Determination of Crystallite Orientation Distribution Function (ODF) From Neutron Diffraction Data

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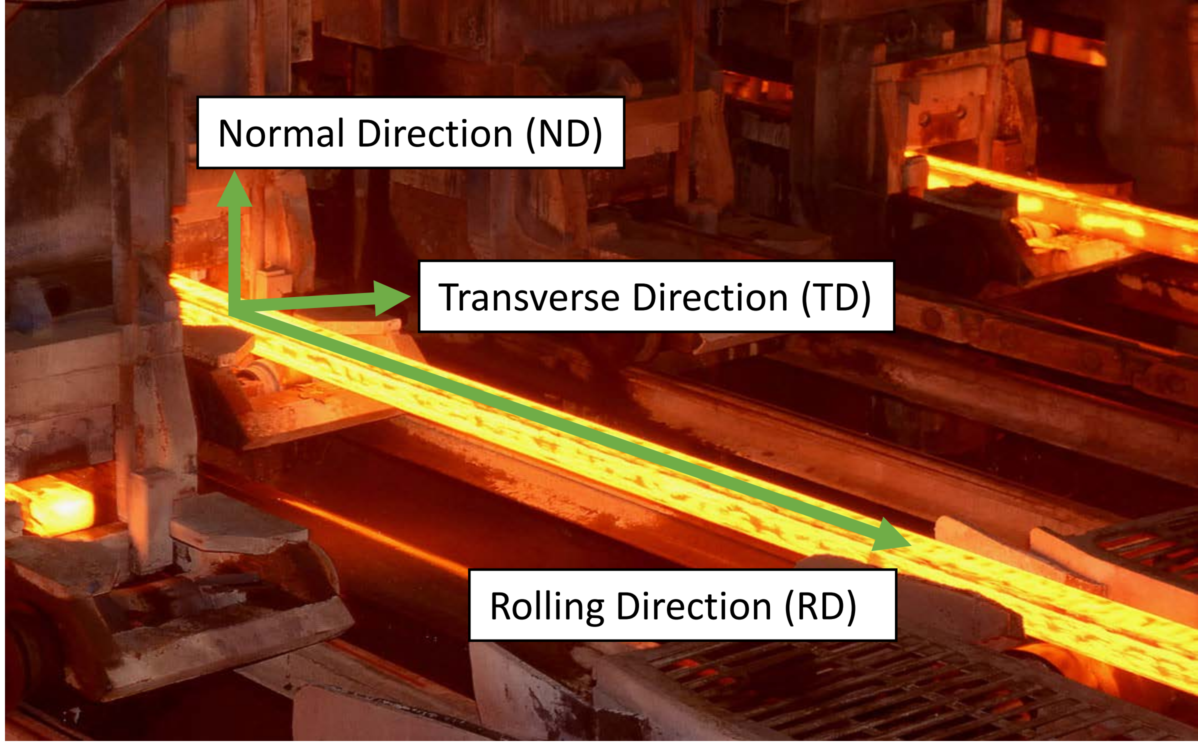
Motivation

- NIST Center for Neutron Research's (NCNR) BT8 Stress and Texture Diffractometer Upgrade
  - x30 increase in performance and data production
  - Requires increased processing capability and quasi-real-time processing of experimental data
- Texture Analysis
  - Prerequisite for optimal stress measurement strategy
  - Allows for prediction of elastic and plastic properties of materials
  - Important to material manufacturing

What is Texture?

- Crystallographic texture is the preferred orientation of grains or crystallites in polycrystalline materials
- Result of thermo-mechanical processing and its interaction with the crystal structure of the constituent grains
- Allows for the identification of the material's anisotropic properties
- Represented qualitatively by pole figures



