Good Diffraction Practice VI:
Texture Analysis with MULTEX

Welcome

Outline

- Fundamentals of Texture Analysis
- Bragg Diffraction and Pole Figures
- Texture with 0D, 1D, and 2D detectors
- Strategies for Pole Figure measurements
- Texture approximation methods
- DIFFRAC.MULTEX
- Application Examples

Speakers

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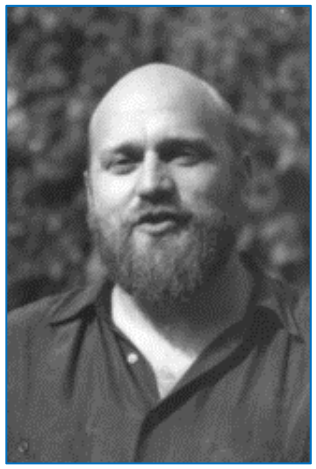

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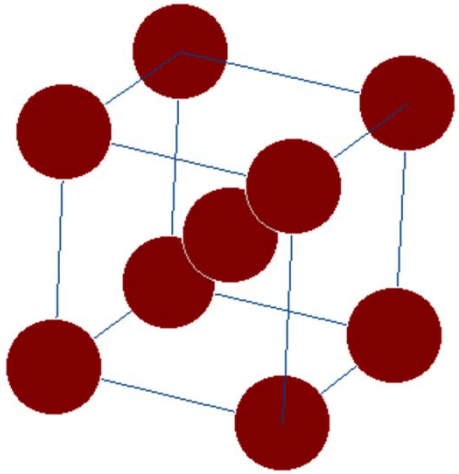
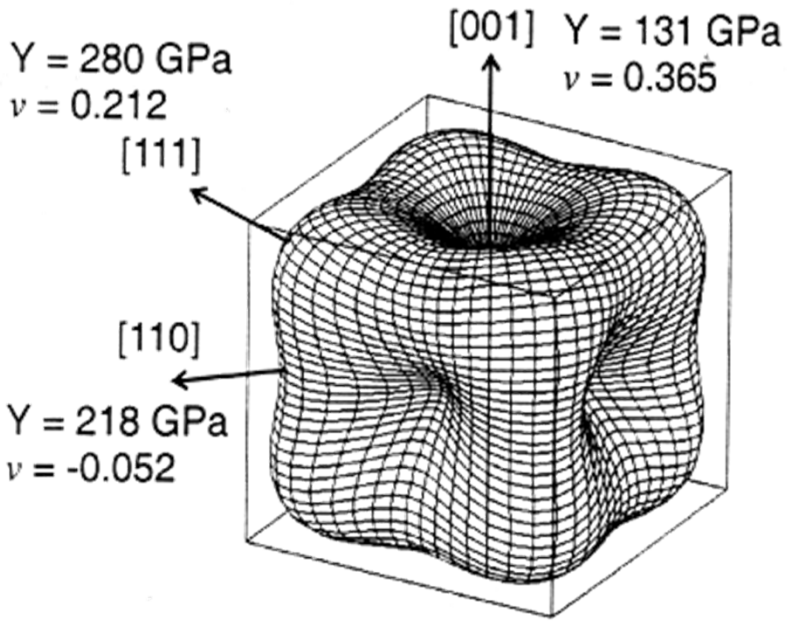
Crystal Structure properties

- Example: Fe crystal

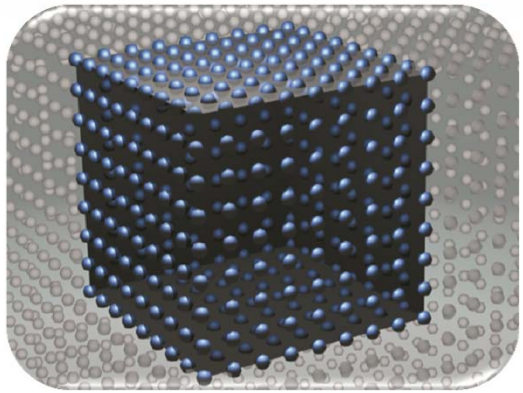


Lattice

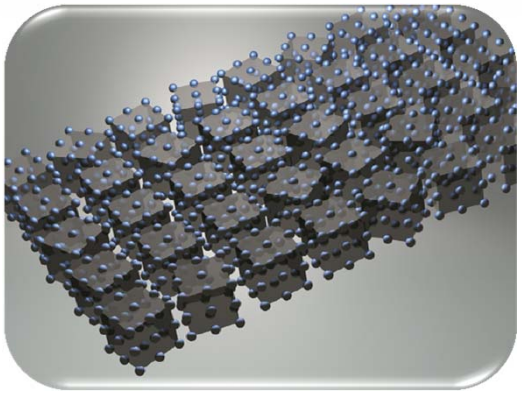


Elastic-Modul

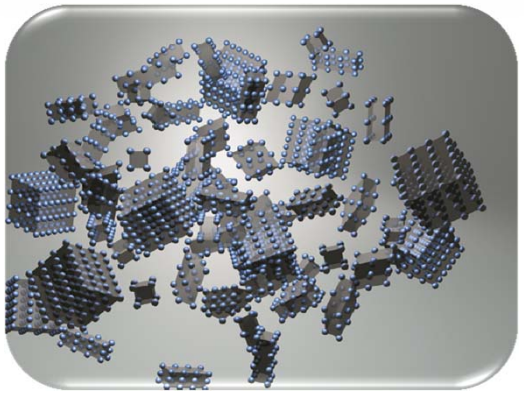
What is Texture?



Single Crystal

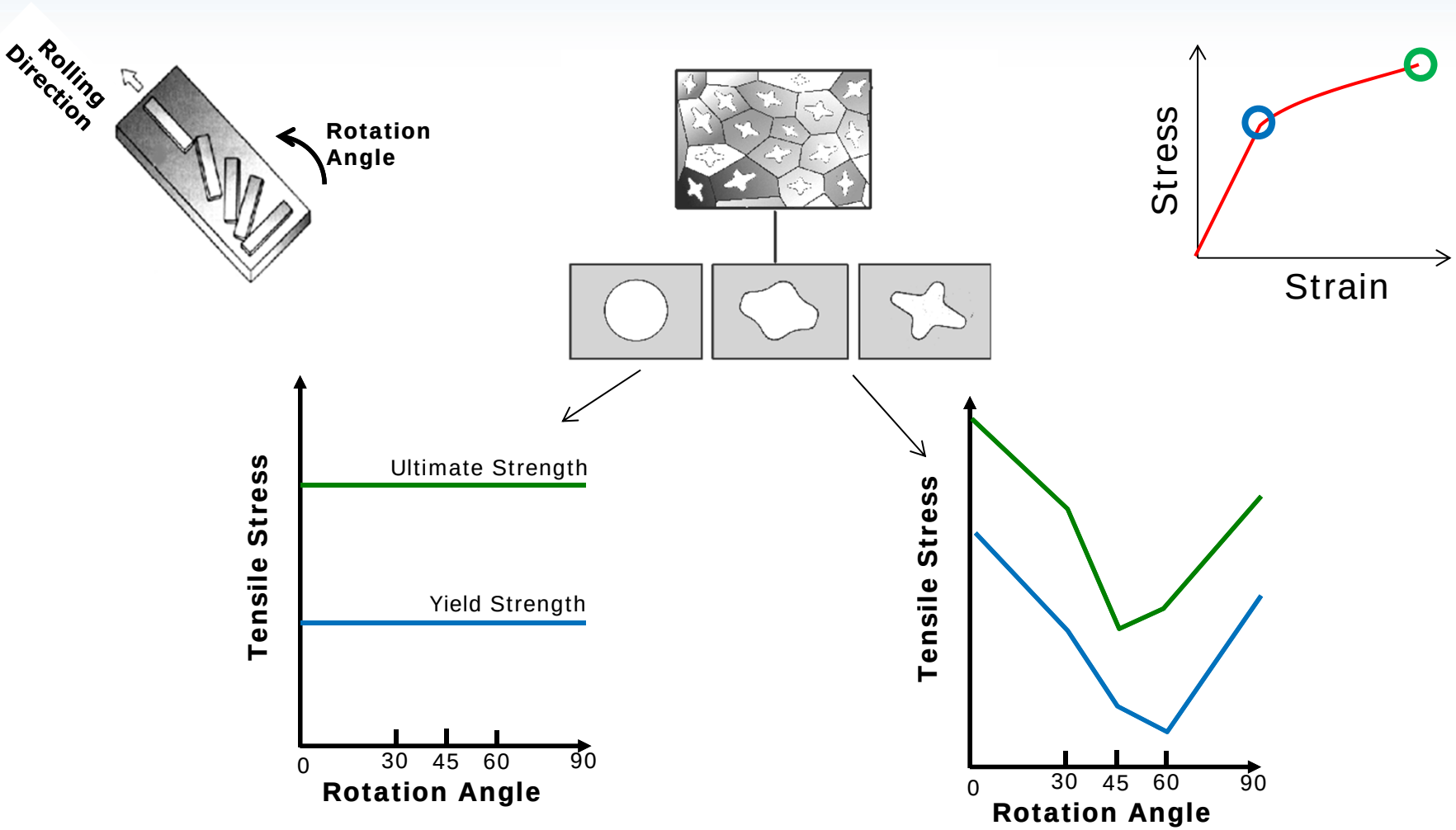


Textured polycrystalline (fiber)

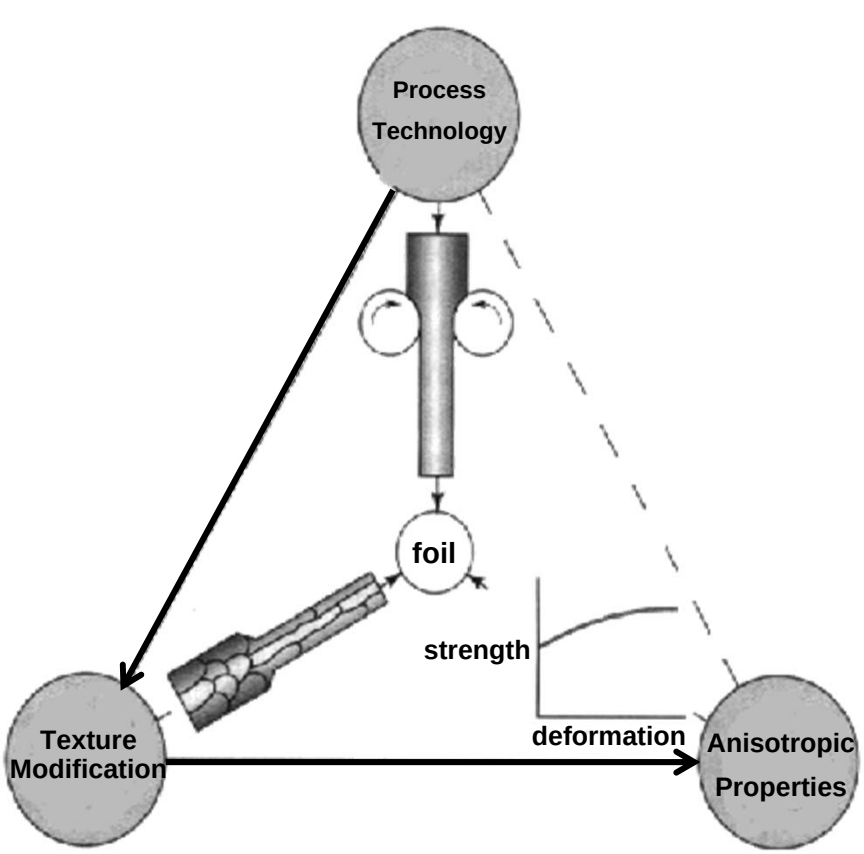


Random (isotropic)

Why do we care?
Anisotropy of polycrystalline materials



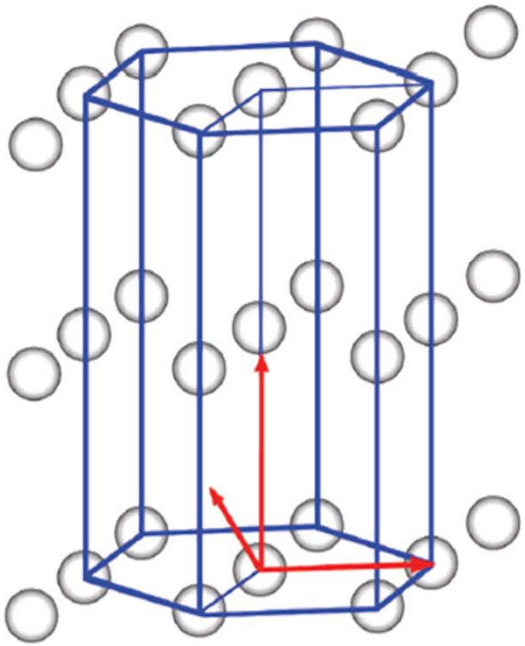
Enhancing materials properties with texture modifications



