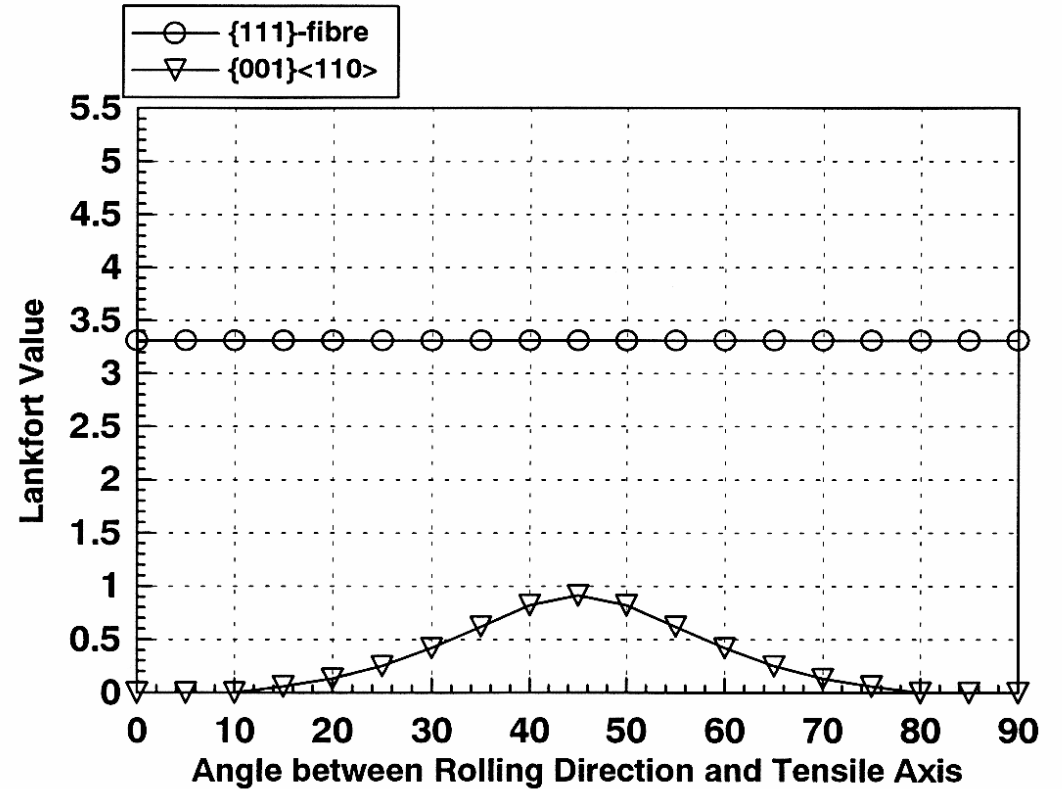
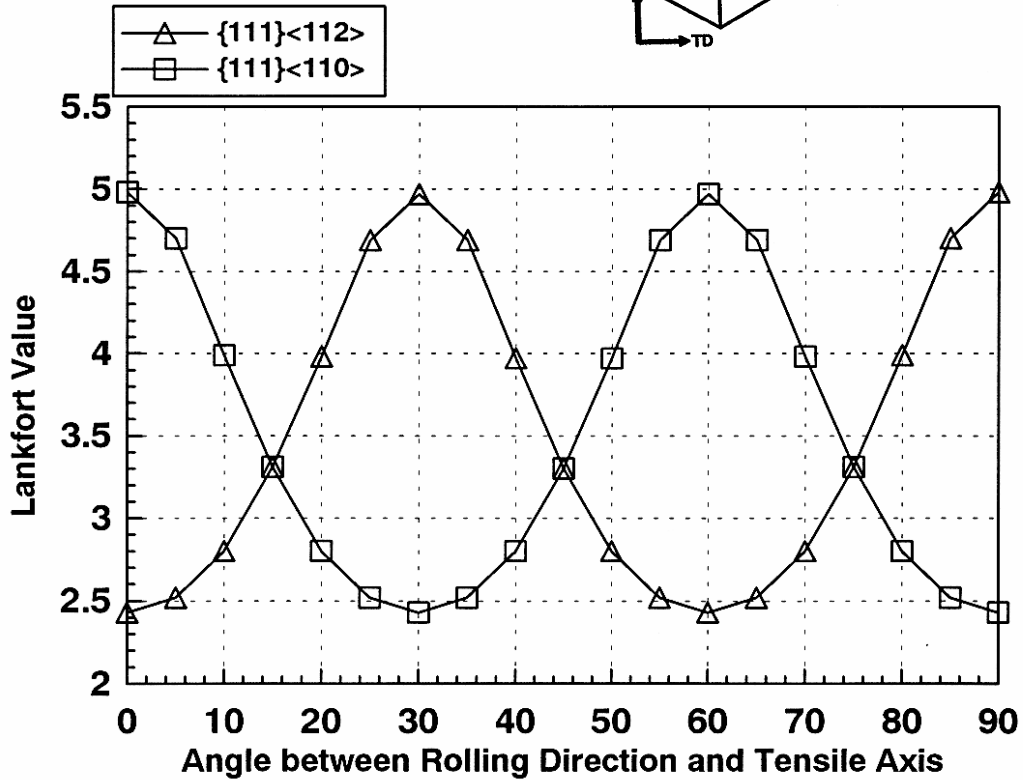
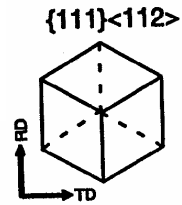
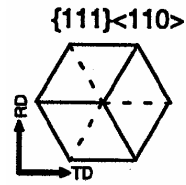




