INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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WORKING PARTY ON
MODELLING THERMOMECHANICAL BEHAVIOUR OF MATERIALS
(29 May - 16 June 1989)

ADDITIONAL MATERIAL FOR LECTURES ON
"MODELLING PLASTIC BEHAVIOUR OF POLYCRYSTALLINE METALS"

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These are preliminary lecture notes, intended only for distribution to participants.

Literature concerning LApp

There is, alas, no complete or up-to-date write-up as yet. Various aspects are covered (sometimes in superseded forms) in the following.

The Relation between Polycrystal Deformation and Single Crystal Deformation

Met. Trans. 1, 1121-1143 (1970).

How Many Slip Systems, and Which?

U. F. Kocks and G. R. Canova
Deformation of Polycrystals: Mechanisms and Microstructures,
N. Hansen, A. Horsewell, T. Leffers, and H. Lilholt, eds.
(Risø National Laboratory, Roskilde, Denmark, 1981), pp. 35-44

NOTE – The assessment of tension is in error: it is an FC case.

Yield Vectors in FCC Crystals

U. F. Kocks, G. R. Canova, and J. J. Jonas
Acta. Met. 31, 1243-1252 (1983).

The Relation between Macroscopic and Microscopic Strain Hardening in FCC Polycrystals

C. Tomé, G. R. Canova, U. F. Kocks, N. Christodoulou, and J. J. Jonas
Acta. Met. 32, 1637-1653 (1984).

NOTE – The RC assessment has changed: the grain rim is now considered to be FC. Also, there are newer exper's & simul's. (see last page)

The Development of Deformation Textures and Resulting Properties of FCC Materials

G. R. Canova and U. F. Kocks
Int'l. Conf. on Textures of Materials, ed. by C. M. Brakman, P. Jongenburger, E. J. Mittemeijer (Netherlands Soc. Mater. Sci. 1984) p. 573-579.

The Yield Surface of HCP Crystals

C. Tomé and U. F. Kocks
Acta Met. 33, 603-621 (1985).

The Yield Surface of Textured Polycrystals

G. R. Canova, U. F. Kocks, C. N. Tomé and J. J. Jonas
J. Mech. Phys. Sol. 33, 371-397 (1985).

Grain Shape Effects on the Slip System Activity and on the Lattice Rotations

S. Tiem, M. Berveiller and G. R. Canova
Acta Met. 34, 2139-2149 (1986)

Constitutive Behavior Based on Crystal Plasticity

U. F. Kocks
Unified Constitutive Equations for Creep and Plasticity,
ed. by A. K. Miller (Elsevier Applied Science, 1987)
pp. 1-88.

H. R. Wenk and U. F. Kocks
Metall. Trans., <u>18A</u>, 1083-1092 (1987)

A Symmetric Set of Euler Angles and Oblique Orientation Space Sections

U. F. Kocks
Proc. <u>Eighth International Conference on Textures of Materials</u>, J. S. Kallend and G. Gottstein, eds. (The Metallurgical Society, Warrendale, PA, 1988) pp. 31-36

Computer Simulation of Pencil Glide in BCC Metals

A. D. Rollett, U. F. Kocks
Proc. <u>Eighth International Conference on Textures of Materials</u>, J. S. Kallend and G. Gottstein, eds. (The Metallurgical Society, Warrendale, PA, 1988) pp. 375-380

Material Dependence of Texture Development in Various Deformation Modes

M. G. Stout, J. S. Kallend, U. F. Kocks, M. A. Przystupa, A. D. Rollett
Proc. <u>Eighth International Conference on Textures of Materials</u>, J. S. Kallend and G. Gottstein, eds. (The Metallurgical Society, Warrendale, PA, 1988) pp. 479-484

The Path Dependence of Deformation Texture Development

T. Takeshita, U. F. Kocks, H.-R. Wenk
Proc. <u>Eighth International Conference on Textures of Materials</u>, J. S. Kallend and G. Gottstein, eds. (The Metallurgical Society, Warrendale, PA, 1988) pp. 445-448

The Sensitivity of Rolling Texture Predictions to the Assumptions Used

U. F. Kocks
Proc. <u>Eighth International Conference on Textures of Materials</u>, J. S. Kallend and G. Gottstein, eds. (The Metallurgical Society, Warrendale, PA, 1988) pp. 285-288

The Effect of the Cube Texture Component on the Earing Behavior of Rolled FCC Metals

A. D. Rollett, G. R. Canova, U. F. Kocks
Symp. on <u>Formability and Metallurgical Structure</u>, A. K. Sachdev and J. D. Embury, eds.
(The Metallurgical Society, Warrendale, PA, 1987) pp. 147-157