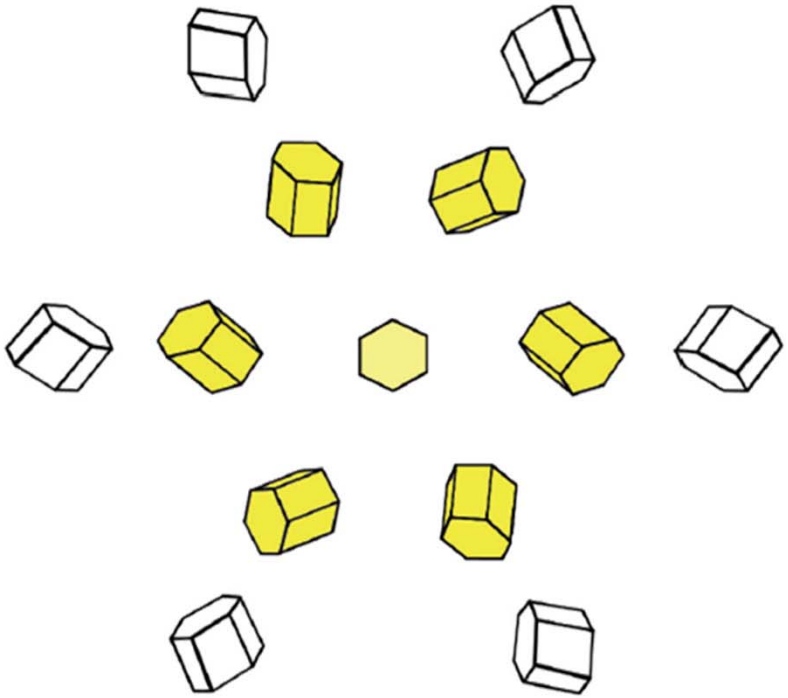
- **Crystalline materials:**
  metals, alloyings, intermetallics, ceramics, composite materials, polymers, semiconductors, nano crystals, superconductors, rocks
- **Texture modification process:**
  deformation, recrystallization, phase transformations, film synthesis with plasma, laser and ion beams, crystallization to boundary surfaces, rigid particle rotation
- **Anisotropic properties:**
  plasticity, elasticity, strength, cleavability, electrical conductivity, thermal extension and conductivity magnetization, corrosion resistance, optical properties

Crystal and Sample symmetry

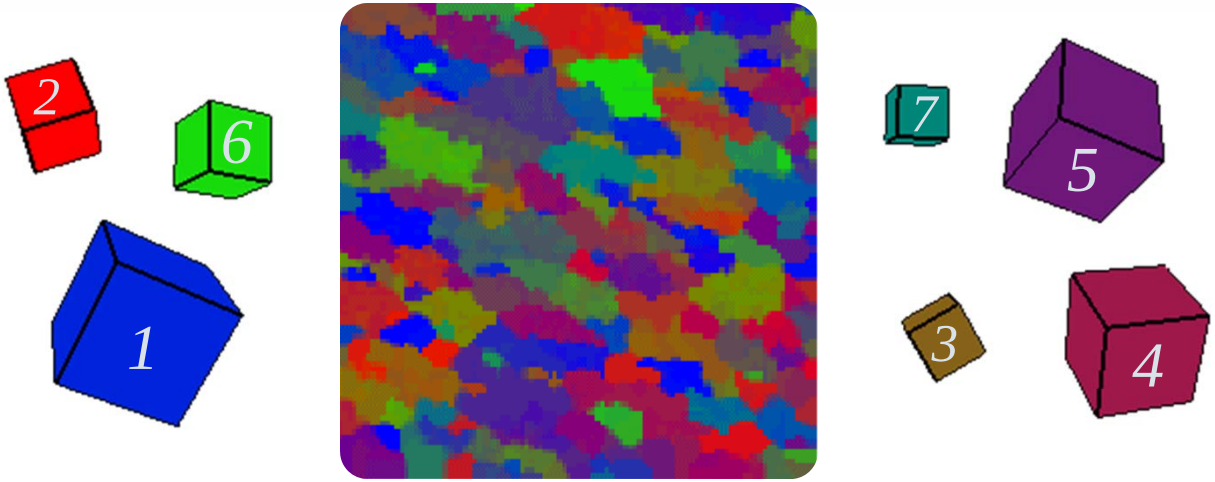
Crystal symmetry D_6



Sample symmetry C_6



Orientation Distribution Function (ODF)



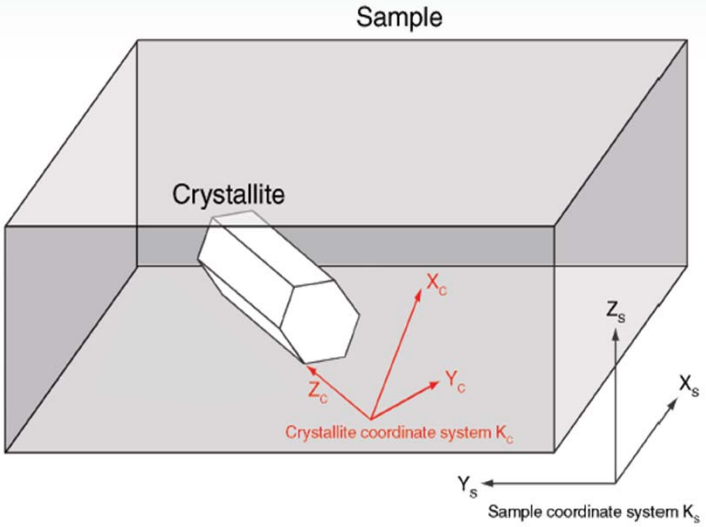
$$N \to \infty$$

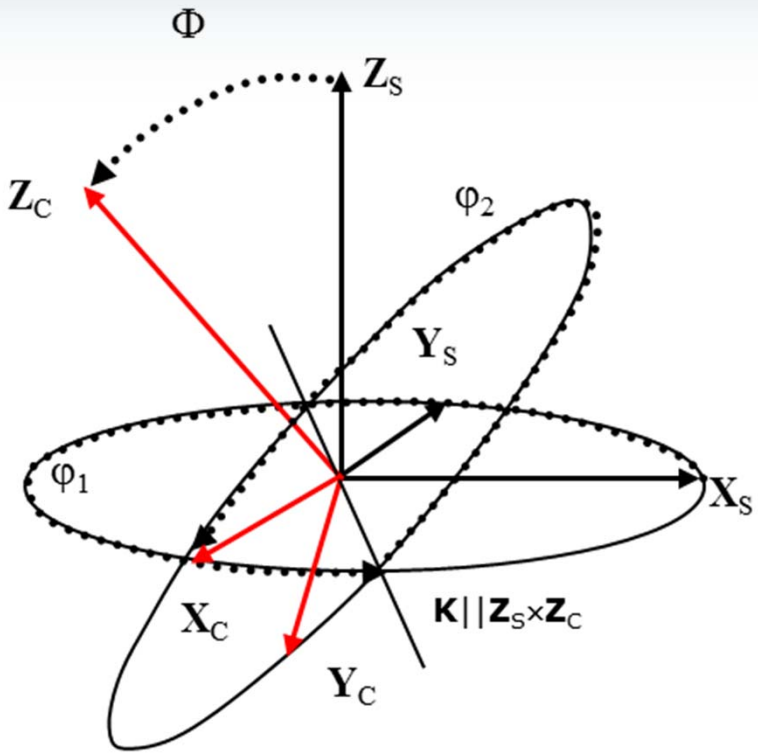
limiting value: $dV(g_1), dV(g_2), \ldots dV(g_N) \quad \Rightarrow \quad f(g)$

$$dg \to 0$$

$$f(g)dg = dV_g / V \geq 0$$

Coordinate systems and Eulerian space



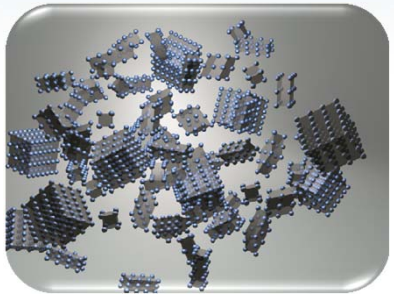


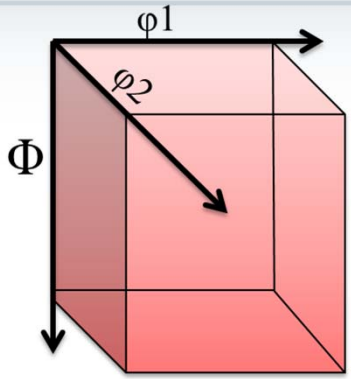
	rotation axis	angle
1. $X_S \Rightarrow K$	Z_S	φ_1
2. $Z_S \Rightarrow Z_C$	K	Φ
3. $K \Rightarrow X_C$	Z_C	φ_2

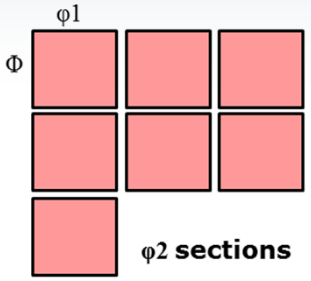
$$0 \le \varphi_1 < 2\pi, \quad 0 \le \Phi \le \pi, \; 0 \le \varphi_2 < 2\pi$$

Real space to Eulerian space
Representing the ODF

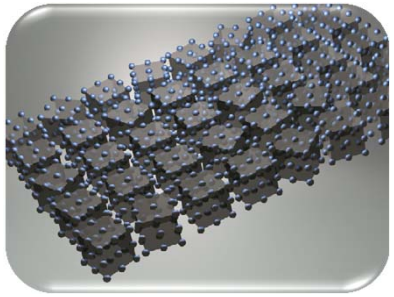
Isotropic

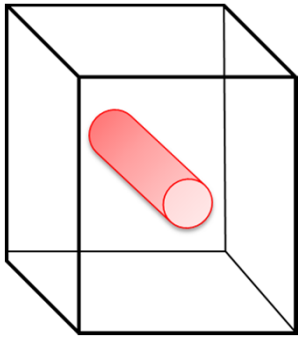


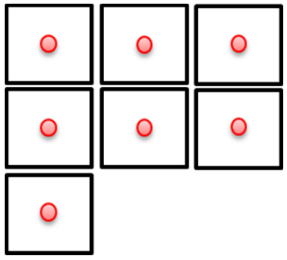




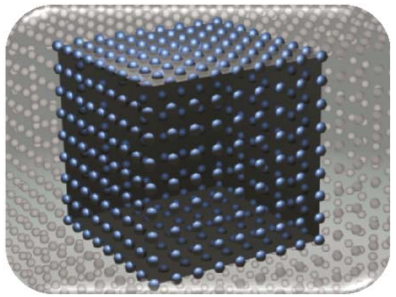
Fiber Texture

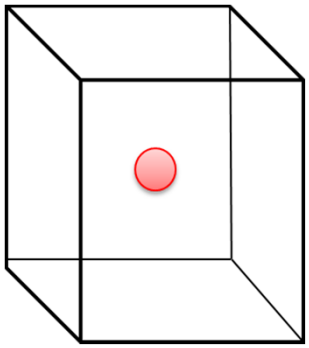


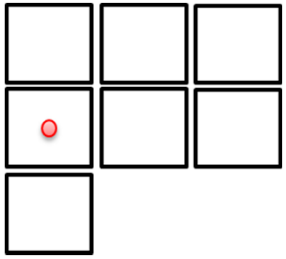




Spherical Texture



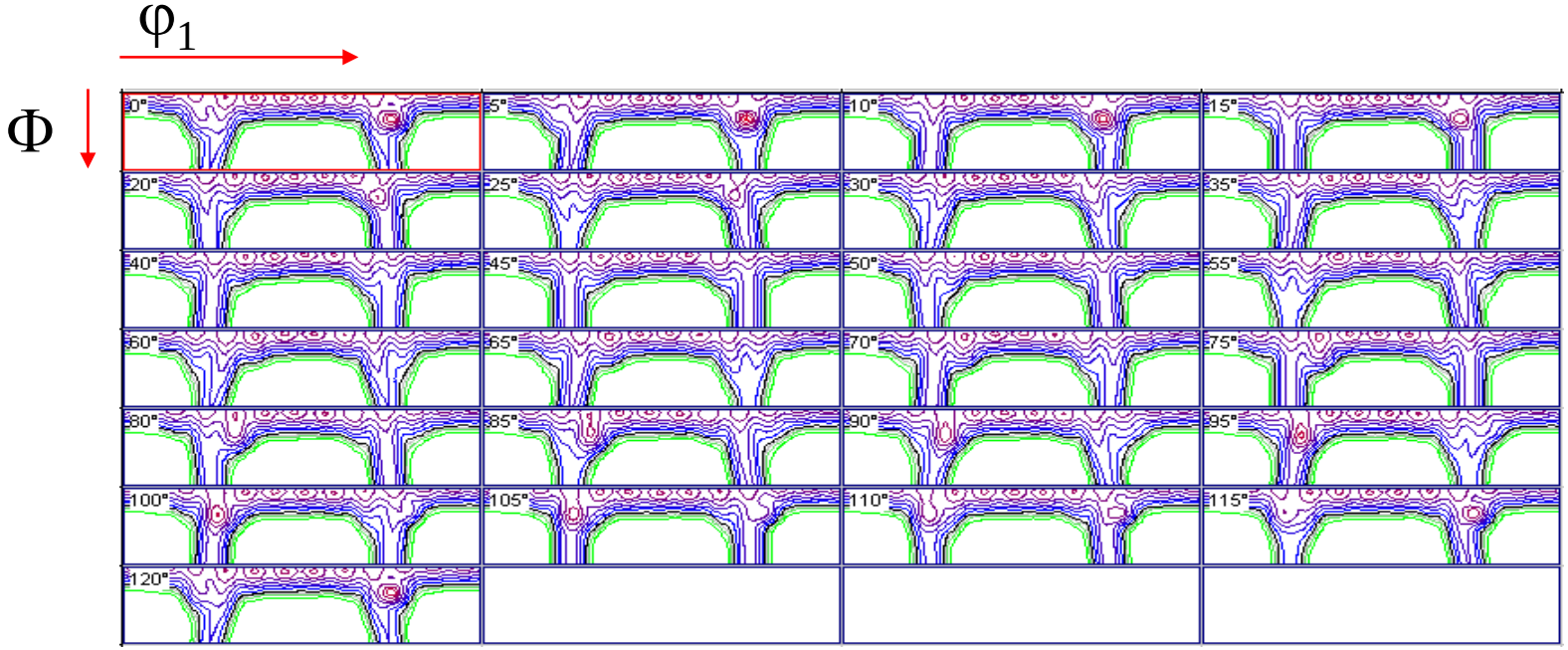




Real world ODF
Eulerian sections

symmetry $\Rightarrow$ reduced fundamental unit in Eulerian space

example: trigonal KS, triclinic sample symmetry
fundamental unit: $0 \le \varphi_1 < 2\pi,\ 0 \le \Phi \le \pi/2, 0 \le \varphi_2 < 2\pi/3$