www.mirion.com

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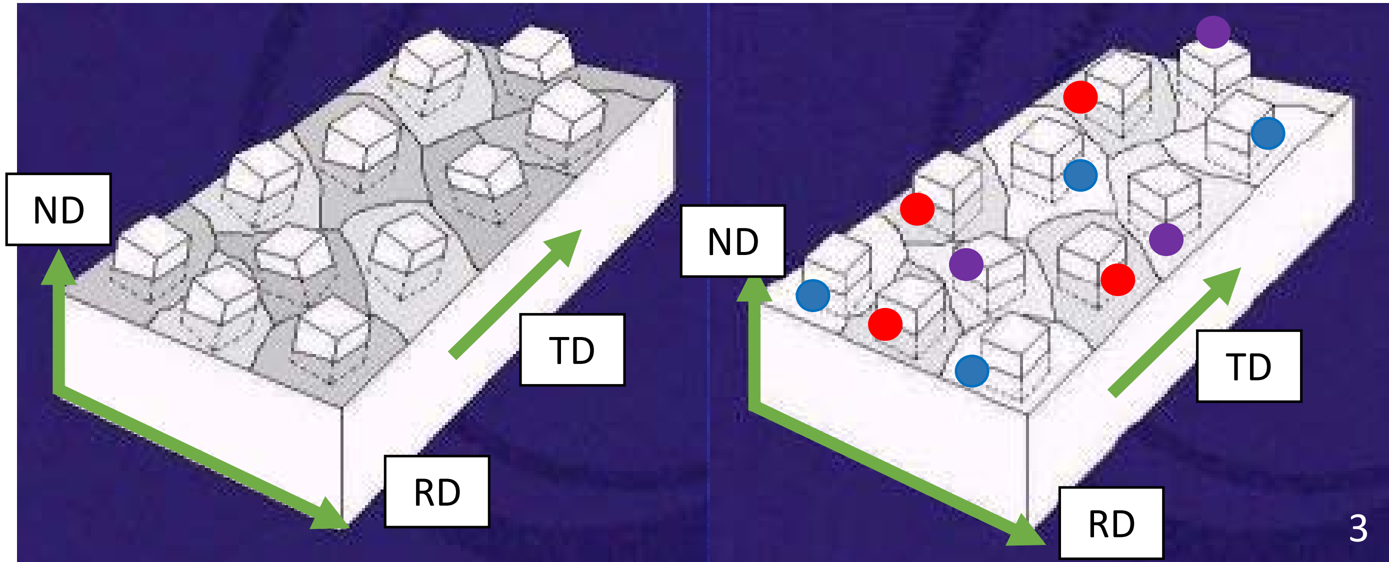
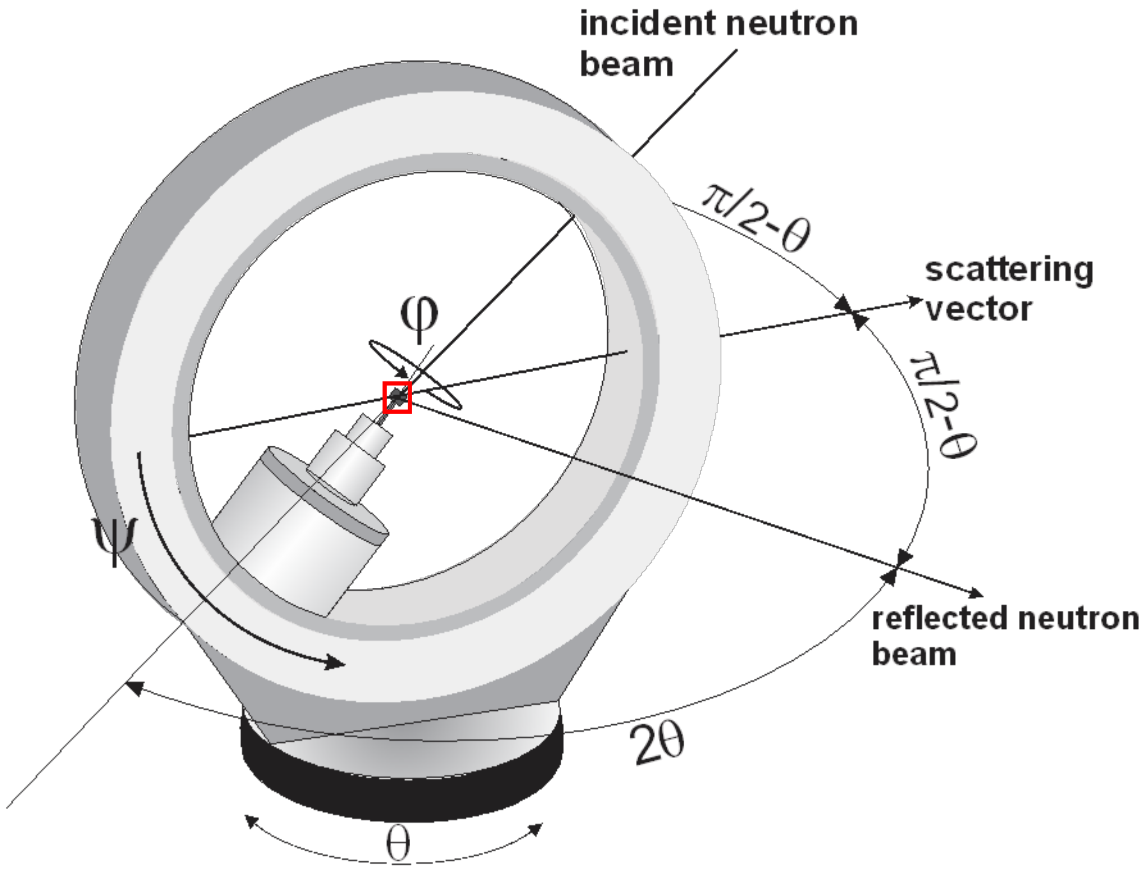