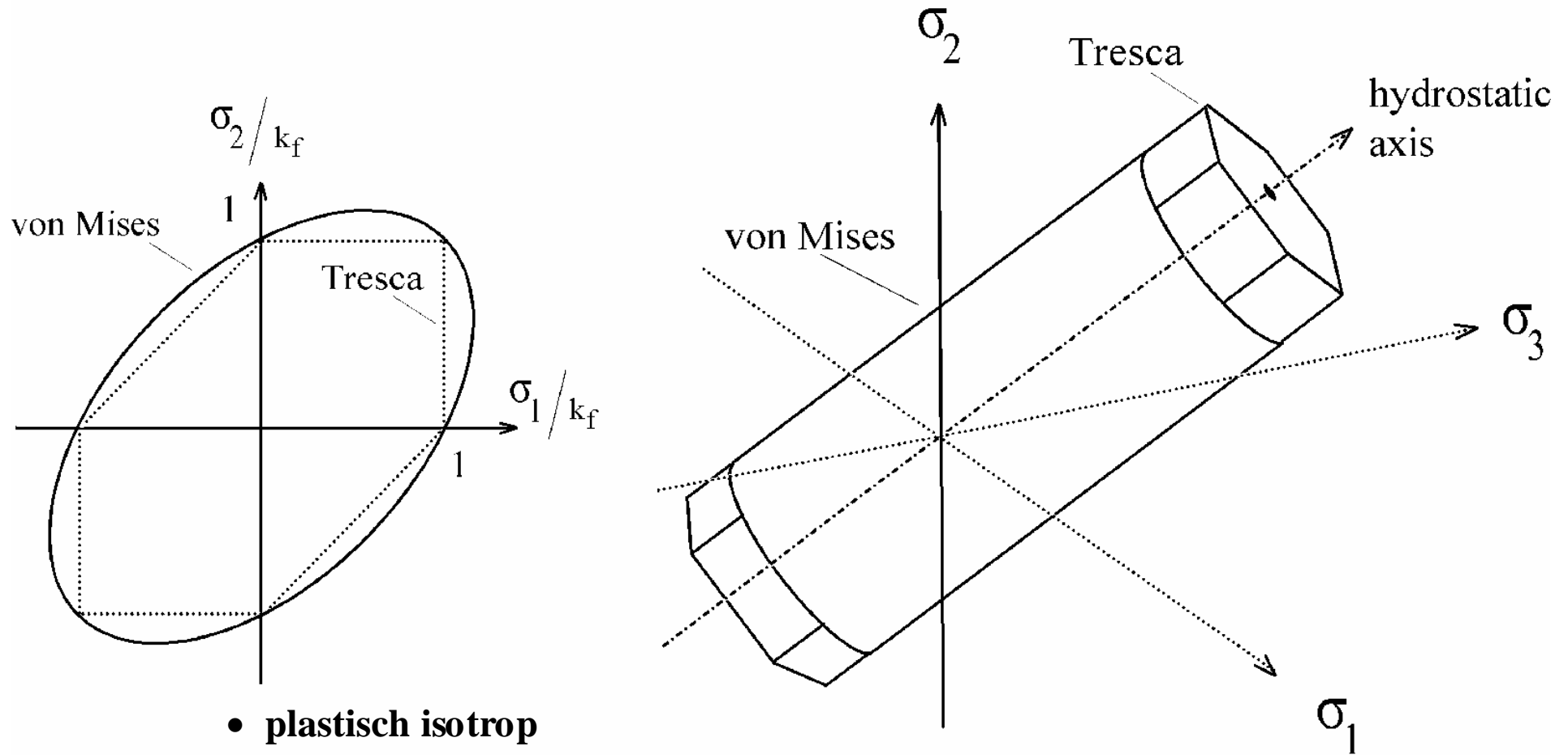
scales of
anisotropy





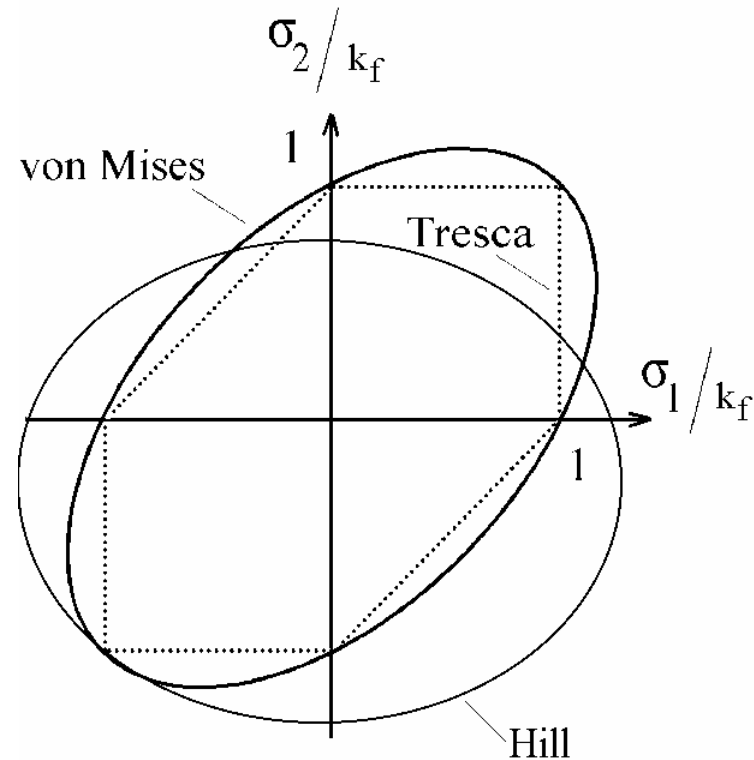


$$\frac{1}{2} \left[(\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 + 6\sigma_{23}^2 + 6\sigma_{13}^2 + 6\sigma_{12}^2 \right] = \sigma_{vM}^2 = k_f^2$$



- **plastisch isotrop**
- **Hypothese zur Berechnung einer Vergleichsspannung**
- **Reduzierung eines Tensors auf einen Skalar**
- **k_f aus 1-achsigen Versuch**