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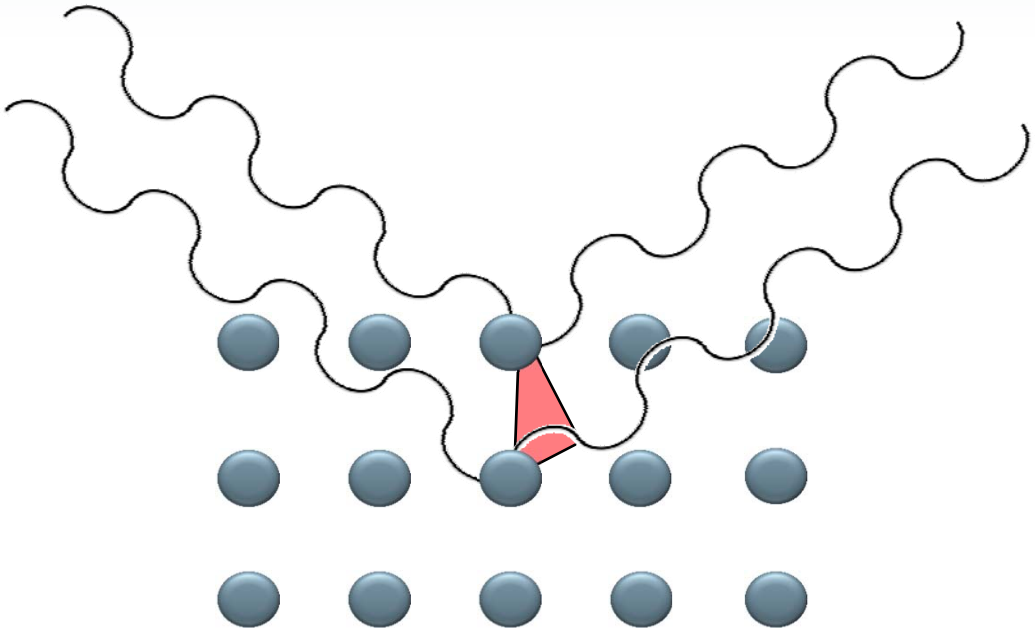
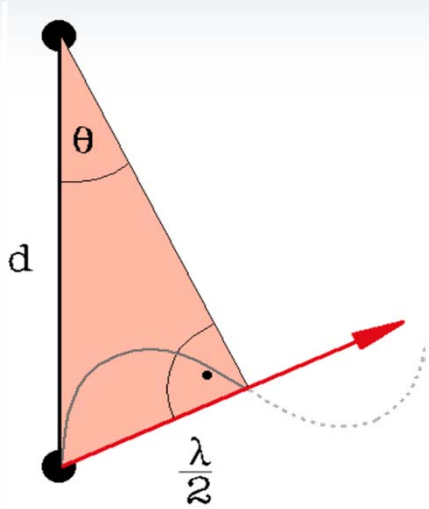
Bragg's Law

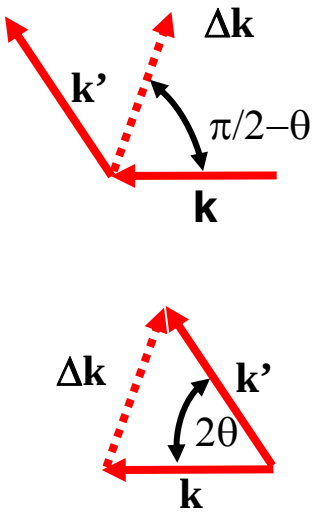




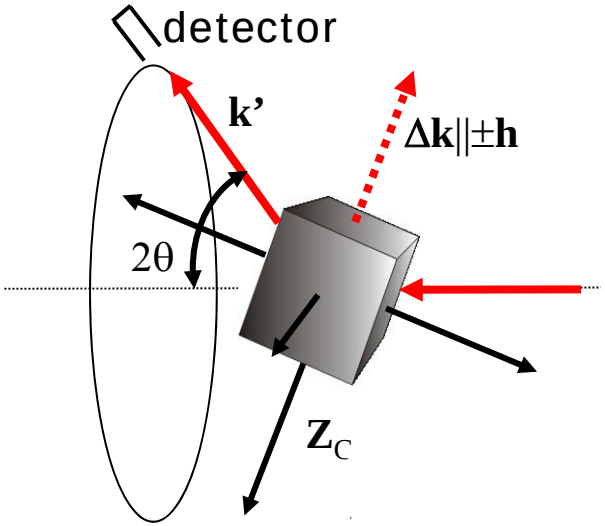
$$\sin\theta = \frac{\lambda/2}{d} = \frac{\lambda}{2d}$$

"Bragg's Law"

Single Crystal diffraction

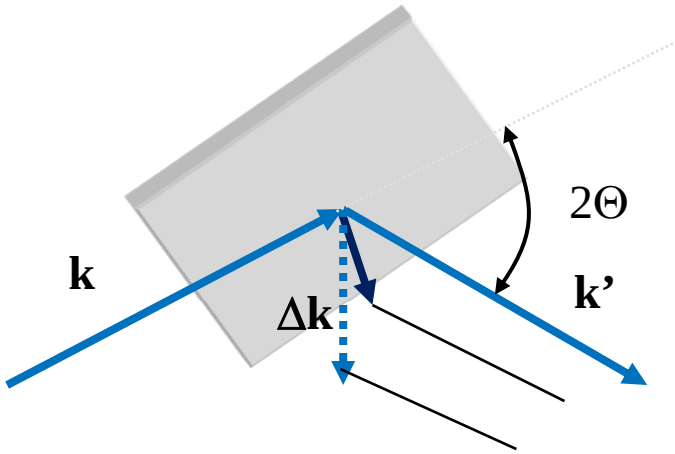


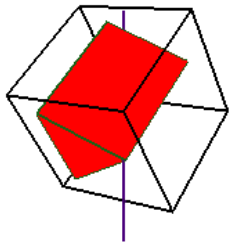
Definition of the diffraction vector $\Delta\mathbf{k} = \mathbf{k'} - \mathbf{k}$



Diffraction on (100) lattice planes of a cubic single crystal.

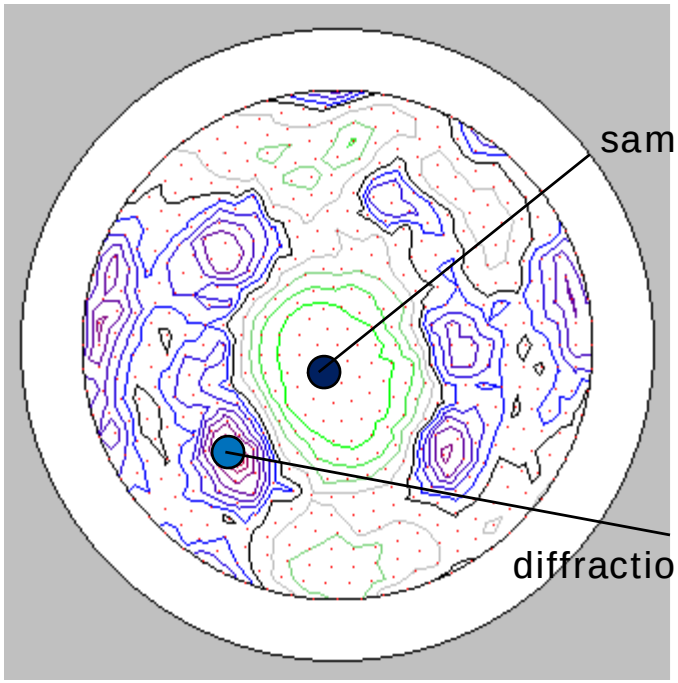
Relating Bragg's Law to Pole Figures





projection: ODF ⇒ pole figure:
orientations with common direction

(hkl) = (101)



Hämatite, point group D_{3d}

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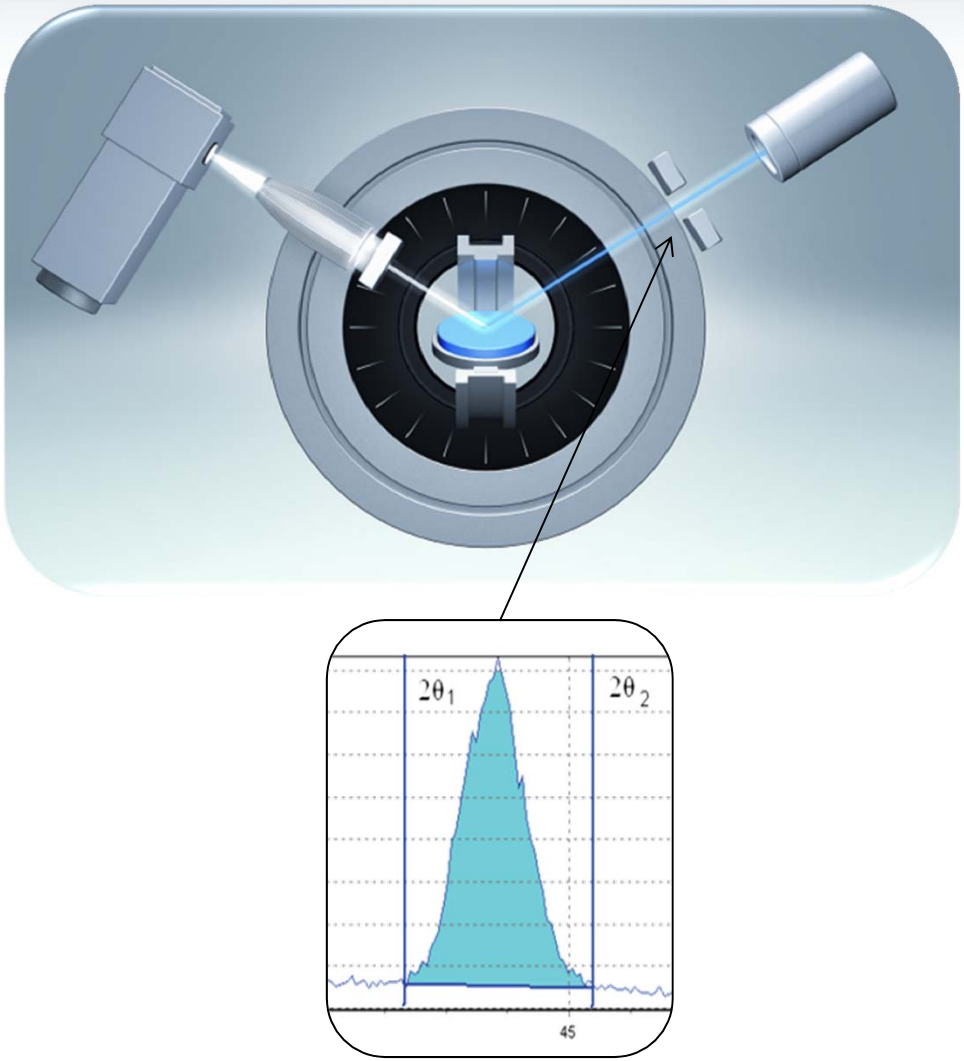
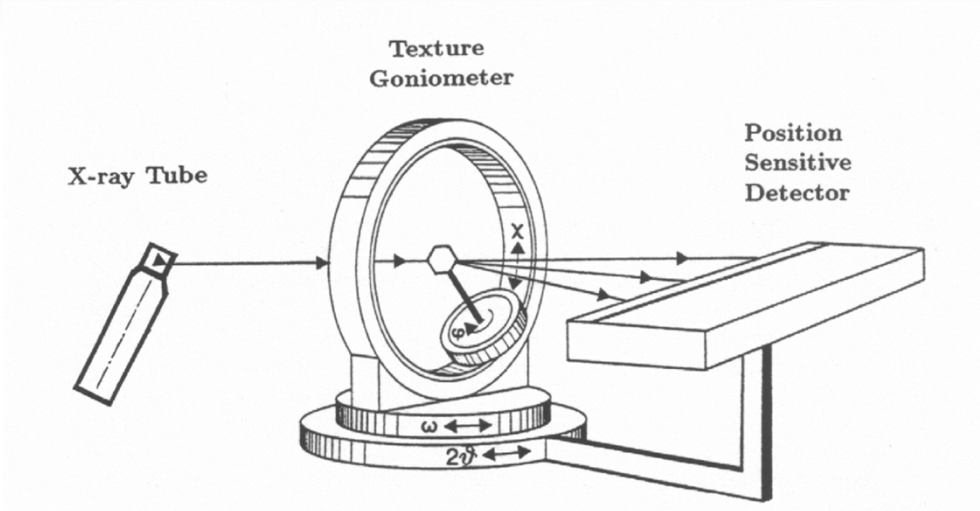
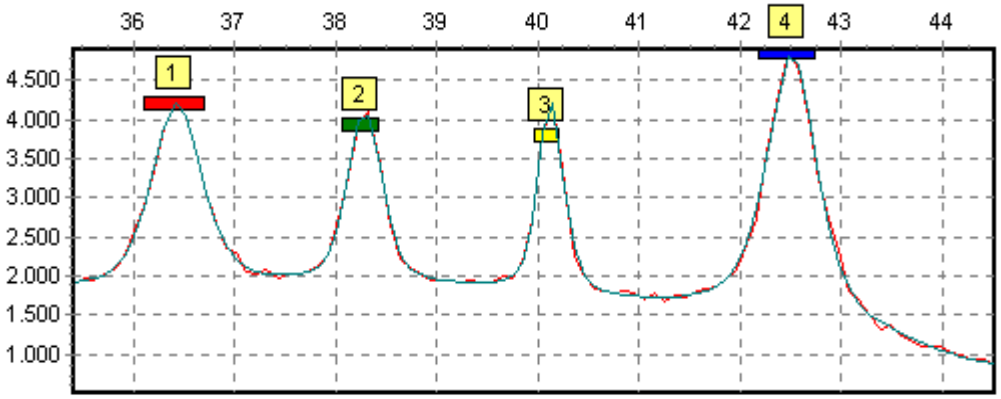
Texture Diffractometer
0D detector



- Single data point used to determine peak intensity.
- Defined by integral intensity passed by detector slit.
- Additional measurement required for background