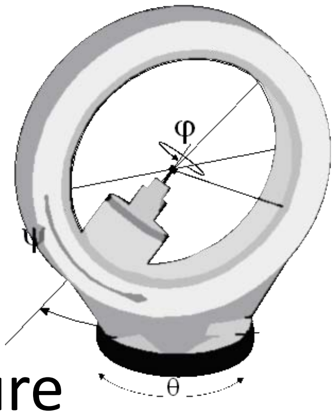
Pole Figure Measurement with Neutrons



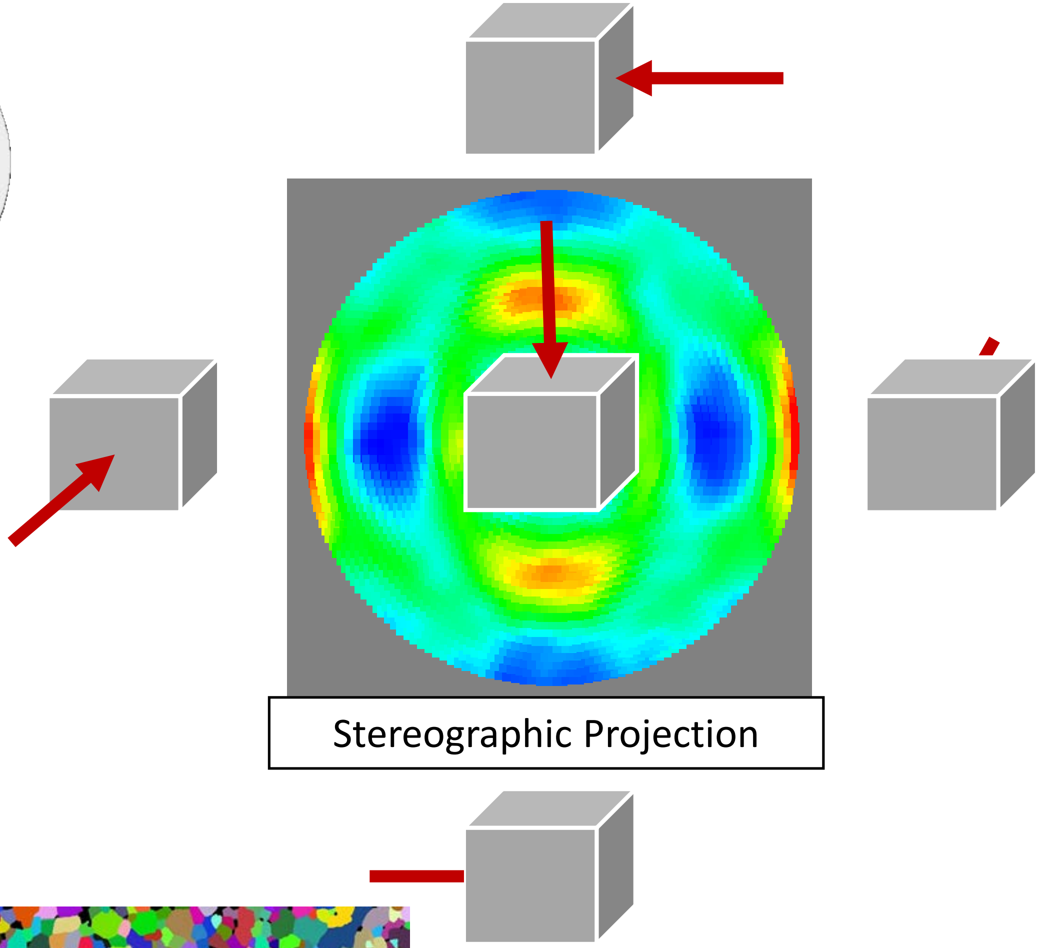
Eulerian Cradle

T. Gnäupel-Herold, et. al., *Neutron Measurements of Stresses in a Test Artifact Produced by Laser-Based Additive Manufacturing*

Pole Figures



- Graphical representation of texture with respect to a sample frame of reference
- Data collection methods
  - X-ray diffraction
  - Electron Backscatter Diffraction
  - Neutron Diffraction
    - Of all measurements methods, neutron diffraction samples the largest number of grains (10^6-10^8 grains)



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Orientation Distribution

- Density of grains in particular orientation
- Three-dimensional statistical description of the texture, f(g)
  - $g=\{\phi_1,\Phi, \phi_2\}$
- Requires two or more pole figures
  - Generalized spherical harmonics