The Effects of Rate Sensitivity on Slip System Activity and Lattice Rotation

G. R. Canova, A. Molinari, C. Fressengeas, U. F. Kocks
Acta Met. <u>36</u>, 1961-1970 (1988)

The Influence of Texture on Strain Hardening

U. F. Kocks, M. G. Stout, A. D. Rollett
Strength of Metals and Alloys (ICSMA 8), P.O. Kettunen, T. K. Lepistö, M. E. Lehtonen, eds. (Pergamon, 1988) pp. 25-34

LAtex: Los Alamos **texture analysis** package (Page 1)

J.S. Kallend, U.F. Kocks, A.D. Rollett, and H.R. Wenk (May 1989)

0. QUIT

1. Get specimen DIRECTORY and VIEW a file

2. **MASSAGE data files:** correct,rotate,symmetrize,smooth,complete,compare

3. WIMV: make spec.SOD; transform to .COD,.SNU,.CNU; pare; recalc.PFs

4. **HARMONIC** analysis

5. **PERMUTATIONS, TRANSFORMATIONS**, other utilities

6. DISPLAYS and plots

7. Derive **PROPERTIES** from .SOD or .WCF files or by SIMULATION

Please enter a number from 0 to 7 -->

MASSAGE DATA FILES (mostly PFs) (LAtex page 2)

0. Quit
1. Return to Page 1

2. **DIGEST Raw Data** (.RAW), with defoc.&bkg (.DFB): make .EPF

3. ROTATE: make .RPF

4. **SYMMETRIZE: make** .QPF or .SPF or .FPF

5. **EXPAND back to full circle** .FPF (needed for **WIMV**)

6. **SMOOTH with Gaussian Filter** (quad, **semi**, or full): make .MPF

7. **COMPLETE rim of pole figure** by **harmonic** method: make .FUL

8. **Take DIFFERENCE between** 2 files (PFs or ODs)

Please enter a number from 0 to 8 ==>

```
 0. Quit
 1. Return to Page 1

 2. Make matrix .WIM for new crystal structure and set of PFs

 WIMV: make .SOD amd recalc. pole figures .WPF  -- for:
    3. cubic, tetra-,hexagonal crystals; sample diad;  up to 3 PFs
    4. general (requires expanded memory)

 5. Make .COD from .SOD file (or .COH from .SOH)
 6. Make OBLIQUE sections from .SOD file: .SNU,.CNU, or .SNH,.CNH from .SOH
 7. Pare to SUBSET for display: make .SOS or .COS (or .SNS,.CNS)

 8. Recalculate POLE FIGURES (even non-measured ones: e.g.to get .WCFs)
 9. Calculate INVERSE pole figures from .SOD: .IPF


 Please enter a number from 0 to 9 -->
```

HARMONIC ANALYSIS (LAtex page 4)

```
0. Quit
1. Return to Page 1

Find harmonic coefficients .WCF, completed PFs (.FUL) for:
   2. Cubic crystal system
   3. Hexagonal, tetragonal or orthorhombic crystal system

4. Compute SOD or COD from harmonic coefficients (slow!)

5. Recalculate pole figures .HPF

6. Inverse pole figures .INV

7. List harmonic coefficients to screen or printer

Please enter a number from 0 to 7 -->
```