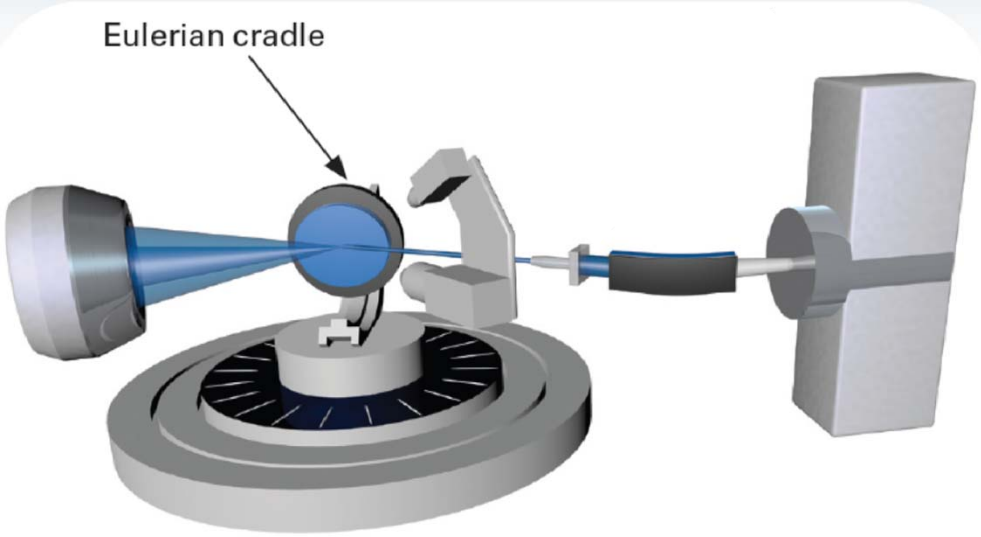
Texture Diffractometer
1D detector

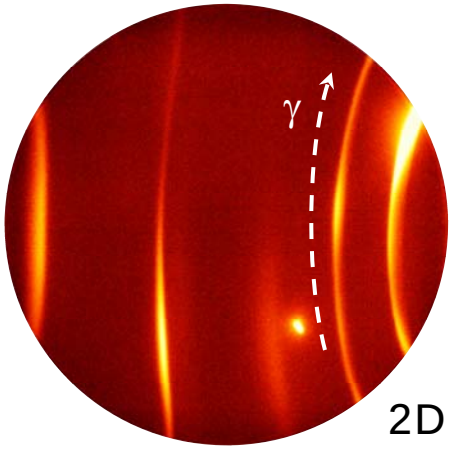




- Simultaneous collection of many data points to accurately define peak(s) intensity.
- Full background available.

Texture Diffractometer
2D detector

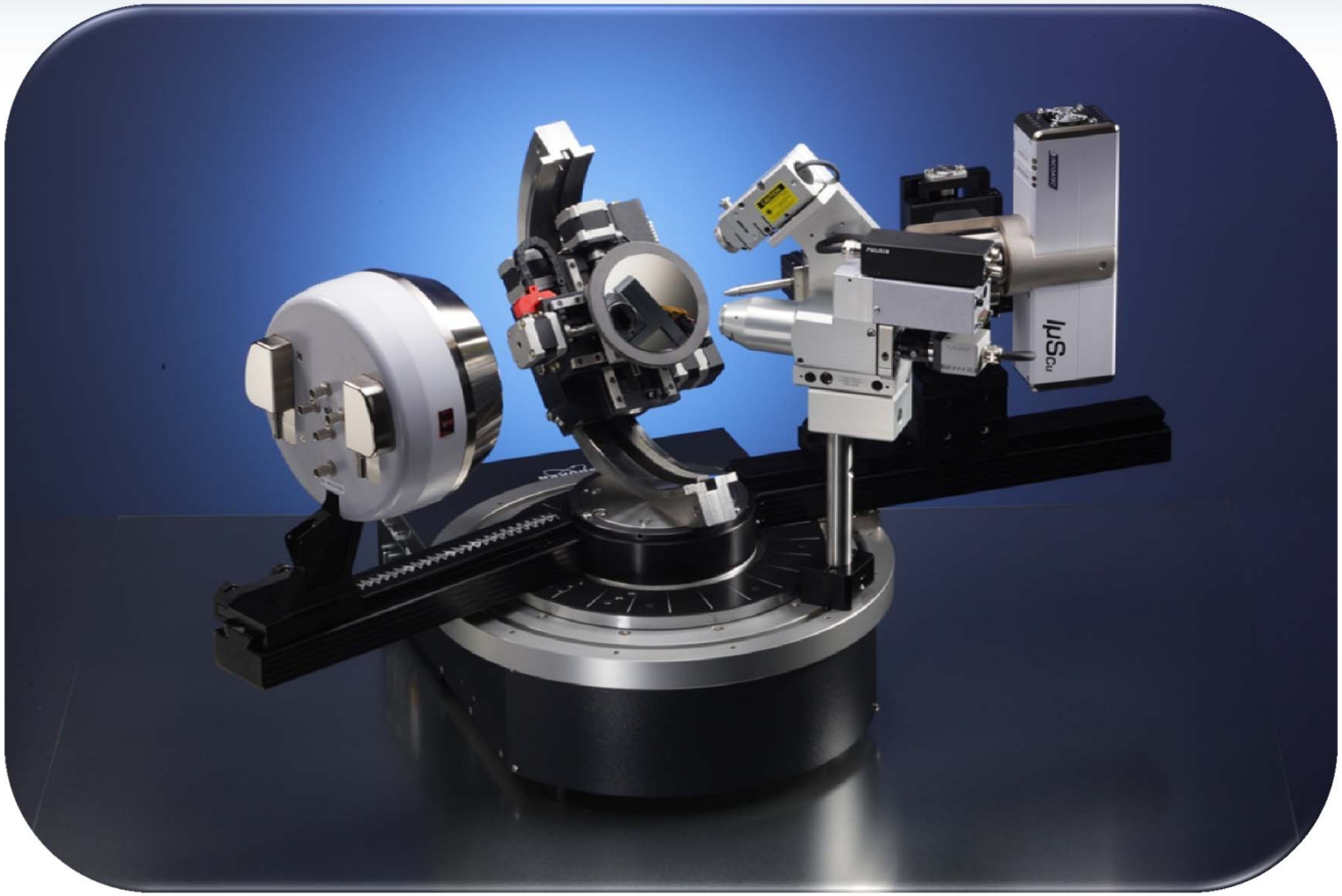




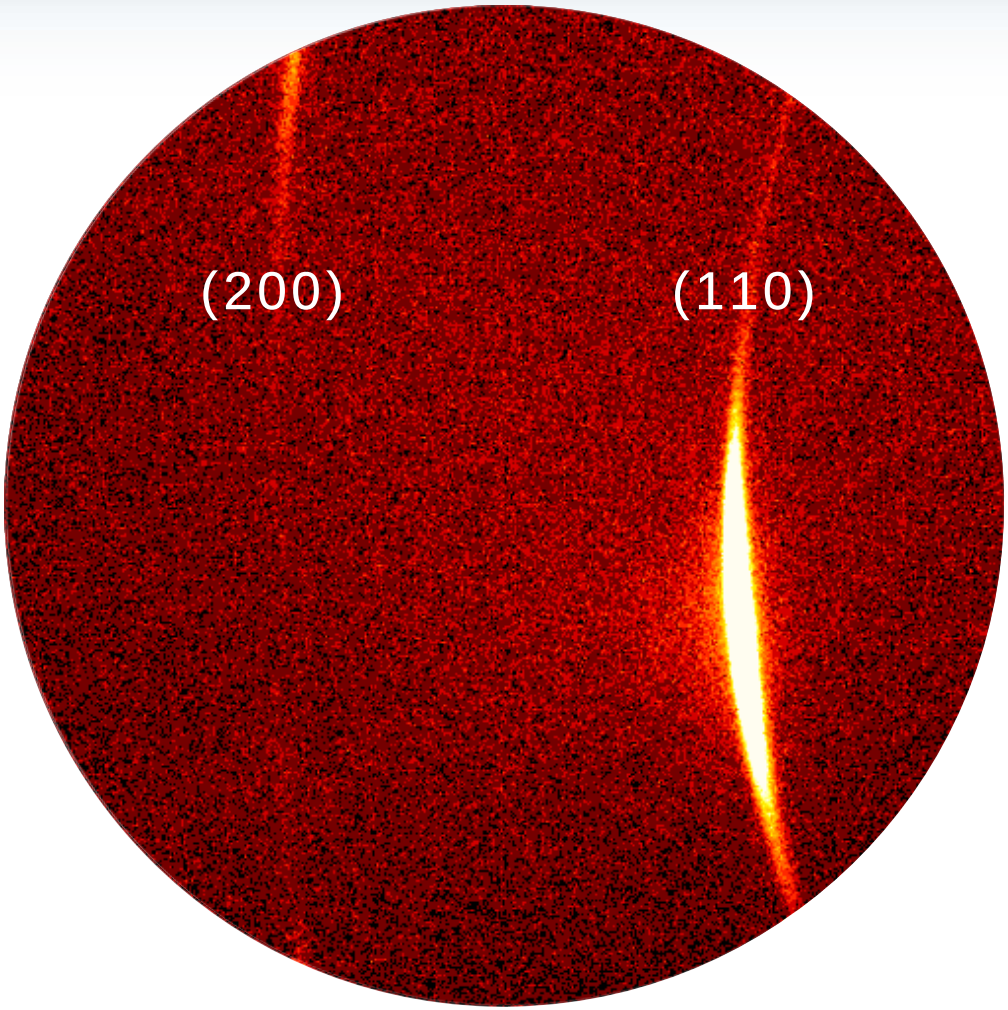
2D detector output

- Simultaneous collection of many data points to accurately define peak(s) intensity.
- Full background available.
- Intensity as function of γ available.