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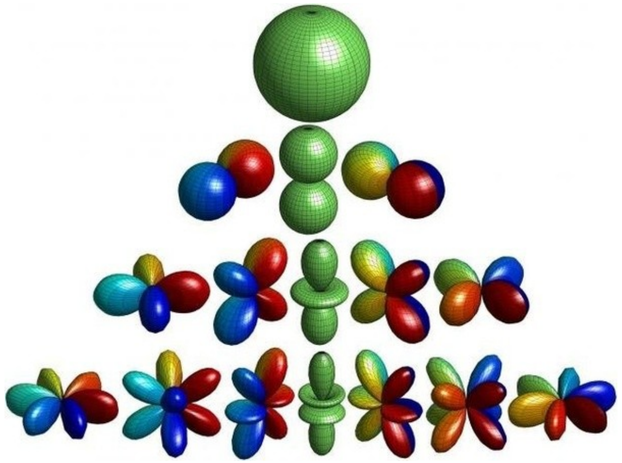
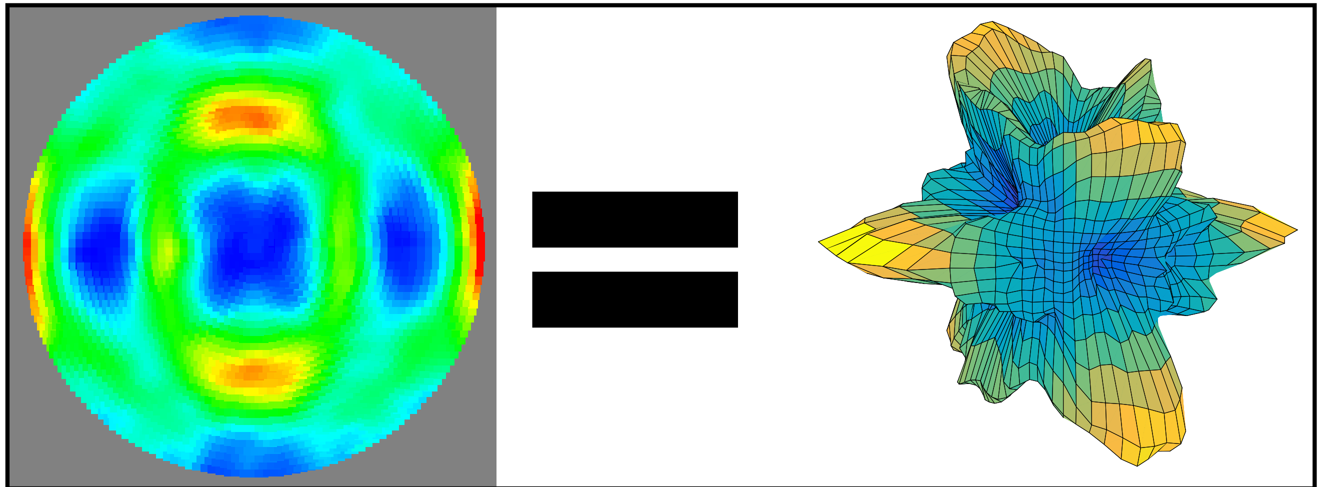
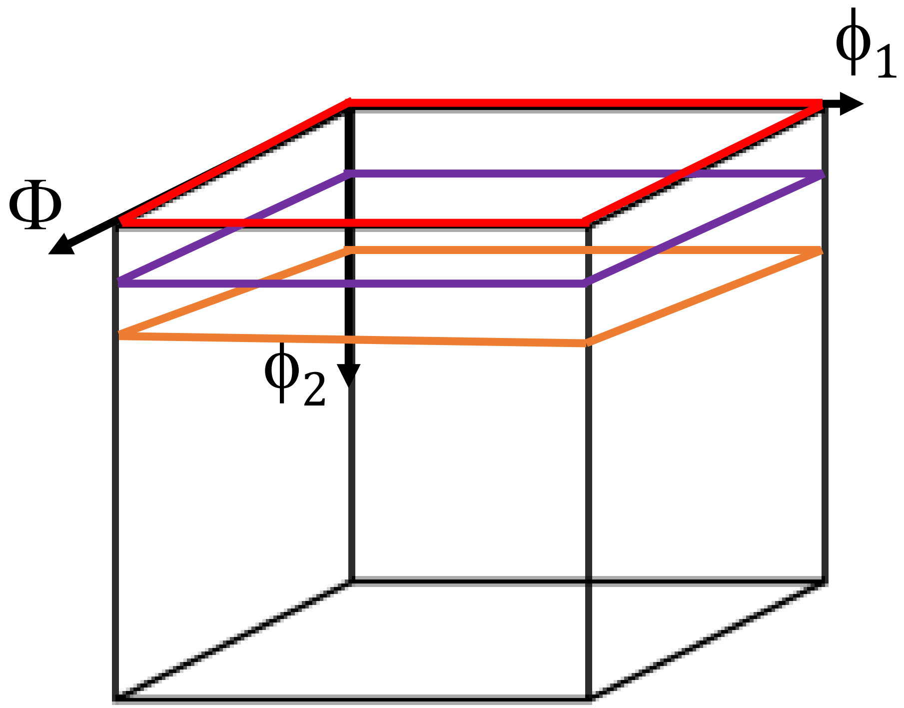
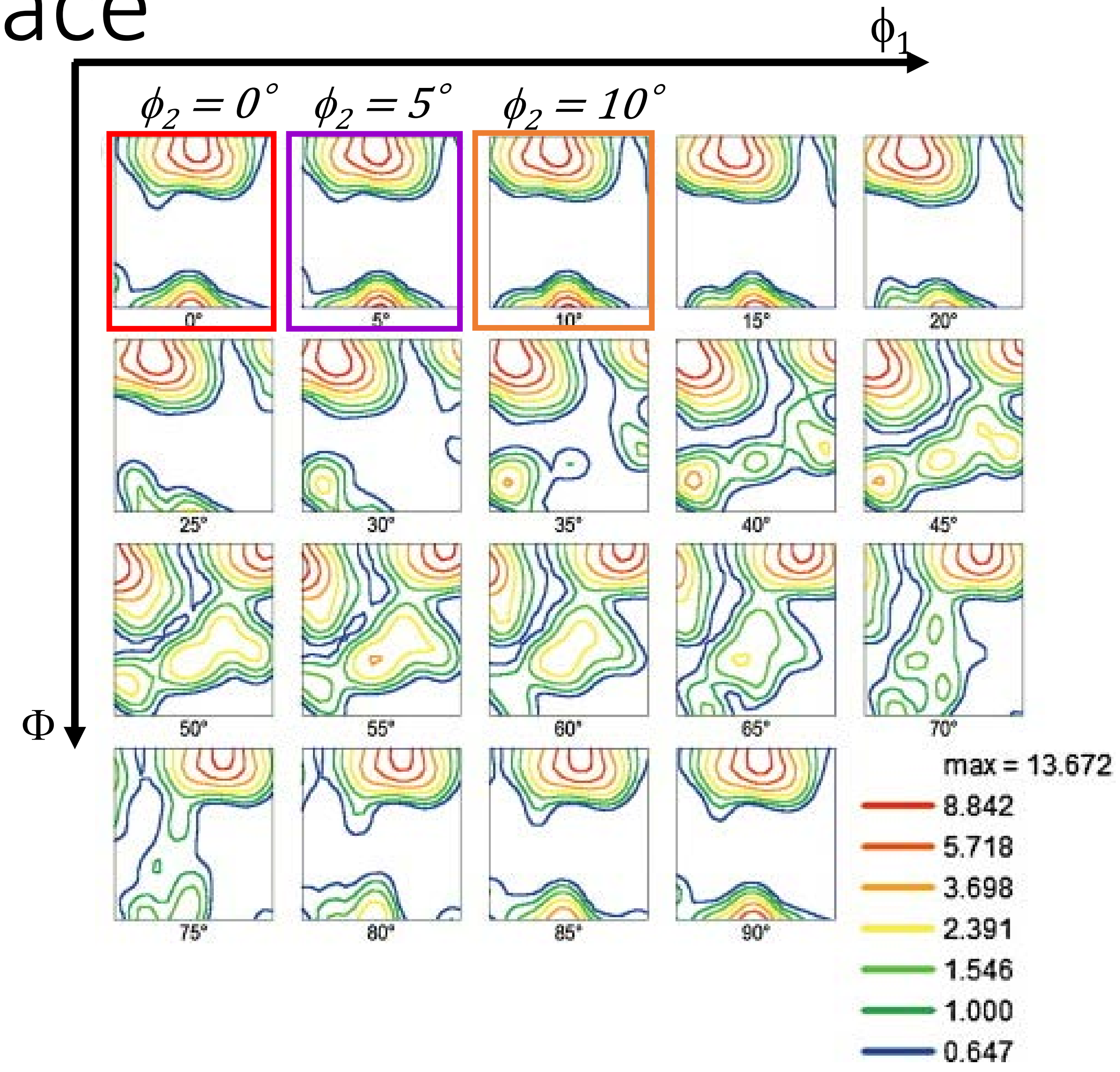