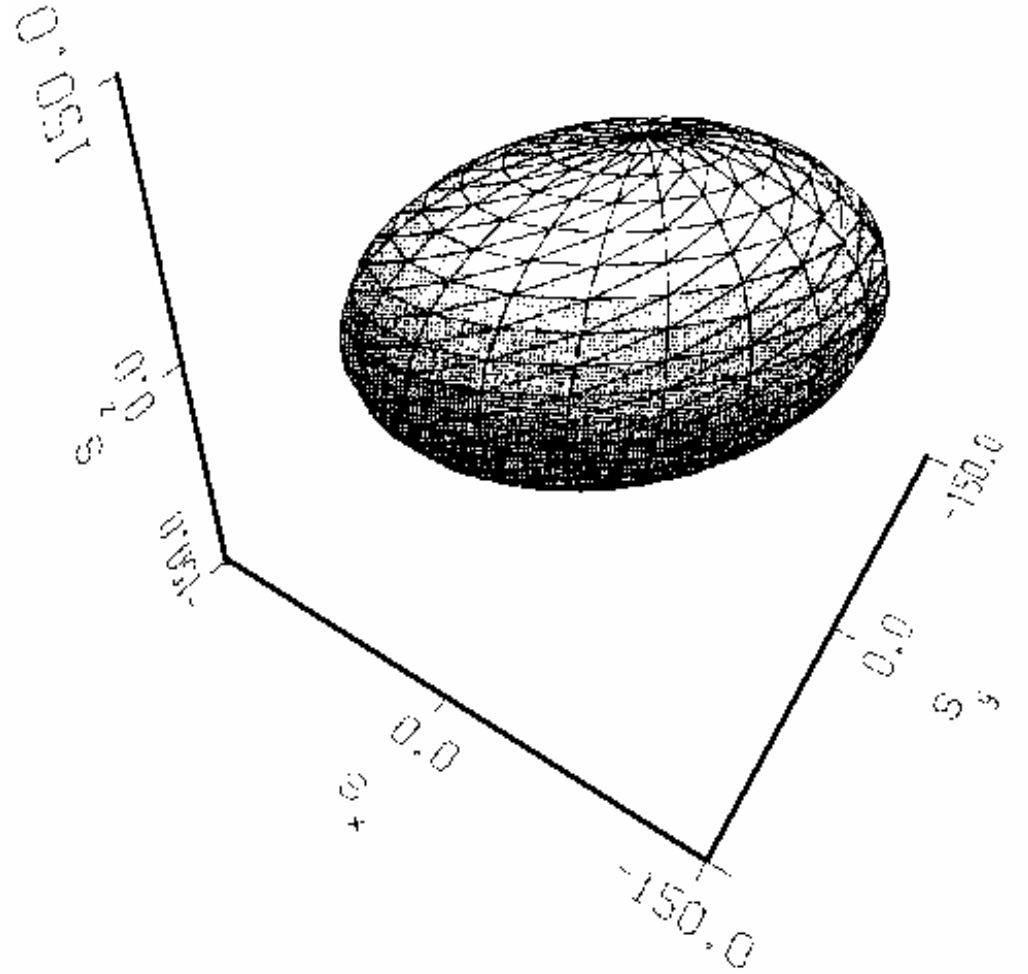
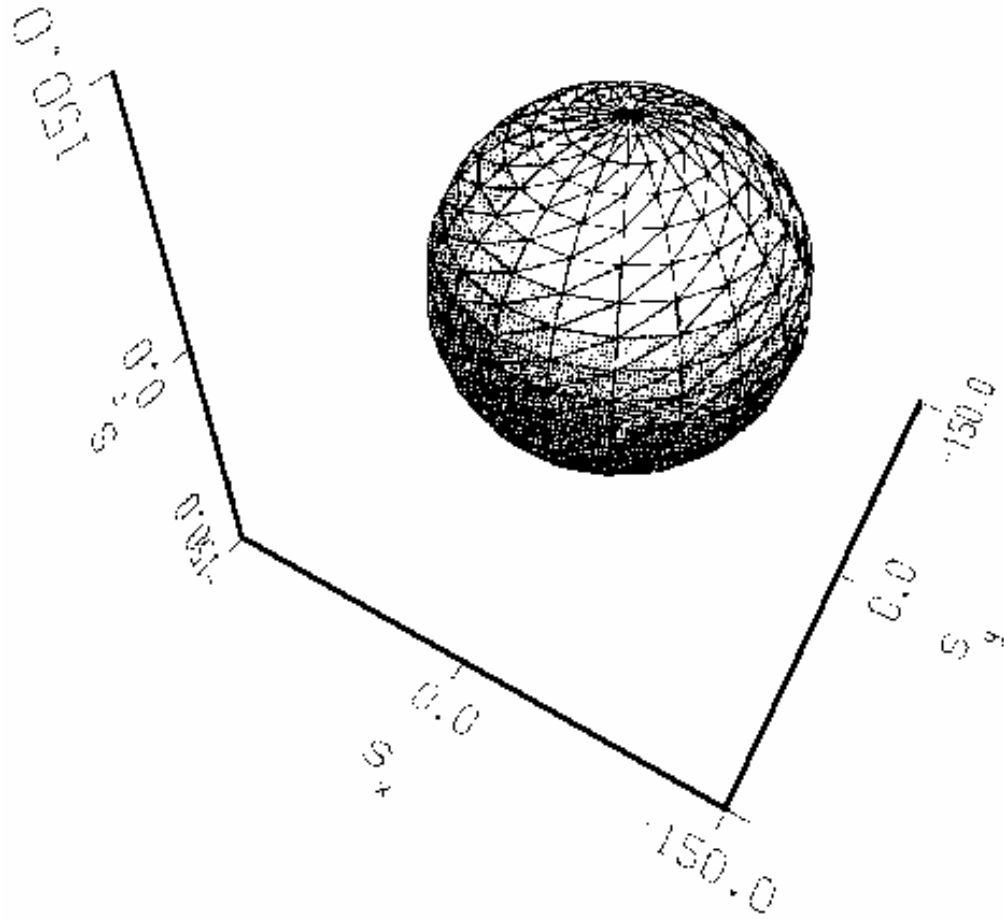
$$\frac{1}{2} \left[H(\sigma_{11} - \sigma_{22})^2 + F(\sigma_{22} - \sigma_{33})^2 + G(\sigma_{33} - \sigma_{11})^2 + 2L\sigma_{23}^2 + 2M\sigma_{13}^2 + 2N\sigma_{12}^2 \right] = \sigma_H^2 = k_f^2$$



- analytisch-empirische Hypothese zur Berechnung einer Vergleichsspannung
- plastisch anisotrop
- Reduzierung eines Tensors auf einen richtungsabhängigen Skalar
- bei Anisotropie eine Funktion aller Spannungs- (bzw. Deviator-)komponenten

von Mises

Hill



Gleitsystem s:

$$n_i^s, b_i^s$$

Orientierungsfaktor für s (Gleitsystem → Kristall):

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

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

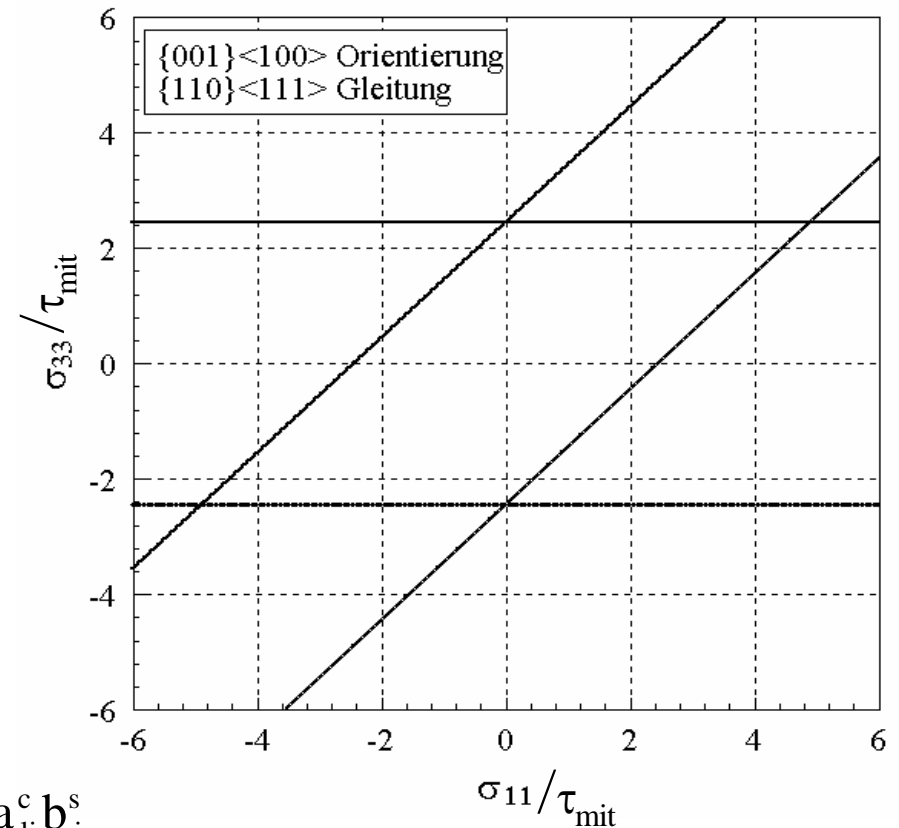
Orientierungsfaktor für s (Kristall → Probe):
$$m_{kl}^s = a_{ki}^c n_i^s a_{lj}^c b_j^s$$