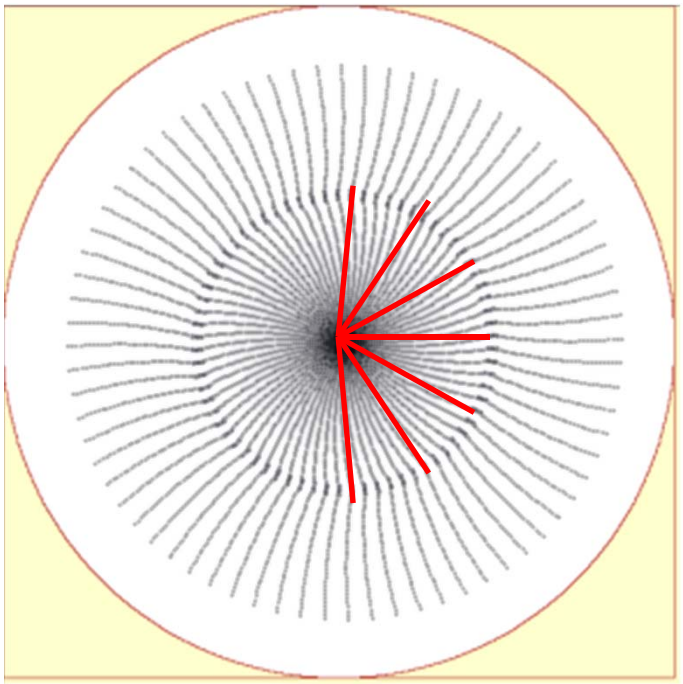
Modern texture diffractometer



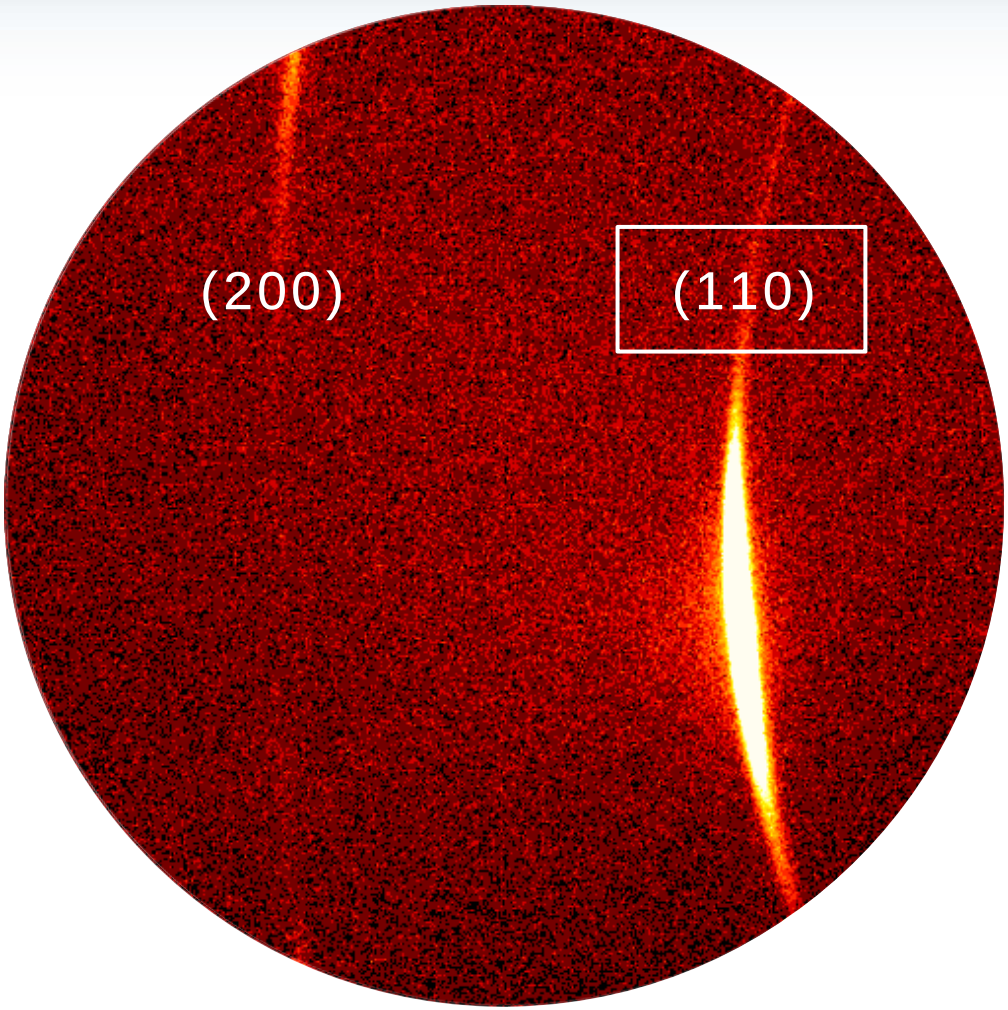
Pole Figures from 2D detector



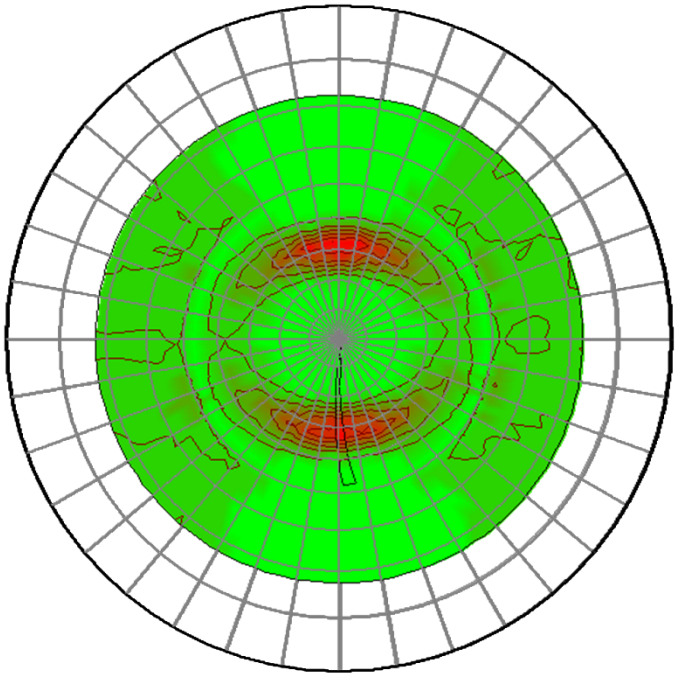
- Steel can
- Intensity variation during ϕ scan



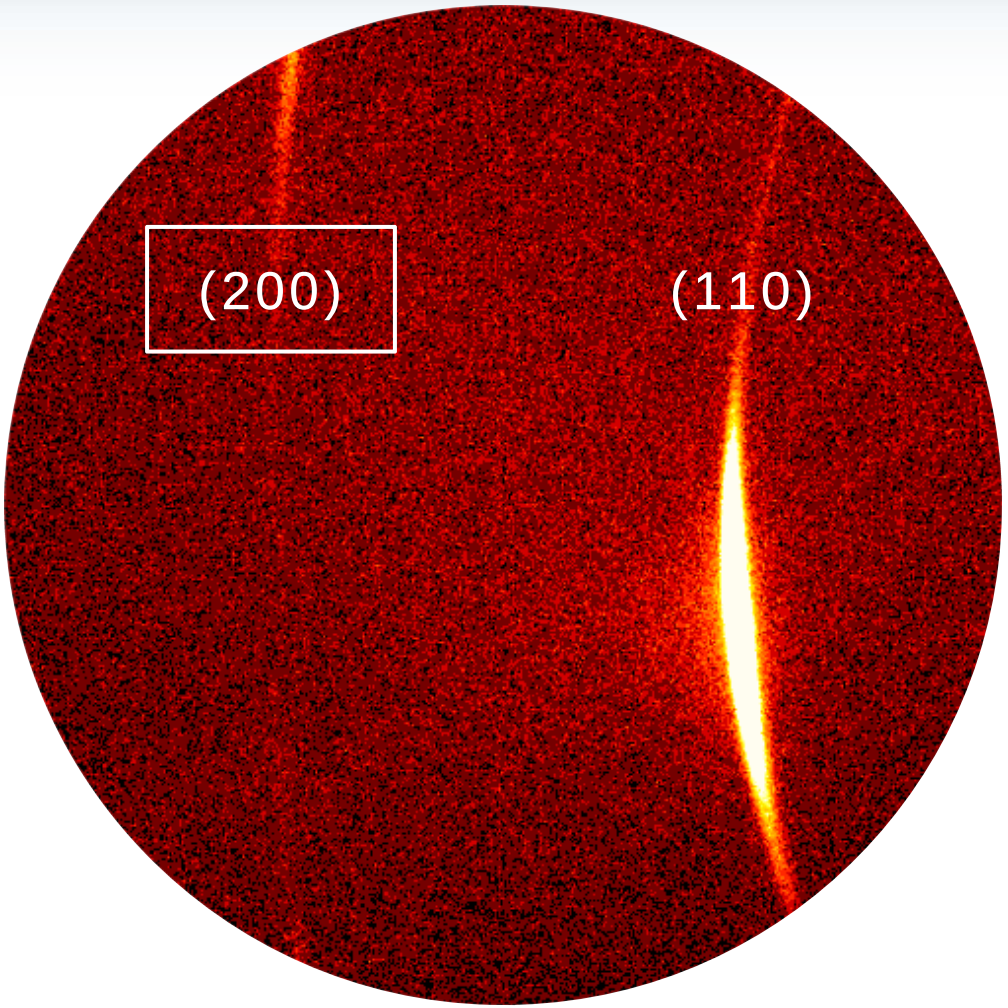
Pole Figures from 2D detector



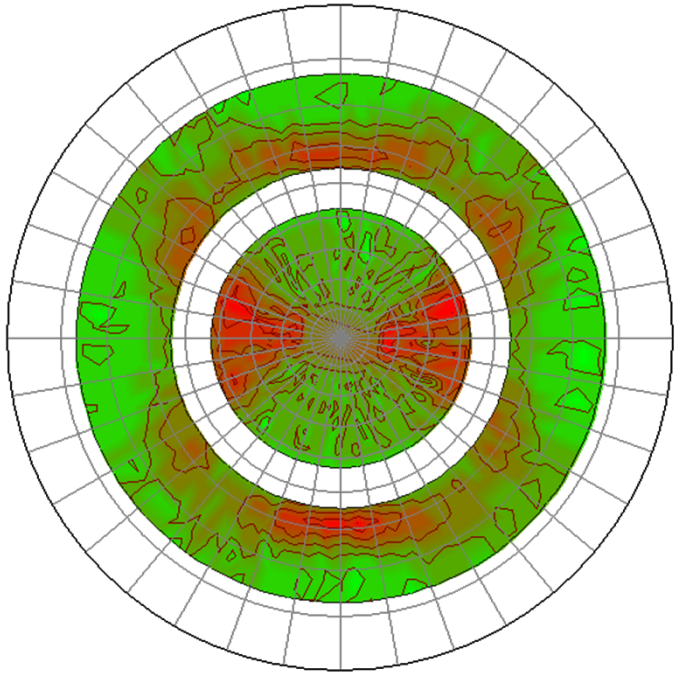
- Steel can
- Intensity variation during ϕ scan



Pole Figures from 2D detector

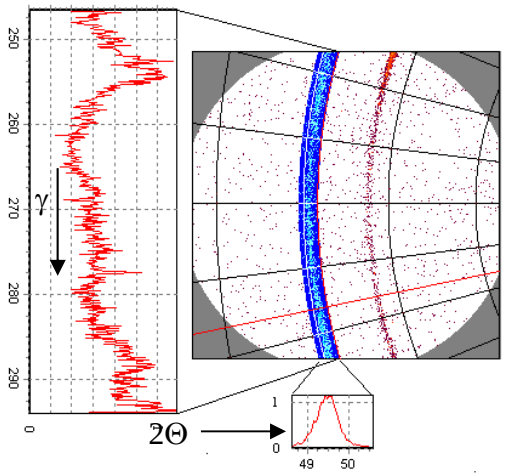


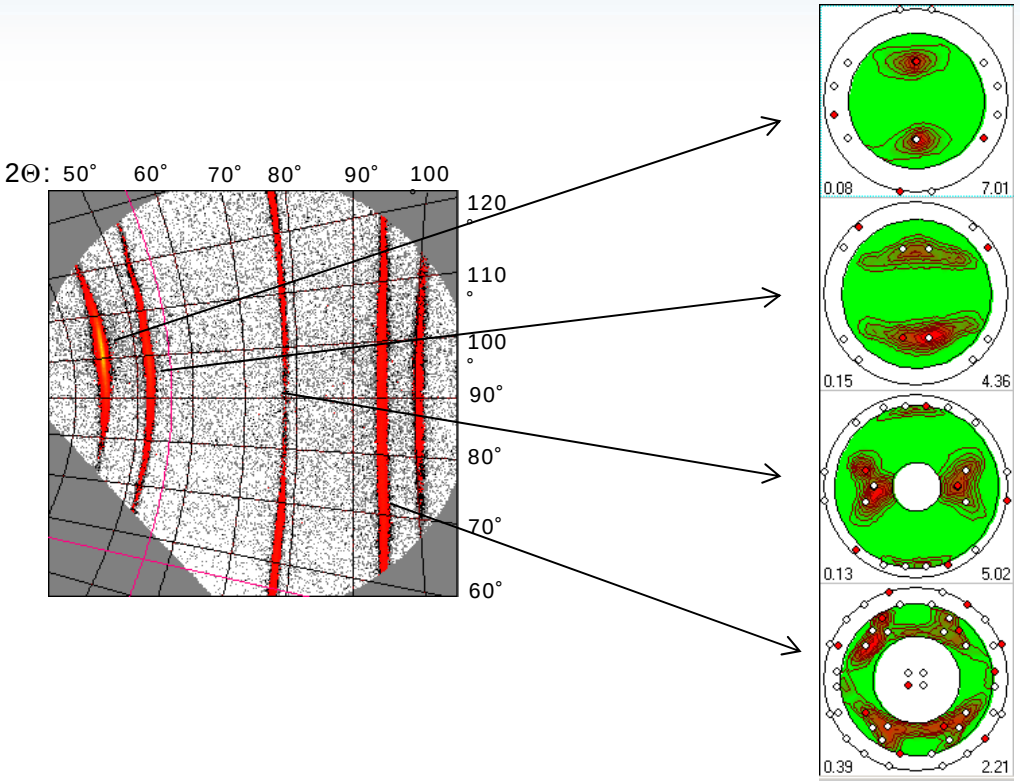
- Steel can
- Intensity variation during ϕ scan



(200) Pole figure

2D detector
Geometry and data frames





2θ- and γ-chart of a cone sector.

Frame with five diffraction sectors and pole figures resulting from 1 Phi scan.

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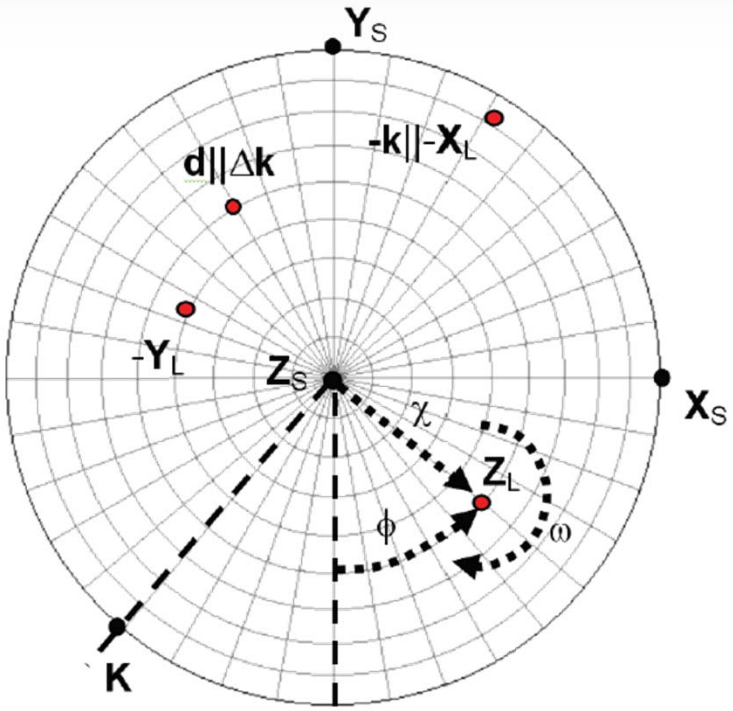
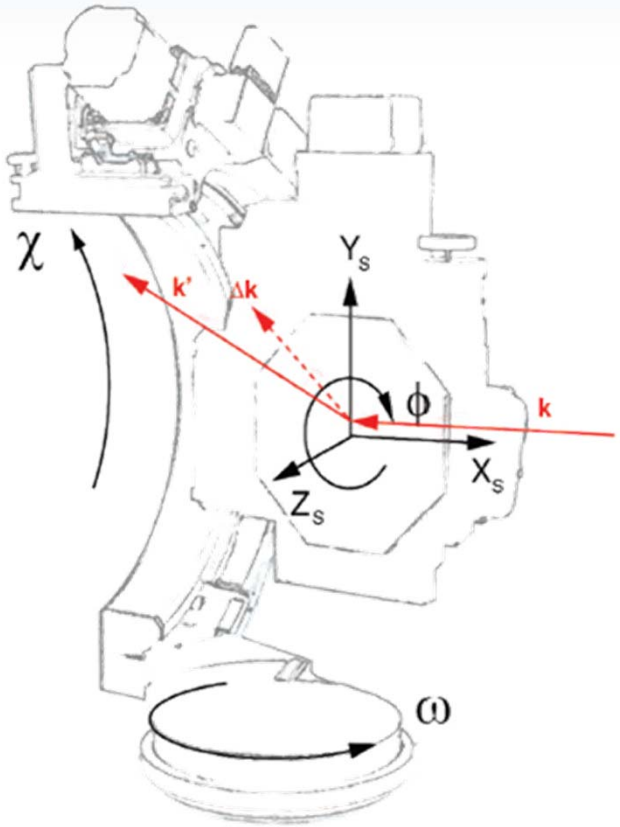
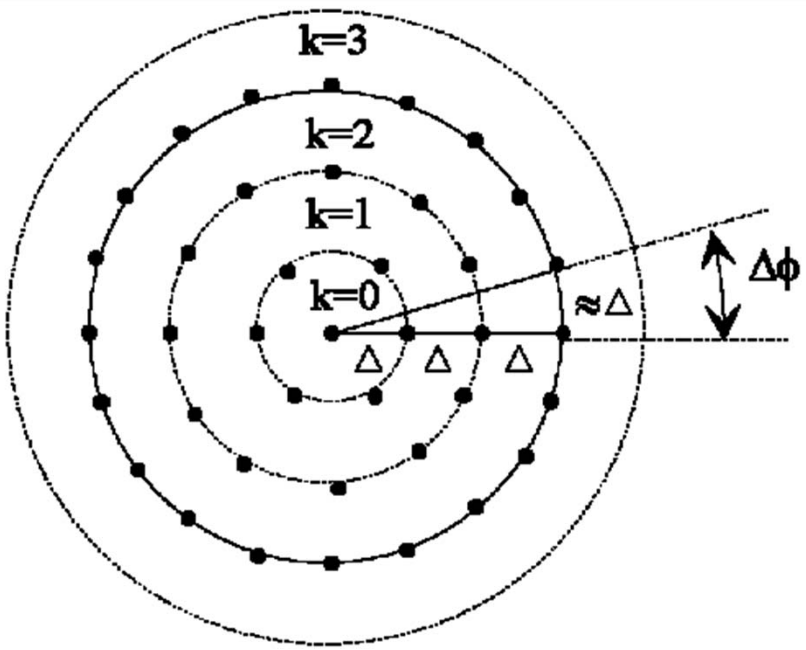
Optimization of pole figure measurements
0D and 1D





Sample rotations ω,χ,ϕ with respect to the pole figure.