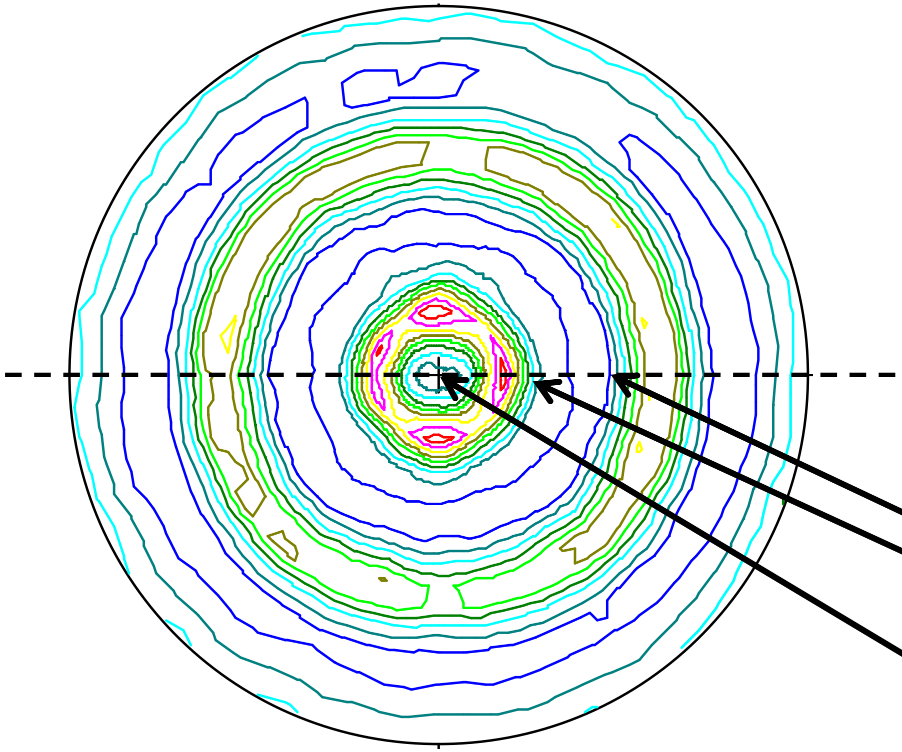


Sections Though OD Space

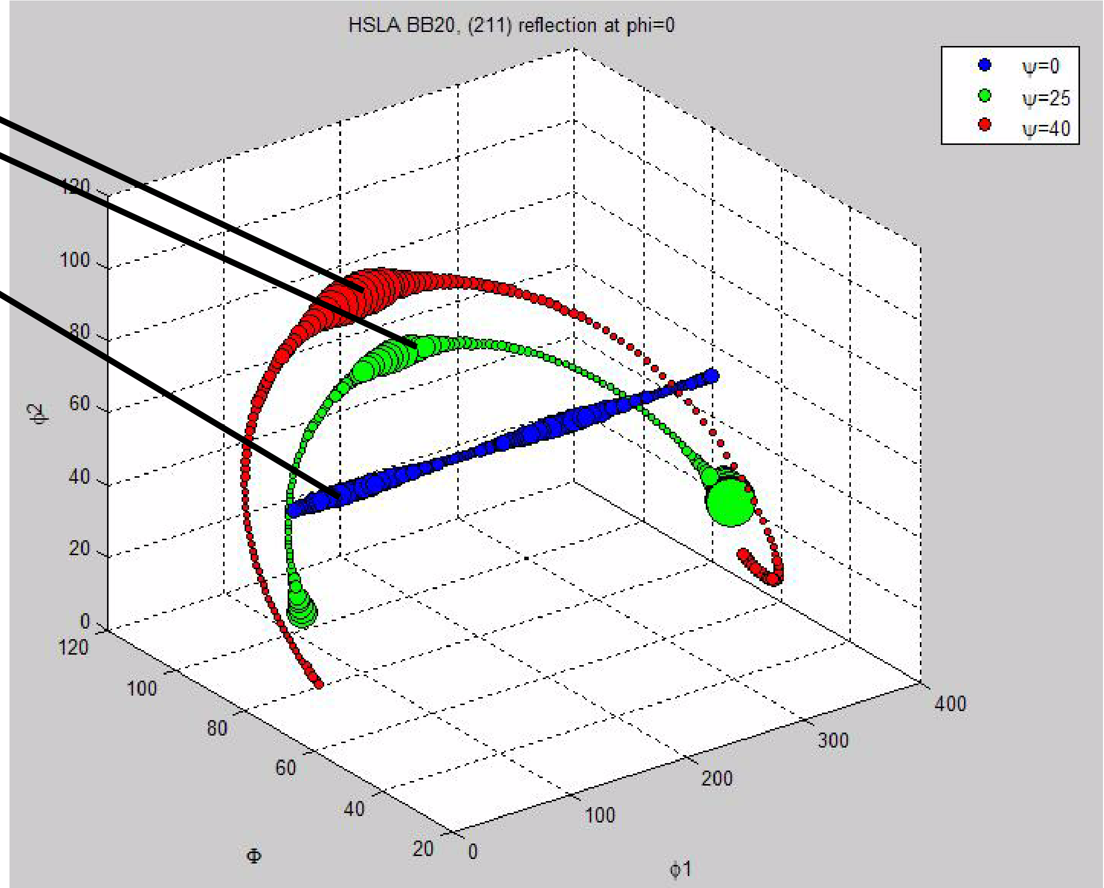




https://doi.org/10.1016/j.fusengdes.2013.04.005



$$P_{hkl}(\alpha,\beta) = \frac{1}{2\pi}\iiint f(g)\,d\phi_1 d\Phi d\phi_2$$



Iron (211) fibers in Euler space – one point in a pole figure is the integral over the ODF intensities along a fiber in Euler space, with the intensity at each coordinate (ϕ_1,Φ, ϕ_2) representing the probability (in units of random density) of a particular grain orientation

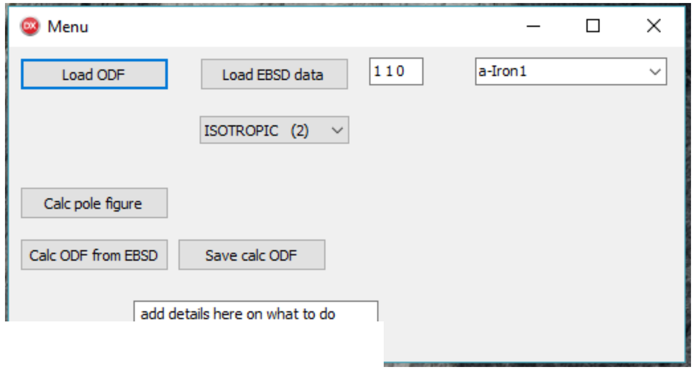
Procedure

www.cyber-tec.org

- Pre-existing code
- Library of Coefficients
- Programs & Subroutines

www.ibm.com

Fortran IV




```
SUBROUTINE COREC
DIMENSION T(19,19),TG(19),TR(19)
COMMON FEX(17,18,4),R(19,19)
COMMON/SET/IN,INP,LIB,IOUT,LTP,LMB
COMMON/DAT/HEAD(22),ACT(10)
COMMON/PAR/LMAX,LFMAX
COMMON/ORG/LIFI,LOK,J1,IB
DATA XCOR/3HCOR/
```