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

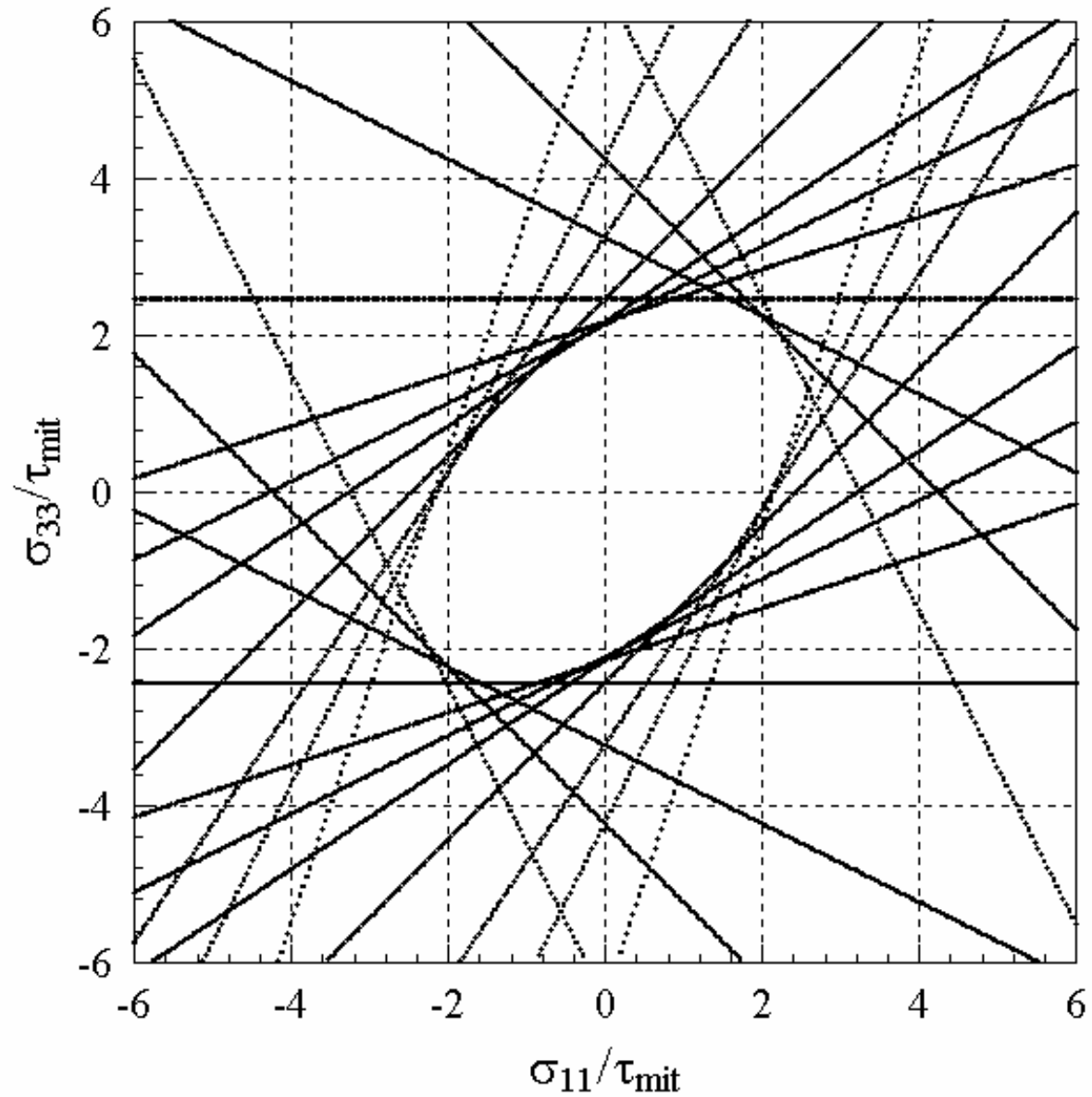


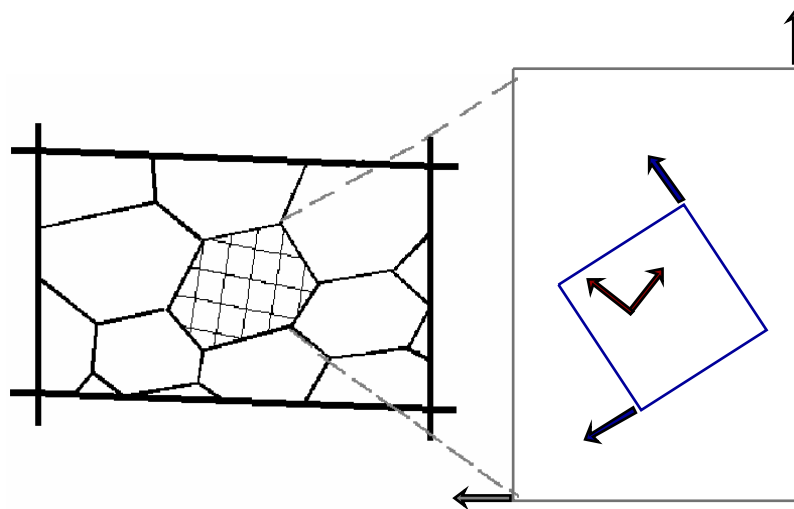
krz, 48 Systeme,
Schnitt

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

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

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





slip systems
 $\bar{n} \bar{b}$

crystal (k,l)
 $m_{kl} = n_k b_l$

sample (i,j)
 $m_{ij} = a_{ik} n_k a_{jl} b_l$

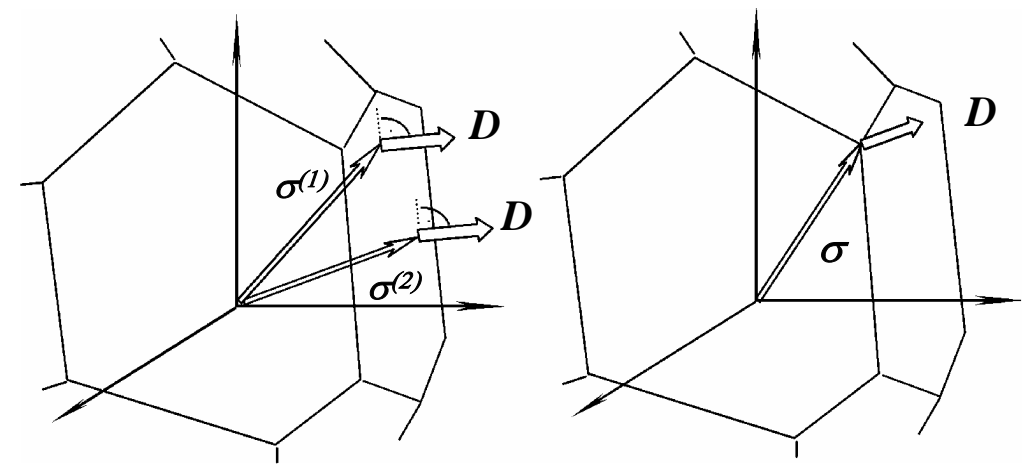
Ein Korn, ein System:

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

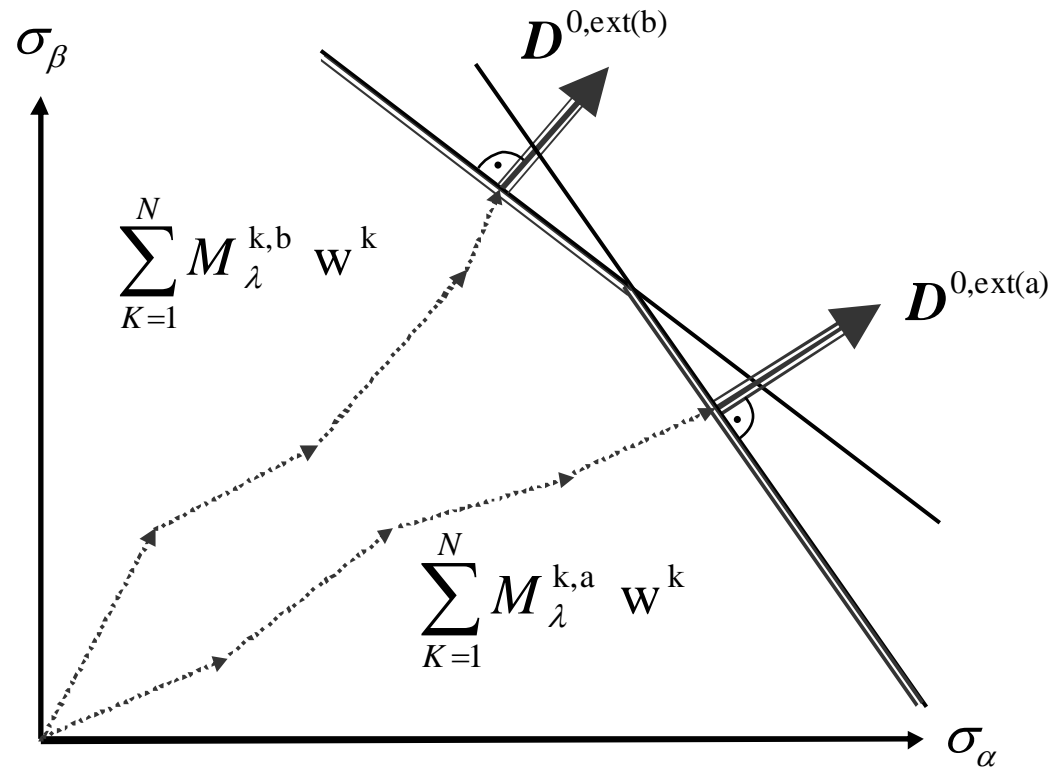
oberhalb FO: existiert nicht

Größe:

M: 2.1 - 4.5



Viele Körner, viele Systeme:

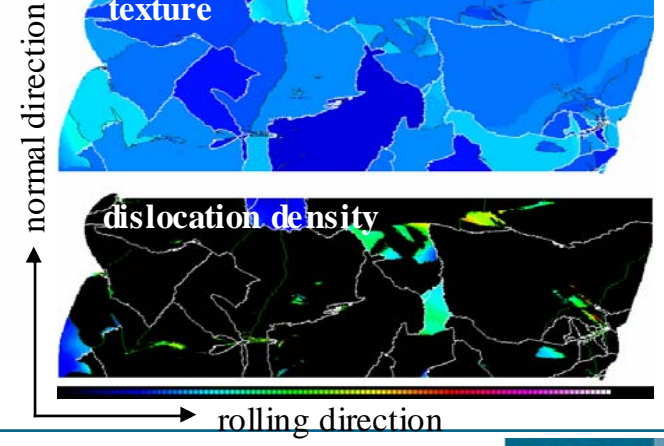
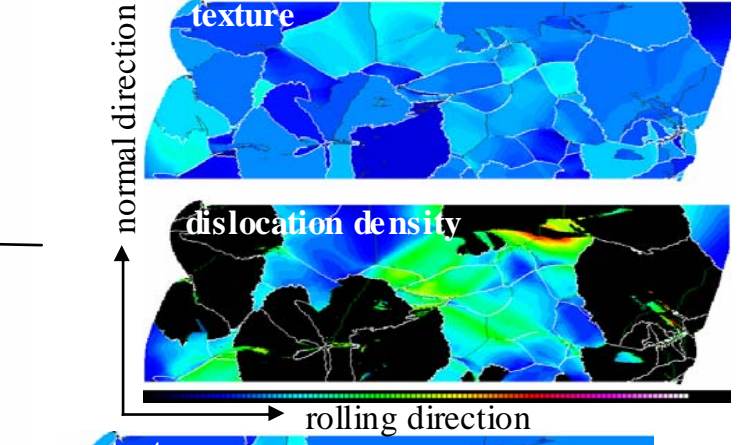
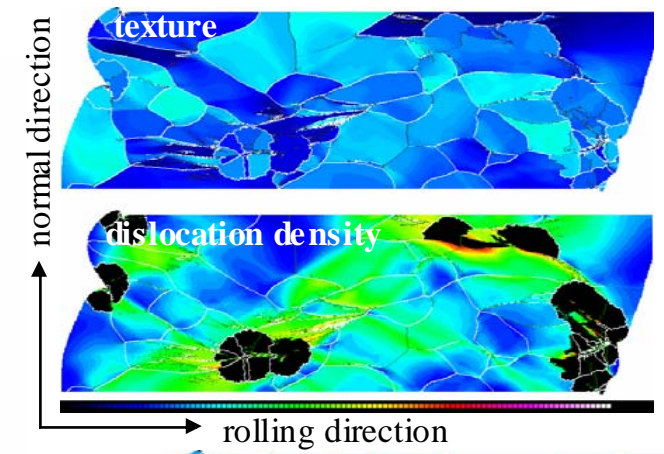
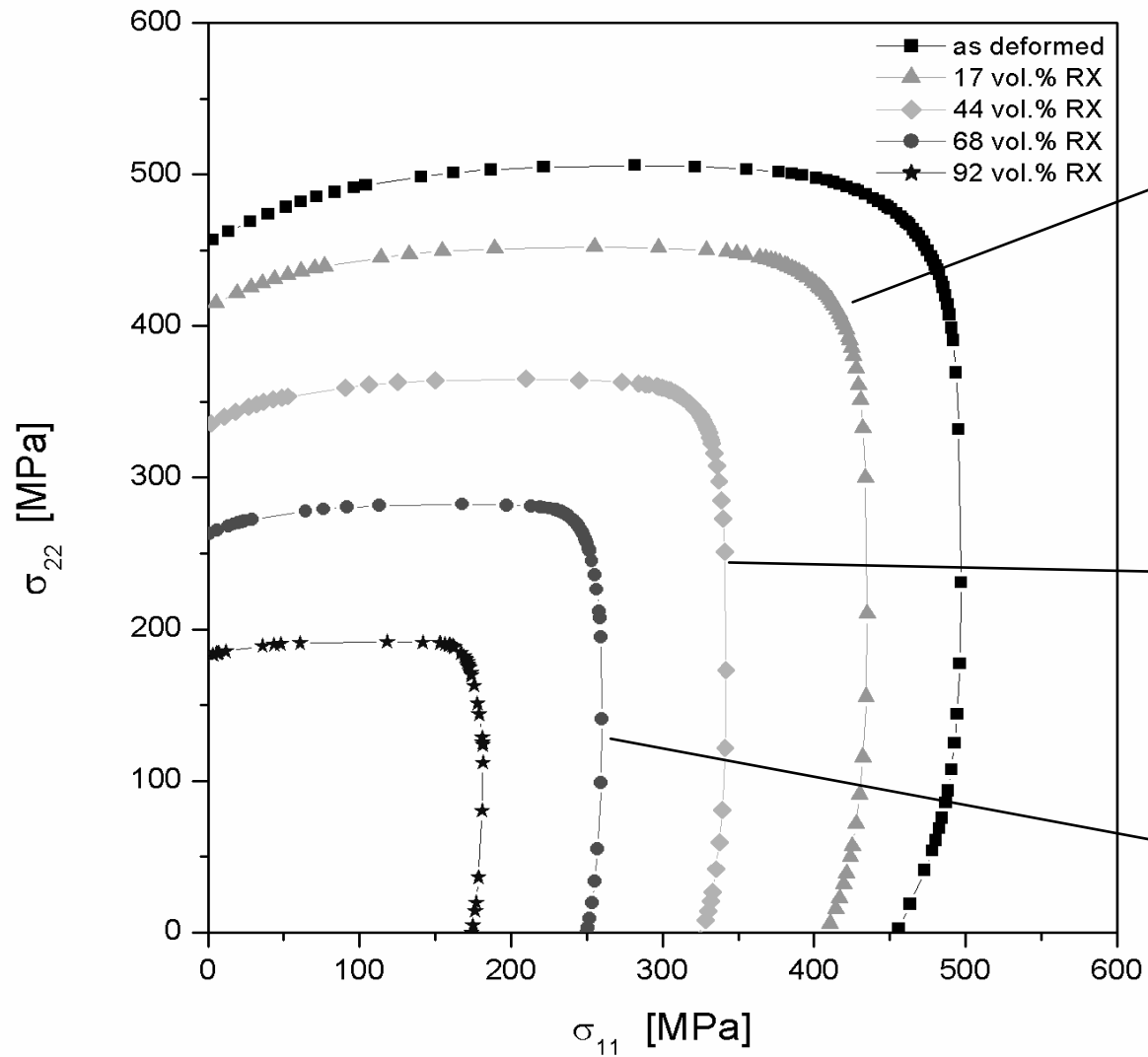