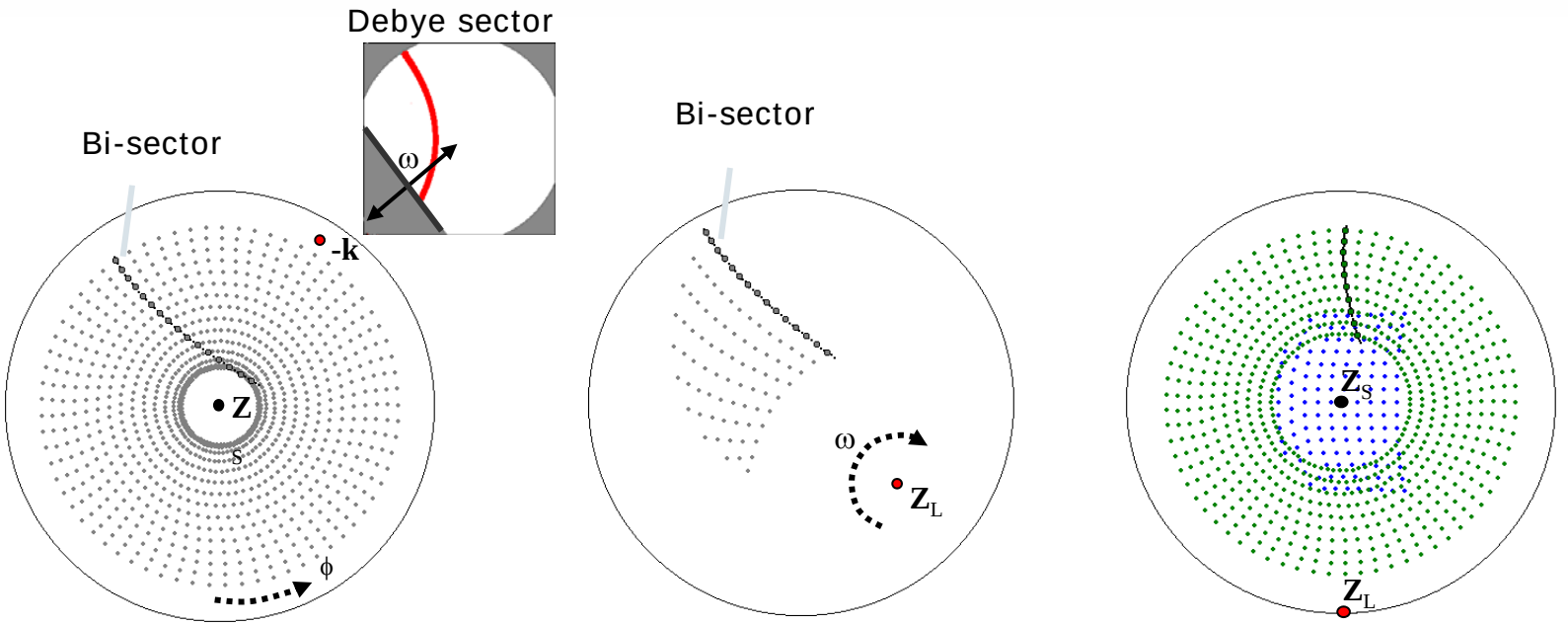
Optimization of pole figure measurements
0D and 1D



- Resolution must match the task to avoid:
  - Long measurement times
  - Resolution too large to resolve texture features
  - Artifacts from bad statistics

$$\Delta\chi = \Delta, \quad \cos\Delta\phi \approx \frac{\cos\Delta - \cos^2 k\cdot\Delta}{\sin^2 k\cdot\Delta}$$

Optimization of pole figure measurements
2D



Combination of

ω-scan and ϕ-scan.

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Texture approximation

- Wigner Functions (series expansion)

$$f(g)=\sum_{l=0}^{L}\sum_{\mu=1}^{L(G_B,l)}\sum_{\nu=0}^{L(G_A,l)}C_l^{\mu\nu}T_{\mu\nu}^{l}(g),\quad L=\frac{360^\circ}{2\Delta\omega}$$

- Texture Components

$$f(g)=F+\sum_{c}I^c f^c_{b_c,g_c}(g)$$

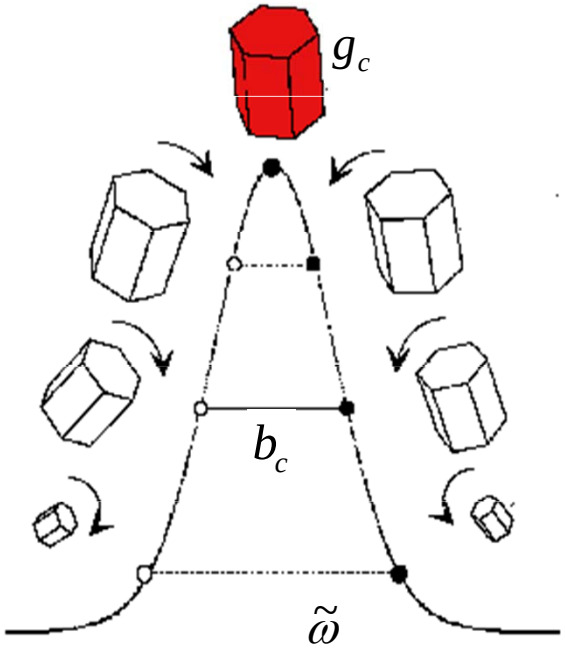
Component method vs Series expansion

- Series expansion method is automatic but is difficult to interpret due to a large number of coefficients in Eulerian space.

- Component method involves user interactive modeling with texture components and results in few, physically meaningful parameters that can be interpreted in direct space.

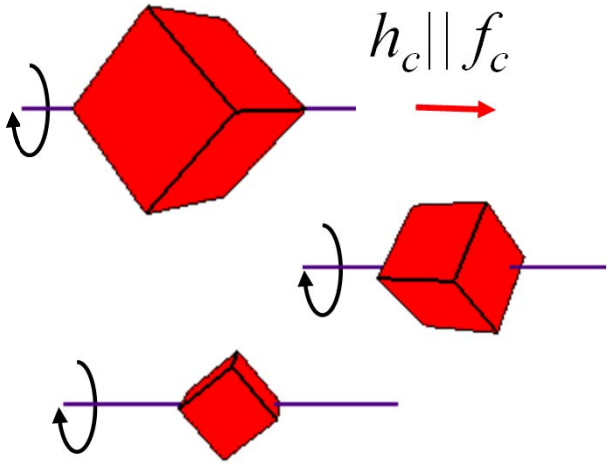
Texture Components

preferred orientation:



$$f^c(g) \propto e^{S_c(b_c)\cos(\tilde{\omega}(\tilde{g}, g_c))}$$

preferred direction:



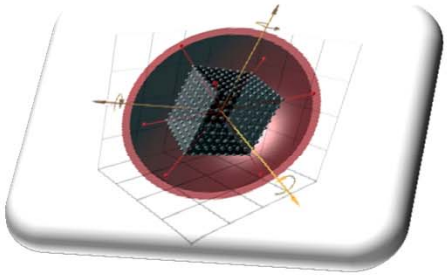
f_c given in K_A, here X
h_c given in K_B, here (111)

$$e^{S_c(b_c)\cos\angle(g \bullet h_c, f_c)}$$

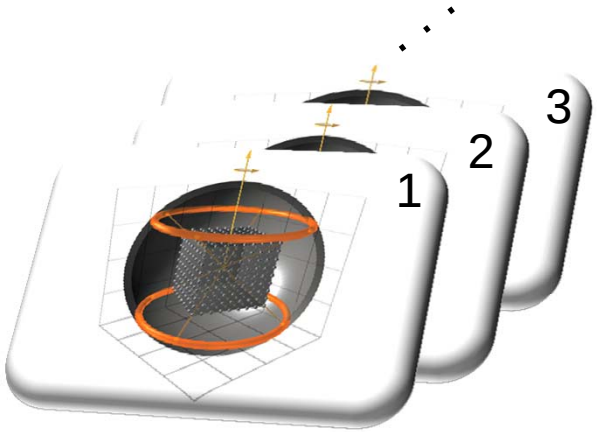
Component Method

=

Real Texture



+



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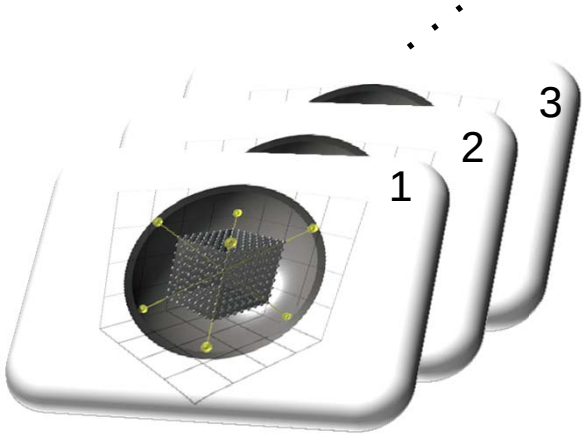


Random

Fiber components

Preferred Orientation (Spherical) components

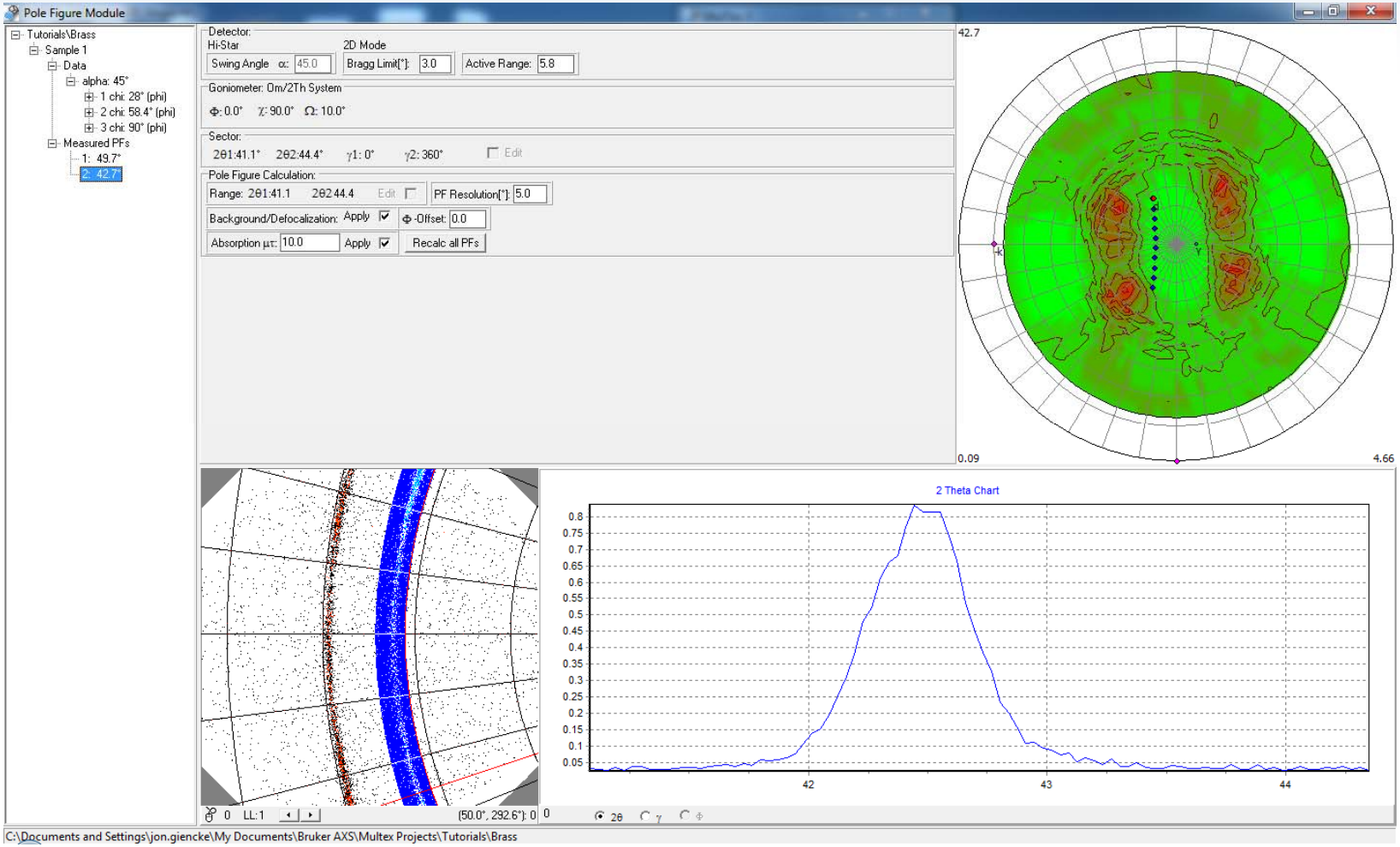
Outline

- Fundamentals of Texture Analysis
- Bragg Diffraction and Pole Figures
- Texture with 0D, 1D, and 2D detectors
- Strategies for Pole Figure measurements
- Texture approximation methods
- DIFFRAC.MULTEX
- Application Examples