TWODIM

```
      SUBROUTINE TWODIM
      DIMENSION DESCRI(19)
      DIMENSION NOR(18)
      DIMENSION D(18,20),P(20),A(40)
      COMMON FEX(17,18,4),R(19,19)
      COMMON/SET/IN,INP,LIB,IOUT,LTP,LMB
      COMMON/DAT/HEAD(22),ACT(10)
      COMMON/PAR/LMAX,LFMAX
      COMMON/ORG/LIFI,LOK,J,I
      EQUIVALENCE (IOUT,LUO)
      EQUIVALENCE (LMAX,L)
      DATA NOR/1,2,3,4,5,6,7,8,9,10,11,12,13,14
      XB=.017453293
      DF=HEAD(LOK-1)
      DFM=HEAD(LOK)
      JP1=J
      IP1=I
      DO 750 JX=1,JP1
750   DESCRI(JX)=DFM*FLOAT(JX-1)
      DO 8 IM=1,IP1
      Y=SIN(FLOAT(IM-1)*DF*XB)
      DO 9 JM=1,JP1
9     P(JM)=R(JM,IM)*Y
      P(JP1)=.5*P(JP1)
      LP1=L+1
      DO 10 N=1,LP1
      X=.5*P(1)
      XNN=FLOAT(N-1)*DFM*XB*2.
      DO 11 JM=2,JP1
11    X=X+COS(FLOAT(JM-1)*XNN)*P(JM)
      D(N,IM)=X
10    CONTINUE
8     CONTINUE
      DO 12 N=1,LP1
12    D(N,IP1)=.5*D(N,IP1)
      X=D(1,1)
      DO 13 IM=2,IP1
13    X=X+D(1,IM)
      Y=12.5663706/(8.*X*DF*DFM*XB*XB)
      DO 201 L20=1,I
      DO 201 L22=1,J
201   R(L22,L20)=R(L22,L20)*Y
      XX=X
      WRITE(LUO,1004) Y
      WRITE(LUO,2201) HEAD(LOK-2)
      WRITE(LUO,3030) (DESCRI(JX),JX=1,JP1)
      DO 20 L20=1,I
      XYZ=DF*FLOAT(L20-1)
20    WRITE(LUO,2020) XYZ,(R(L22,L20),L22=1,J)
      LN1=L+1
      WRITE(LUO,1005) (NOR(K),K=1,LN1)
      ISRD=2
      IF(DF.EQ.5.) ISRD=1
      IF(ISRD.EQ.1) GO TO 710
      DO 711 I=1,188
711   READ(LIB)
710   CONTINUE
```


```
      DO 10 N=1,LP1
      X=.5*P(1)
      XNN=FLOAT(N-1)*DFM*XB*2.
      DO 11 JM=2,JP1
11    X=X+COS(FLOAT(JM-1)*XNN)*P(JM)
      D(N,IM)=X
10    CONTINUE
8     CONTINUE
      DO 12 N=1,LP1
12    D(N,IP1)=.5*D(N,IP1)
      X=D(1,1)
      DO 13 IM=2,IP1
13    X=X+D(1,IM)
      Y=12.5663706/(8.*X*DF*DFM*XB*XB)
      DO 201 L20=1,I
      DO 201 L22=1,J
201   R(L22,L20)=R(L22,L20)*Y
```


www.cyber-tec.org

H. J. Bunge, *Texture Analysis in Material Science: Mathematical Methods*

Coefficient Equations

$$\mathrm{Q}_\ell^{mn} = i^{m+n}\mathrm{P}_\ell^{mn}(\pi/2)$$

$$\overline{\mathrm{P}_\ell^m}(\phi) = i^{-m}(2\ell+1)^{1/2}P_\ell^{mo}(\phi)$$

$$\dot{\dot{k}}_\ell^\mu(h_i) = \sum_{m=0}^{\ell} \dot{\dot{\mathrm{B}}}_\ell^{m\mu}\,\overline{\mathrm{P}_\ell^m}(\phi_i)\cos(m\beta_i)$$

$$\dot{\dot{\mathrm{B}}}_\ell^{m\mu} = (2\pi)^{-1/2}\dot{\dot{\mathrm{A}}}_\ell^{\prime m\mu}$$

$$\mathrm{a}_\ell^{\prime ms} = \varepsilon(4\ell+2)^{1/2}\mathrm{Q}_\ell^{ms}\mathrm{Q}_\ell^{so}$$