$$R_{ij}^P = \frac{1}{V} \int_V \underbrace{M_{ij}^{\text{hom}}(\mathbf{g}, D_{ij})}_{\text{Kinematik}} \underbrace{\tau_{\text{crit}}(s^1, \dots, s^m, S_{ij}^1, \dots, S_{ij}^n, T, D_{ij}^{\text{Kon}}, \mathbf{g})}_{\text{Kinetik}} dV \approx \sum_{k=1}^N M_{ij}^{\text{hom},k} \tau_{\text{crit}}^k w^k$$

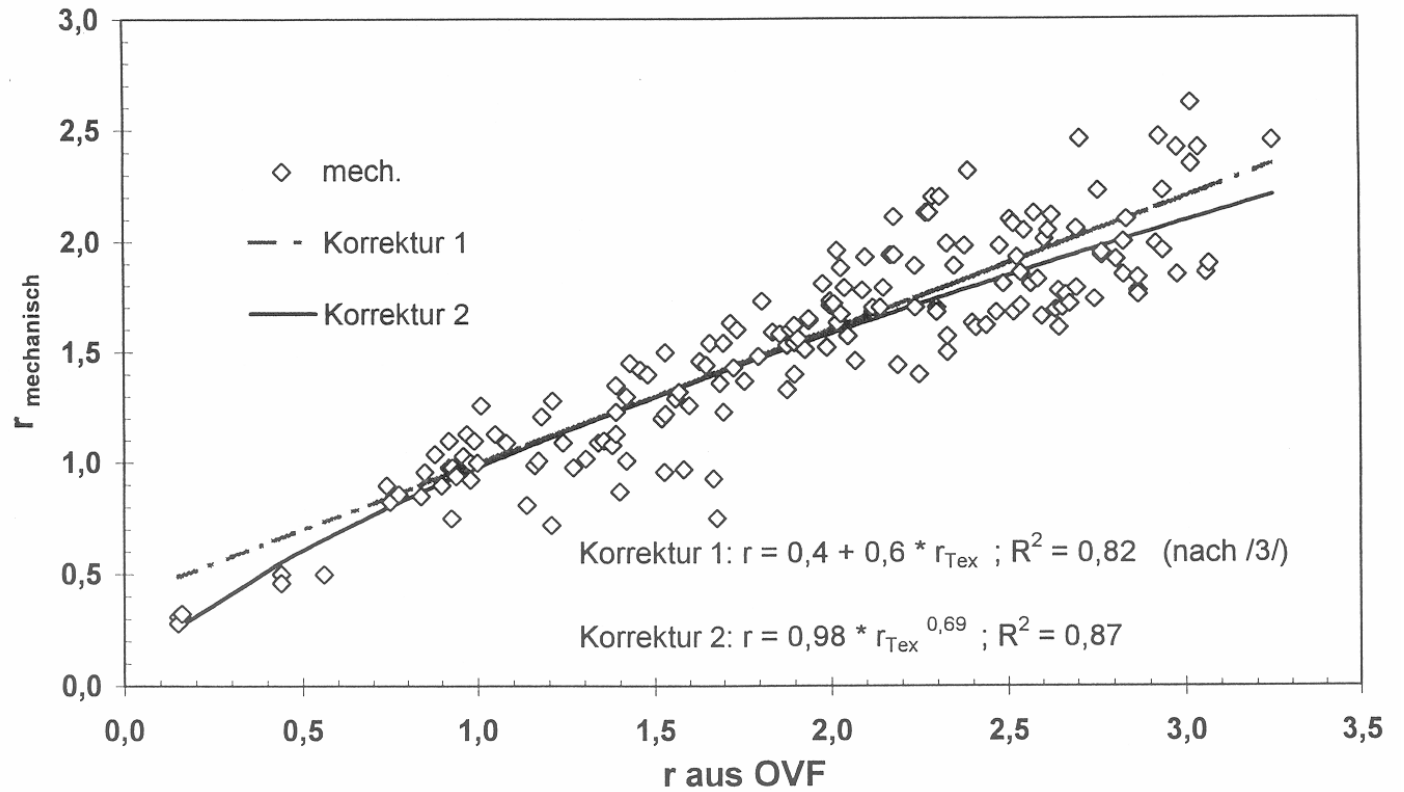
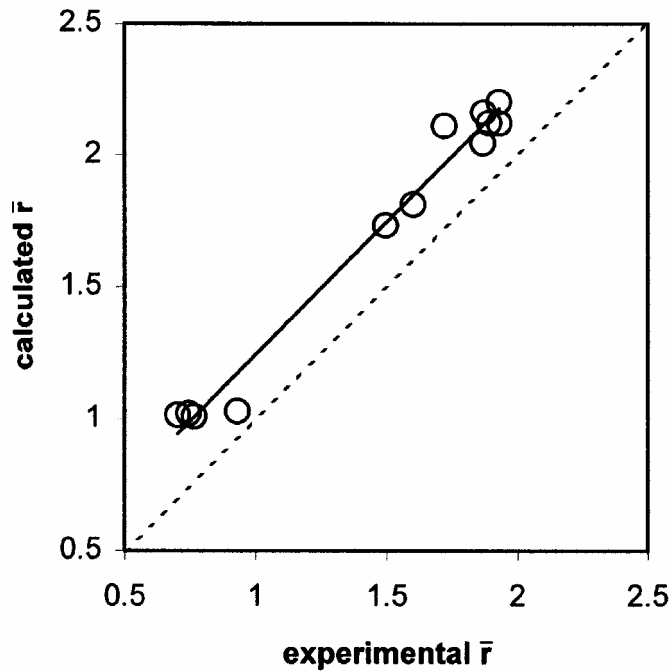
Kinematik