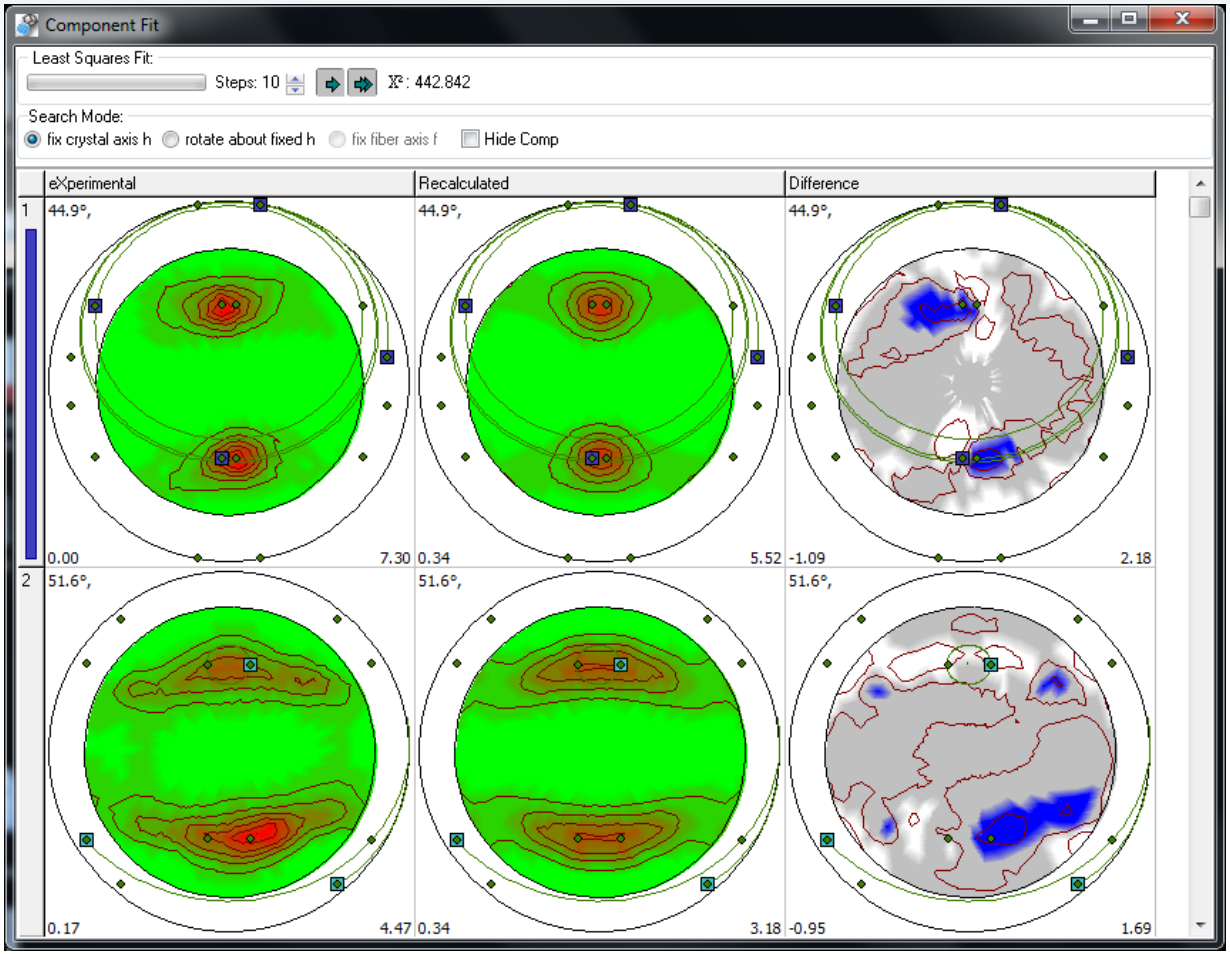
DIFFRAC.MULTEX

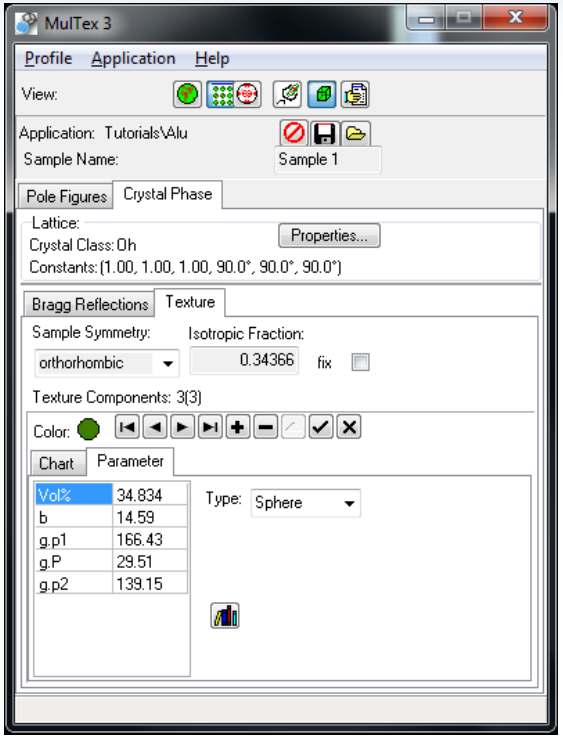
- Planning measurement with 0D/1D/2D detector
- Extended background and absorption handling
- Component Method Approach for texture analysis
- Pole Figure, Inverse Pole Figure, and ODF calculation

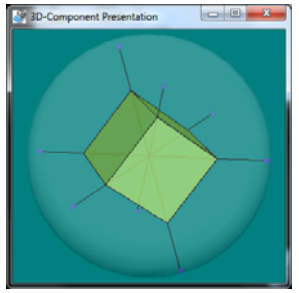
DIFFRAC.MULTEX
Pole Figure creation



DIFFRAC.MULTEX
Component creation







Outline

- Fundamentals of Texture Analysis
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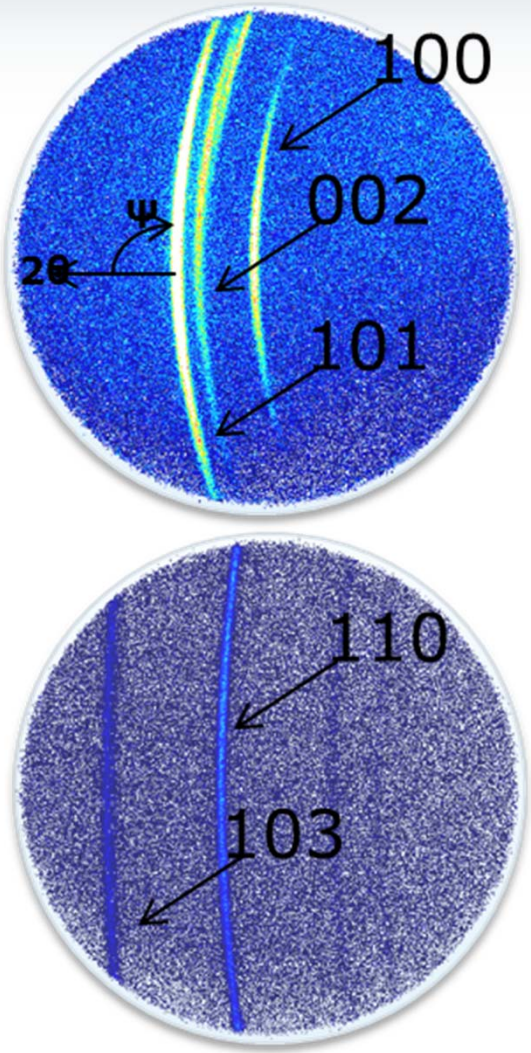
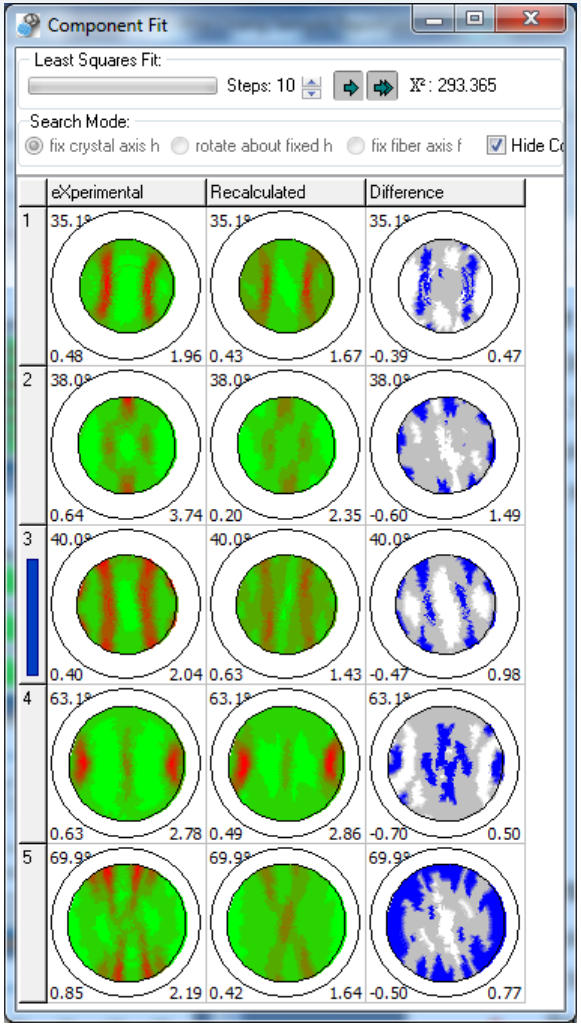
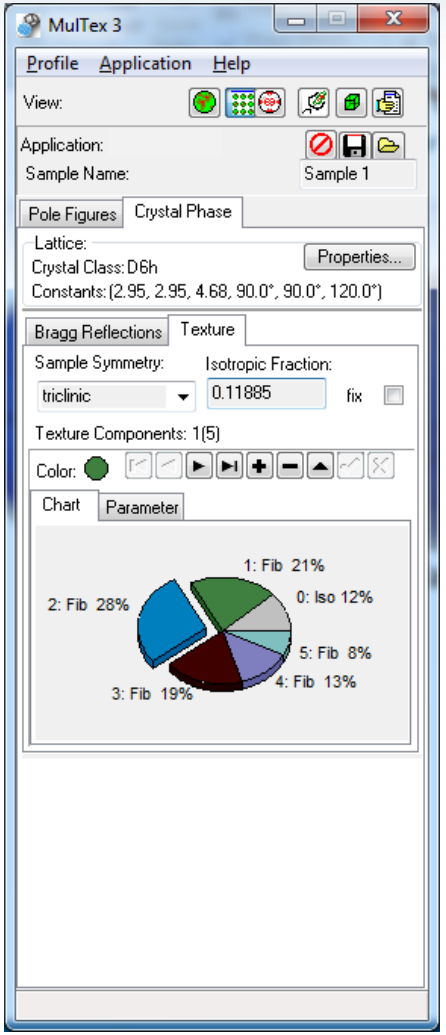
- DIFFRAC.MULTEX
- Application Examples

Application Example 1
Texture of rolled Ti alloy

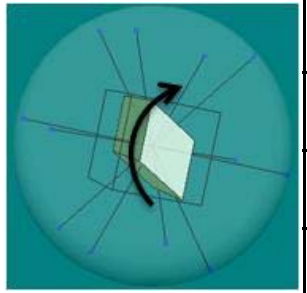






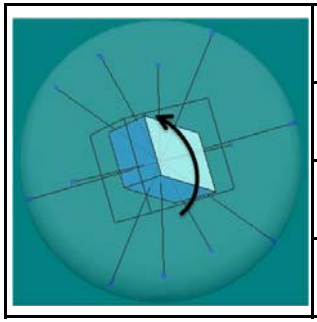
Application Example 1
Texture of Ti alloy

Component 1



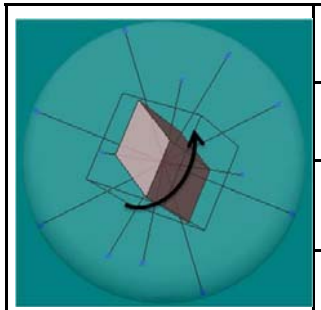
Vol%: 20.67
b=15.6°
h=(71.0, 89.9)
f=(90.3, 168.4)

Component 2



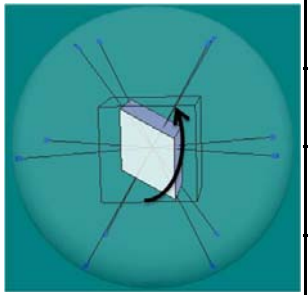
Vol%: 28.09
b=21.4°
h=(64.0, 80.5)
f=(90.4, 204.6)

Component 3



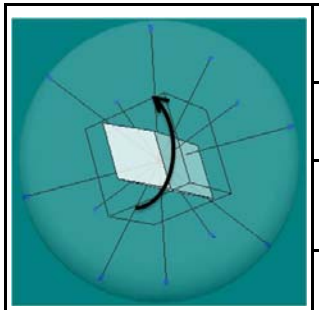
Vol%: 19.14
b=25.8°
h=(121.4, 284.6)
f=(91.0, 145.2)