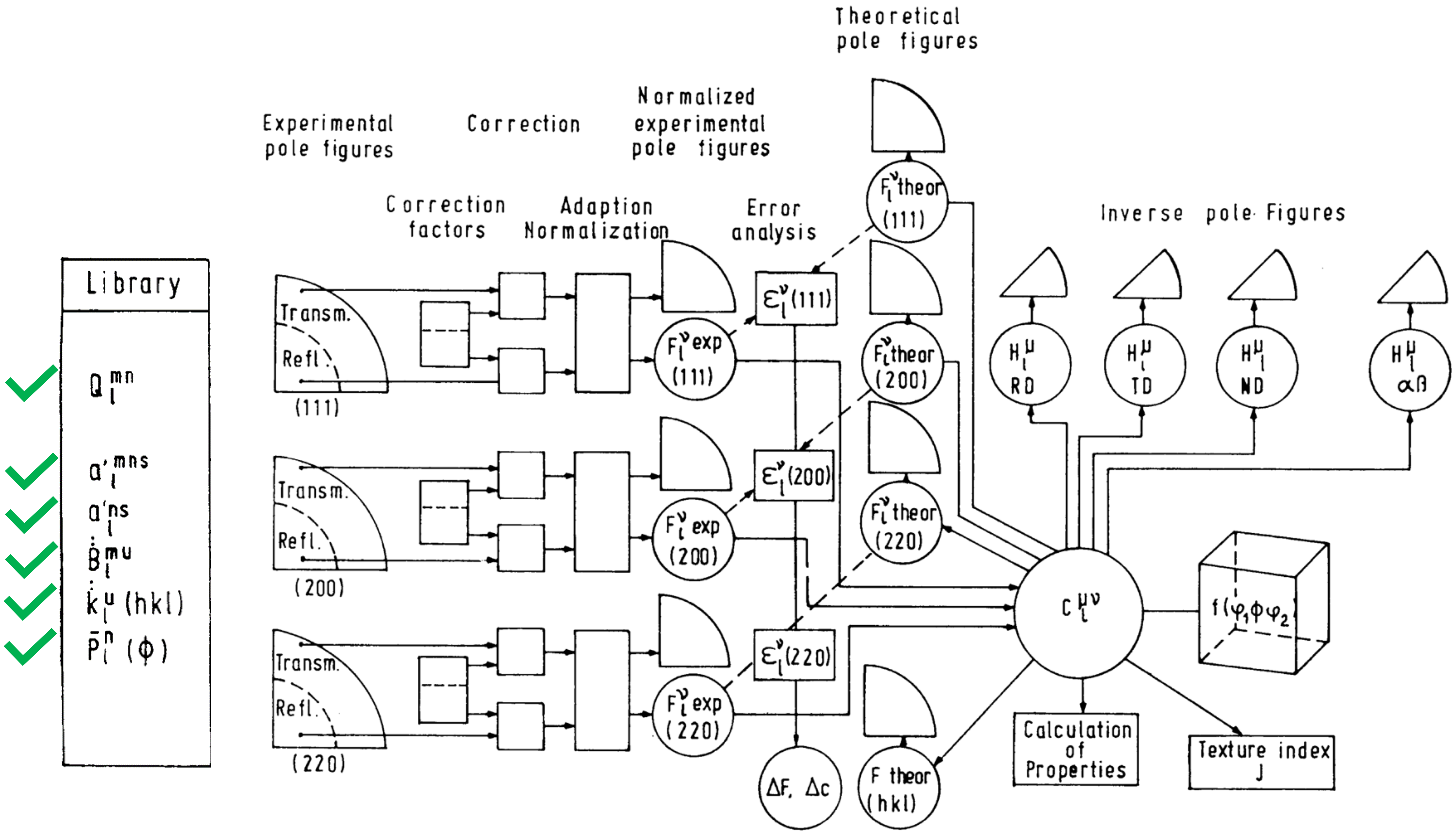
$$\mathrm{a}_\ell^{\prime mns} = \varepsilon\mathrm{Q}_\ell^{ms}\mathrm{Q}_\ell^{sn}$$

Where...

$\ell = 2, LMAX, 2$
$m = 0, \ell, IDN$
$n = 0, m, IDN$
$\phi = 0, 90^\circ, \Delta\phi$
$\mu = 1, M(\ell), 1$
$h_i = (\phi_i, \beta_i)$
$s = 0, \ell, 2$

$\varepsilon = (-1/2)^{m/2}$ if $s = 0$
$\varepsilon = (-1)^{m/2}$ if m is even
$\varepsilon = (-1)^{(m-1)/2}$ if m is odd

$\varepsilon = 1$ if $s = 0$
$\varepsilon = 2$ if $m + n$ is even
$\varepsilon = 2i$ if $m + n$ is odd



Theoretical pole figures
Experimental pole figures
Correction
Normalized experimental pole figures
Correction factors
Adaption Normalization
Error analysis
Inverse pole Figures
Library
Transm.
Refl.
(111)
(200)
(220)
F_l^ν theor (111)
F_l^ν theor (200)
F_l^ν theor (220)
F_l^ν exp (111)
F_l^ν exp (200)
F_l^ν exp (220)
ε_l^ν(111)
ε_l^ν(200)
ε_l^ν(220)
H_l^μ RD
H_l^μ TD
H_l^μ ND
H_l^μ αβ
$C_l^{\mu\nu}$
$f(\varphi_1 \phi \varphi_2)$
ΔF, Δc
F theor (hkl)
Calculation of Properties
Texture index J

Summary

- All programs and subroutines were transcribed into text files
  - Work was started in transcribing, debugging and updating Fortran IV to Fortran 95 syntax
- The following coefficients were confirmed from the library program output transcribed in Fortran 95:
  - Symmetry Coefficients, $\dot{\dot{B}}_l^{m\mu}$ for cubic symmetry
  - Fourier Coefficients, Q_l^{ms}
  - Cubic Spherical Harmonics, $\dot{\dot{k}}_l^{m}(hkl)$
  - Fourier coefficients, $a_l'^{ms}$ of the associated Legendre function $P_l^m(\Phi)$
  - Fourier coefficients, $a_l'^{mns}$ of the associated Legendre function $P_l^m(\Phi)$

Future Work

- Continue debugging Fortran 95 programs and subroutines
  - Optimize code
  - Ensure validity of output data
- Transcribe Fortran 95 programs and subroutines into a modern language
  - Produce a user-friendly GUI
- Integrate into NCNR code data base for future neutron data analysis and simulation

Acknowledgements

- National Institute of Standards and Technology (NIST)
- NIST Center for Neutron Research (NCNR)
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