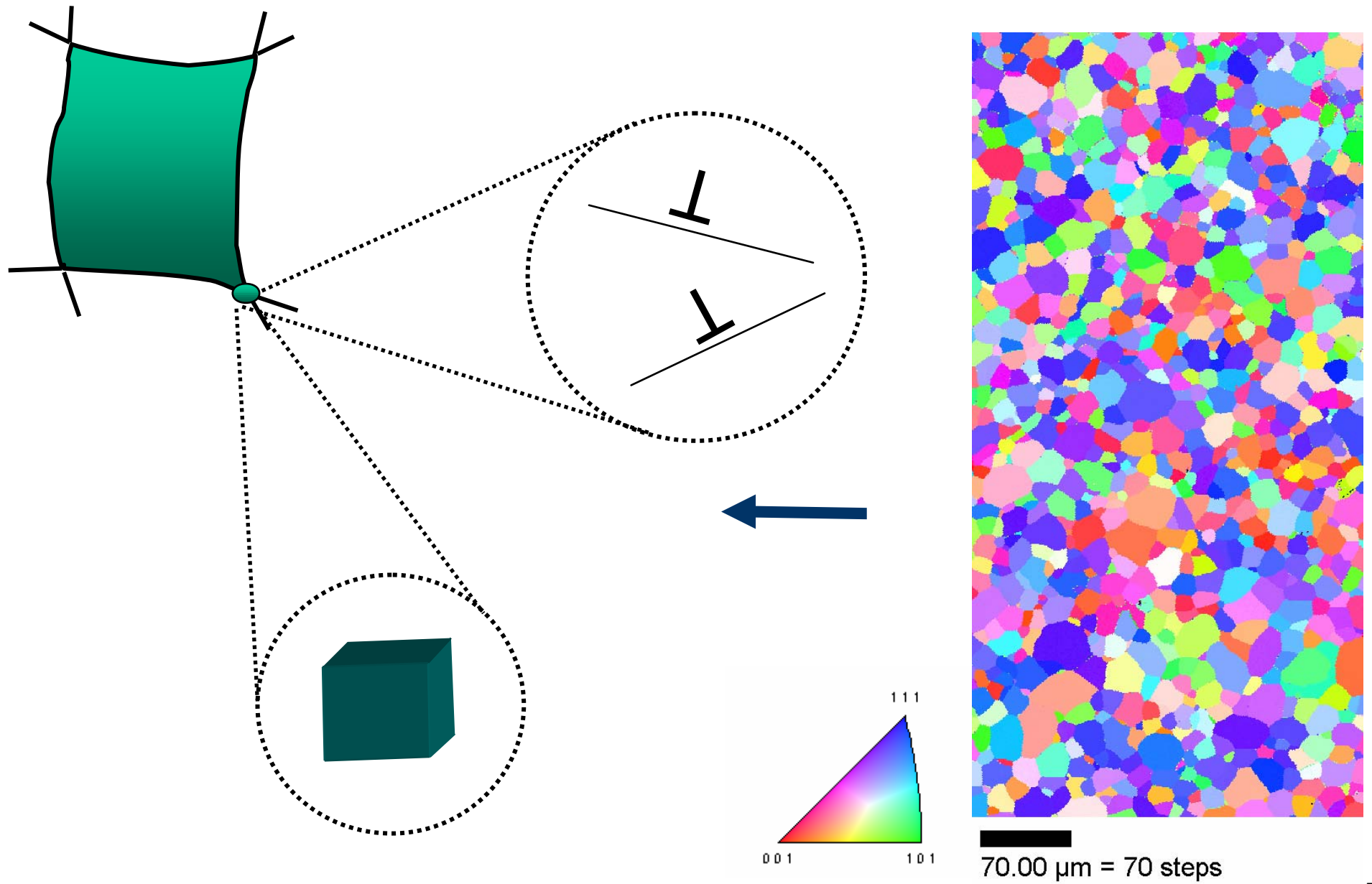
Kinetik

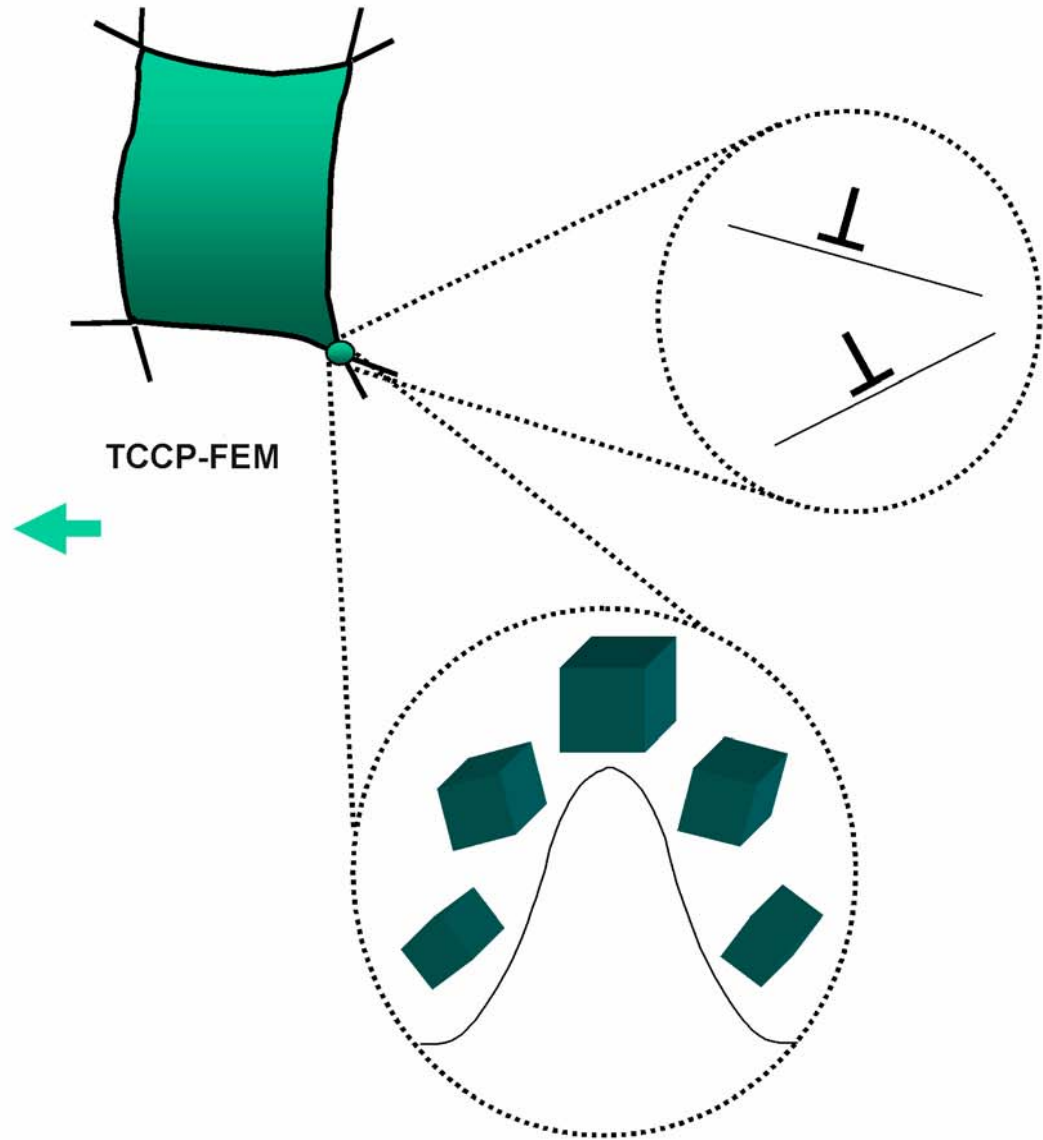
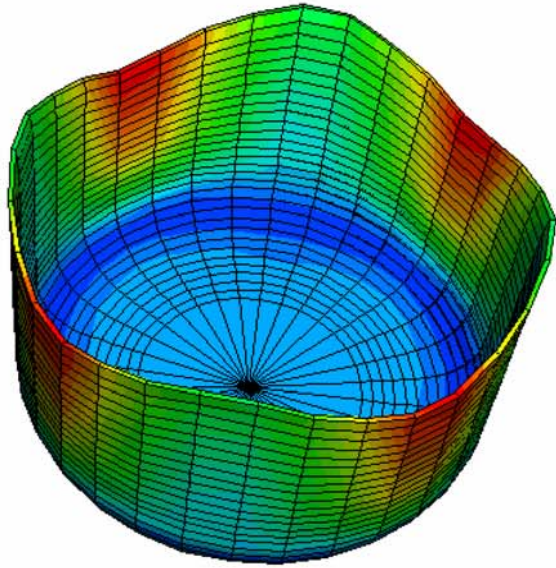