Component 4



Vol%: 12.55
b=10.6°
h=(95.2, 270.0)
f=(90.6, 181.5)

Component 5



Vol%: 7.67
b=11.8°
h=(118.8, 112.8)
f=(90.0, 175.1)

b = Broadening

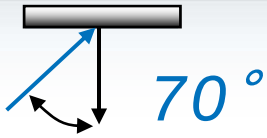
h=Crystal Axis

f = Fiber Axis

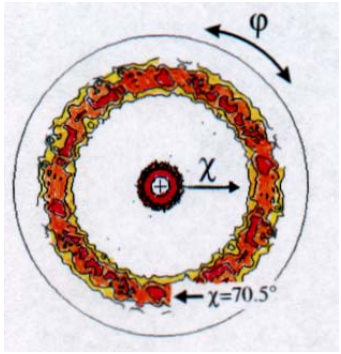
Application Example 2
Ion Beam Assisted PVD

Ion current density: J_I

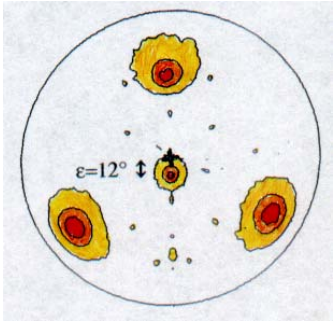
Ion beam



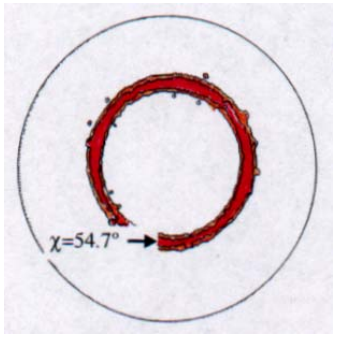
$J_I = 10 \mu A/cm^2$



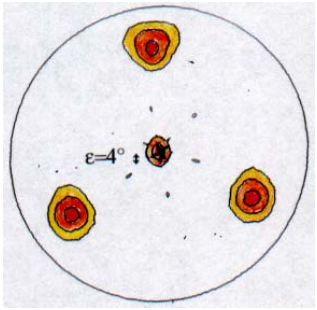
$J_I = 12 \mu A/cm^2$



$J_I = 150 \mu A/cm^2$



$J_I = 70 \mu A/cm^2$



Q & A

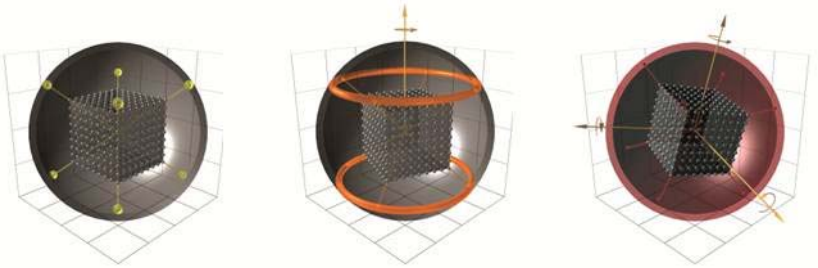
Any questions?

Please type any questions you may have for our speakers in the Q&A panel and click Send.

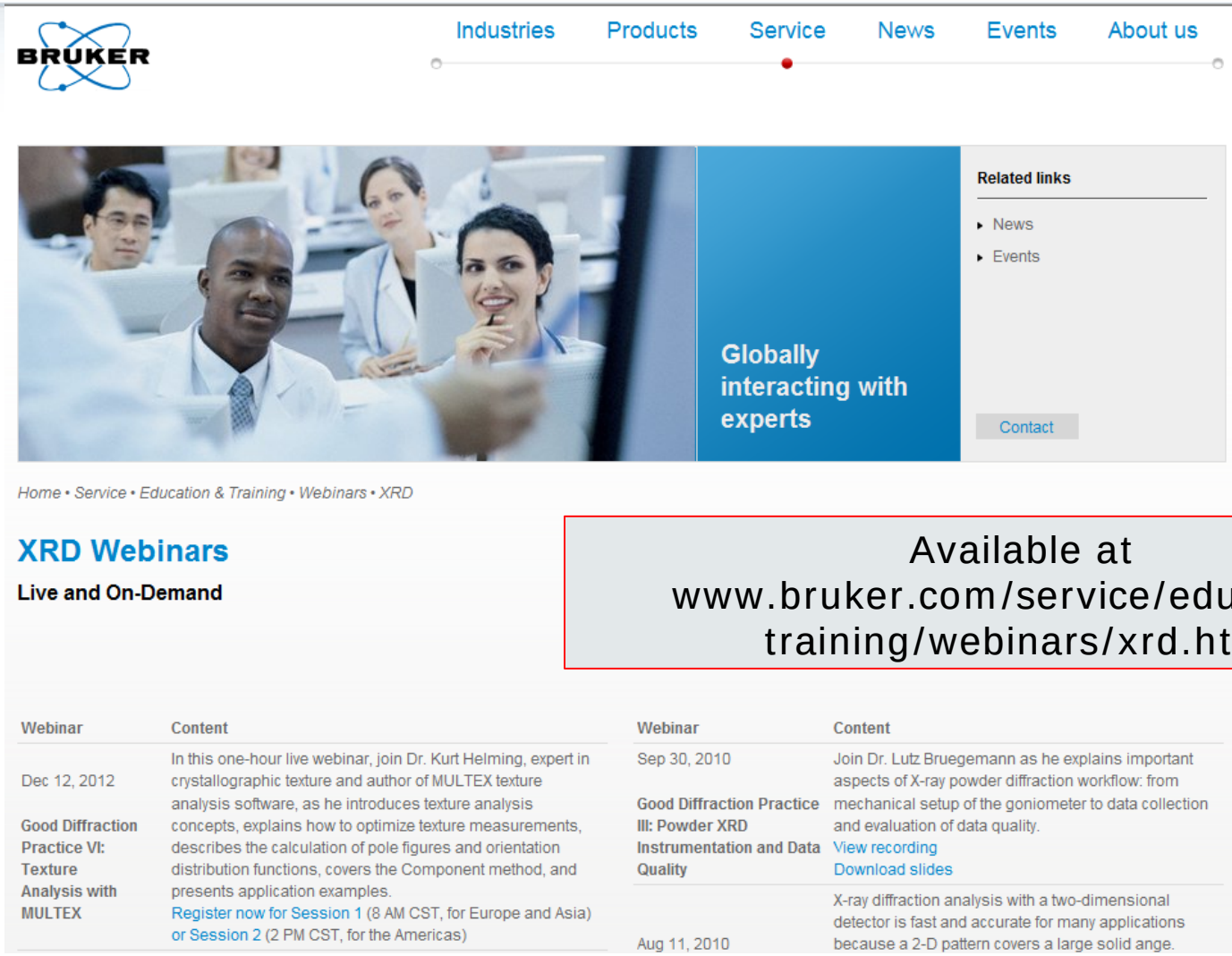
How did we do?

When you exit the webinar, please fill out our evaluation survey to let us know. We appreciate your feedback.

Thank you!



Past and Future XRD Webinars

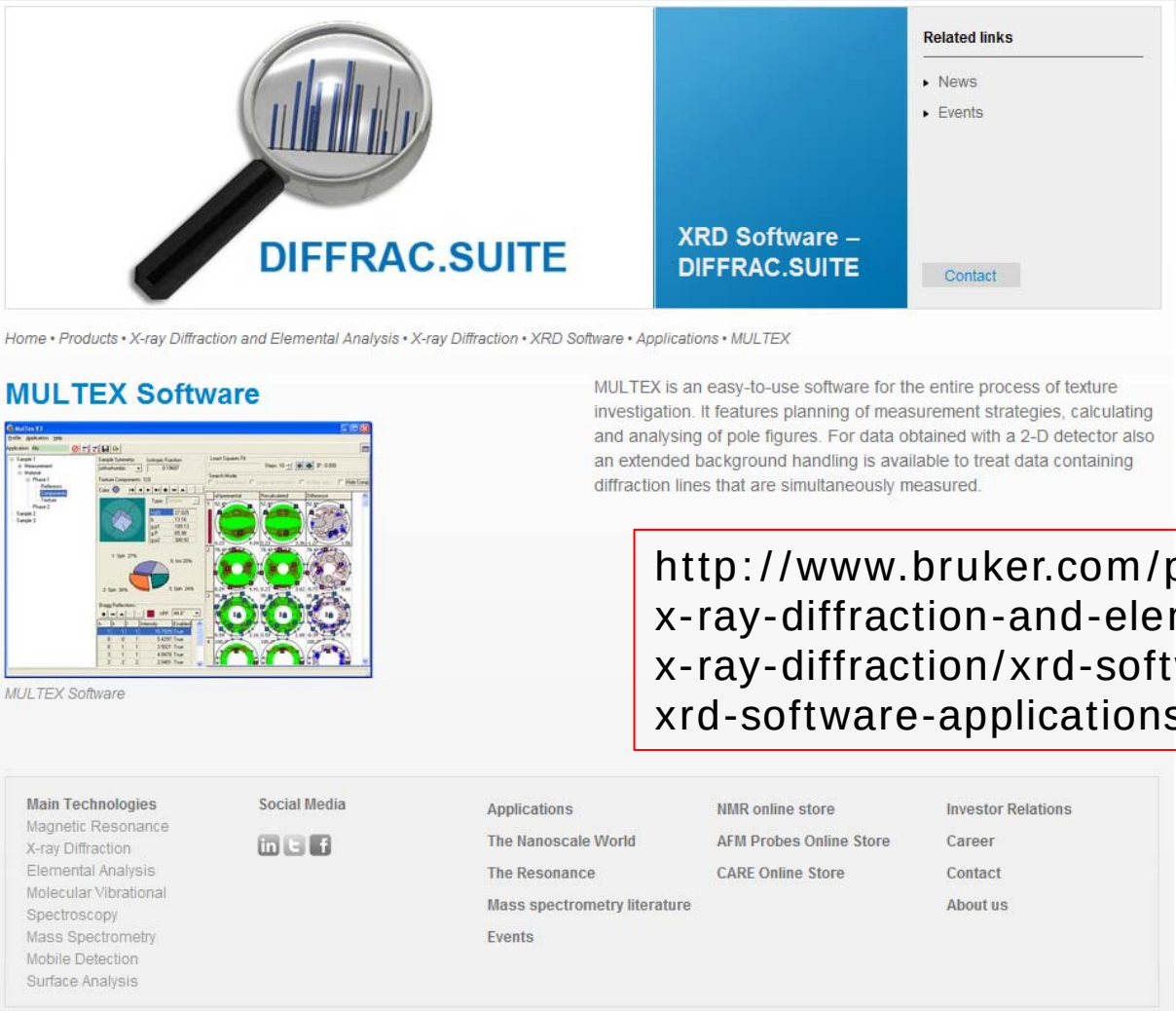


Available at www.bruker.com/service/education-training/webinars/xrd.html

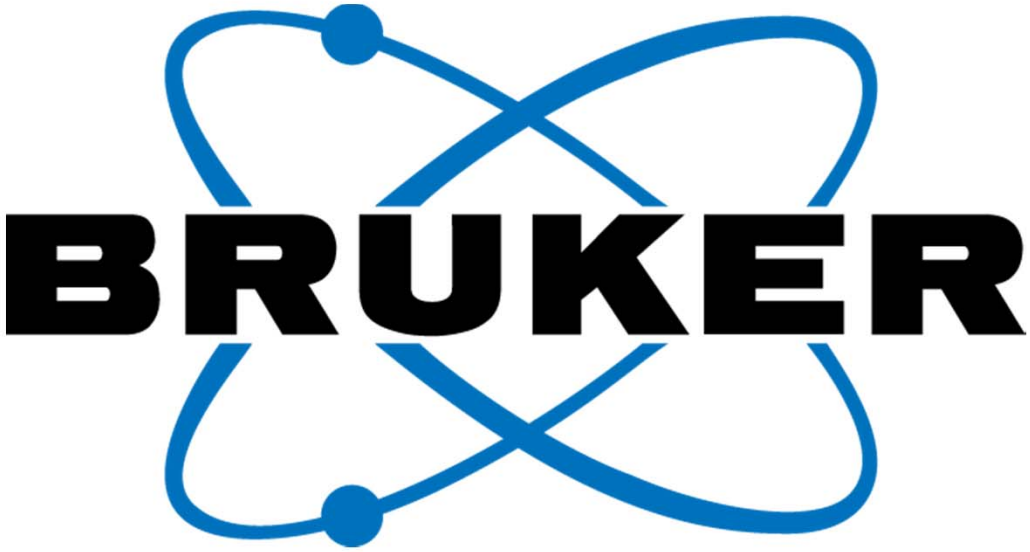
Webinar	Content
Dec 12, 2012 **Good Diffraction Practice VI: Texture Analysis with MULTEX**	In this one-hour live webinar, join Dr. Kurt Helming, expert in crystallographic texture and author of MULTEX texture analysis software, as he introduces texture analysis concepts, explains how to optimize texture measurements, describes the calculation of pole figures and orientation distribution functions, covers the Component method, and presents application examples. Register now for Session 1 (8 AM CST, for Europe and Asia) or Session 2 (2 PM CST, for the Americas)

Webinar	Content
Sep 30, 2010 **Good Diffraction Practice III: Powder XRD Instrumentation and Data Quality**	Join Dr. Lutz Bruegemann as he explains important aspects of X-ray powder diffraction workflow: from mechanical setup of the goniometer to data collection and evaluation of data quality. View recording Download slides
Aug 11, 2010	X-ray diffraction analysis with a two-dimensional detector is fast and accurate for many applications because a 2-D pattern covers a large solid ange.

MULTEX Software – More Information



http://www.bruker.com/products/x-ray-diffraction-and-elemental-analysis/x-ray-diffraction/xrd-software/applications/xrd-software-applications/multex.html



Innovation with Integrity

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