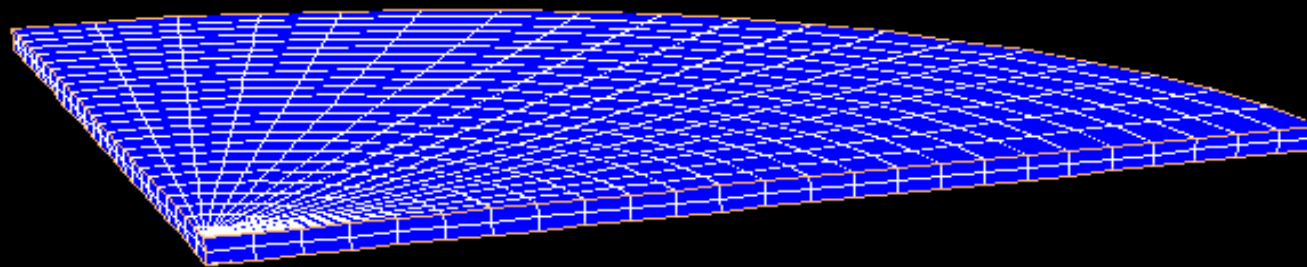
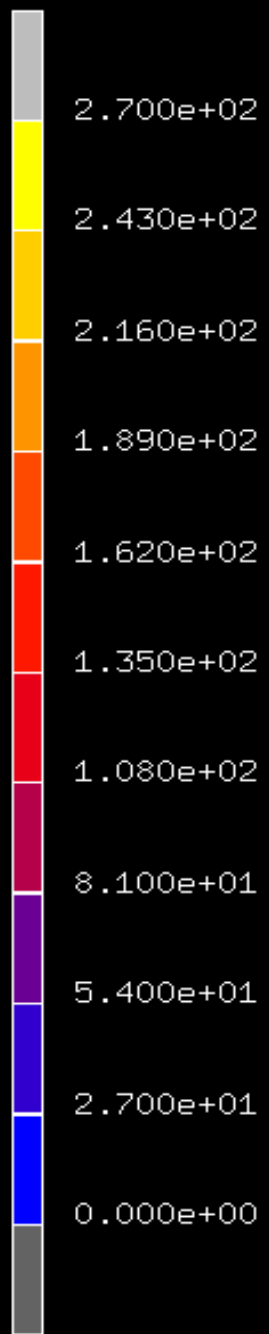


Empirischer Abgleich mechanisch und aus Texturen (OVF) ermittelter r-Werte

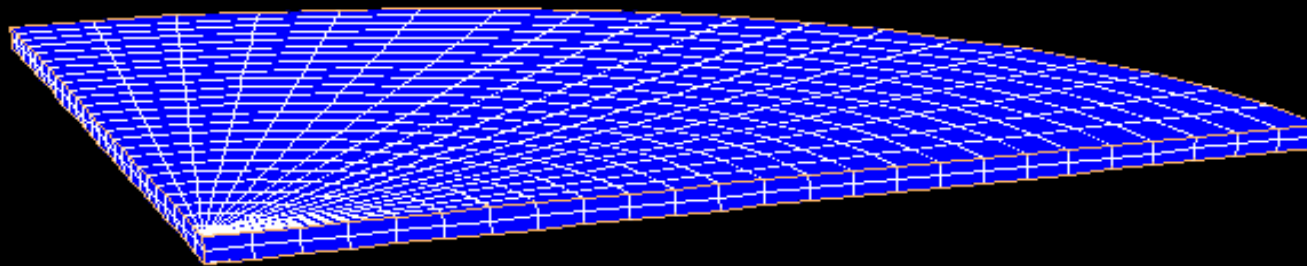
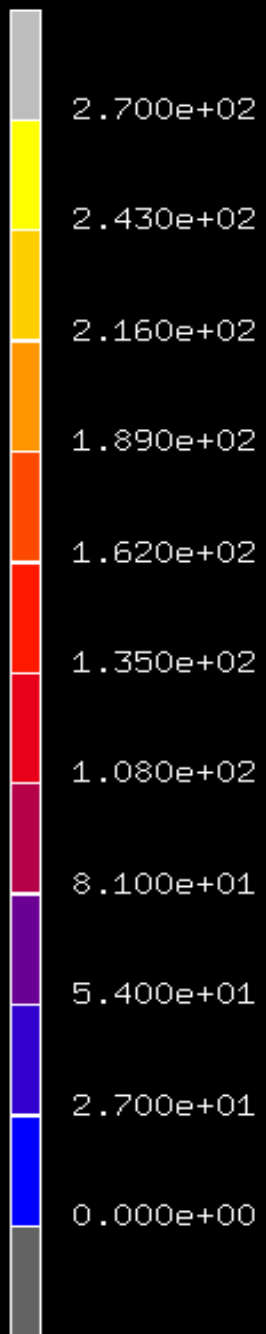








vaw1sr1



vaw2sr