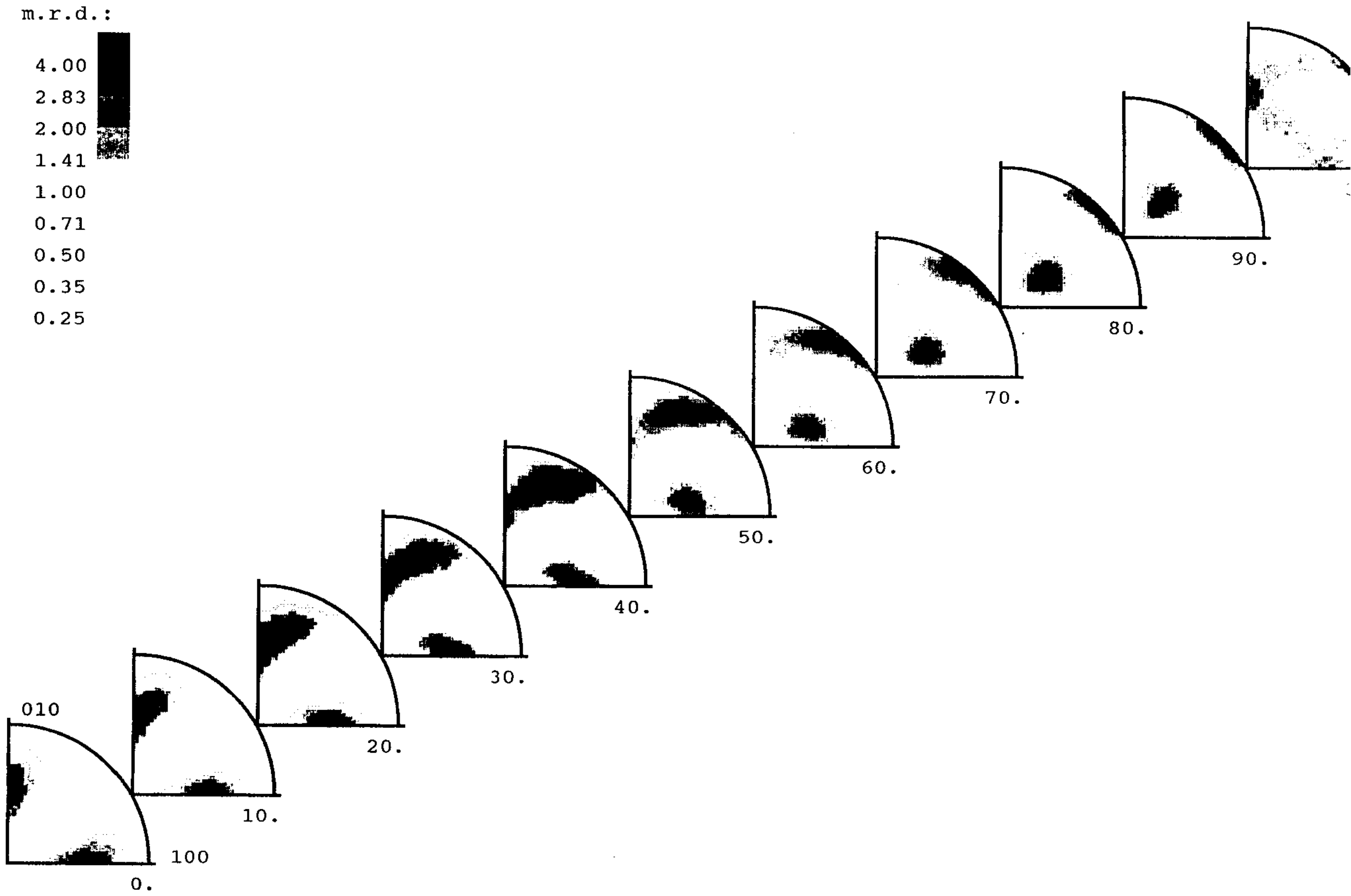
```
PERMUTATIONS, TRANSFORMATIONS, other utilities        (LAtex page 5)

 0. QUIT
 1. RETURN to Page 1

--- ORIENTATION DENSITY FILES ---

 2. Permute axes in pole figures
 3  Permute axes in .SOD

--- DISCRETE ORIENTATION FILES ---

 4. Add crystal and sample symmetries, permute axes, change Euler
    angle convention, or make DENSITY file from DISCRETE angles file

 5. Convert generic MILLER INDICES to any Euler angles (Rollett)

--- HARMONIC COEFFICIENTS FILES ---

 6. Establish coefficients for a given ROTATION
 7. Apply ROTATION to given coefficients


 Please enter a number from 0 to 7  -->
```

```
DISPLAYS AND PLOTS                                    (LAtex page 6)

 0. Quit
 1. Return to Page 1

 --------- POLAR REPRESENTATION (Wenk and Kocks) ---------
 DENSITY PLOTS:
    2. POP: colors or gray-shades on EGA (need VDIDY010.SYS)
                                  or VGA (need VDIDY012.SYS)
       or gray-shades on hp-LASERJET+ or II or to POSTSCRIPT (slow)
 CONTOUR PLOTS:
    3. OD sections from density files (Wenk program)
    4. single PFs from density file (Kallend program)
 DISCRETE ORIENTATION PLOTS:
    5. PFs, points or contours (Tome/Wenk program, Canova angles)
    6. all OD sections and projections (DIOR)
       (general crystal, sample symmetries and permutations)

--------- SQUARE SECTIONS (Kallend) ---------
    7. Colors on screen
    8. Contours on hp-Laserjet

 9. CURVES on screen or hp by GRAPHER (need data as file.DAT)

 Please enter a number from 0 to 9 -->
```

```
PROPERTIES                                        (LAtex page 7)

 0. Quit
 1. Return to Page 1

 Assign WEIGHTS to discrete grain file for simulation:

    2. from .SOD (or .SOH) -- Kocks-style Euler angles only
    3. from harmonic coefficients directly (Canova angles only)

 4. SIMULATION of polycrystal plasticity from weighted grain file

    5. Plot resulting 2-D yield surface sections or projections
    6. Plot resulting 3-D yield surface section for sheets

 SHEET properties directly from harmonic coeff's.(cubic only):

    7. Young's moduli
    8. Lankford coefficients (sheet normal=3, RD= )
    9. Yield locus section (11,22), for any angle in plane


 Please enter a number from 0 to 9 -->
```

MSCR11 8/3/88 9 WIMV iters to RP= 5.0 2-MAY-89

SODK Psi= min= 1; max= 1619; median= 23



al26r00 .WTS file from its SOD and texlat3 27-JUL-88

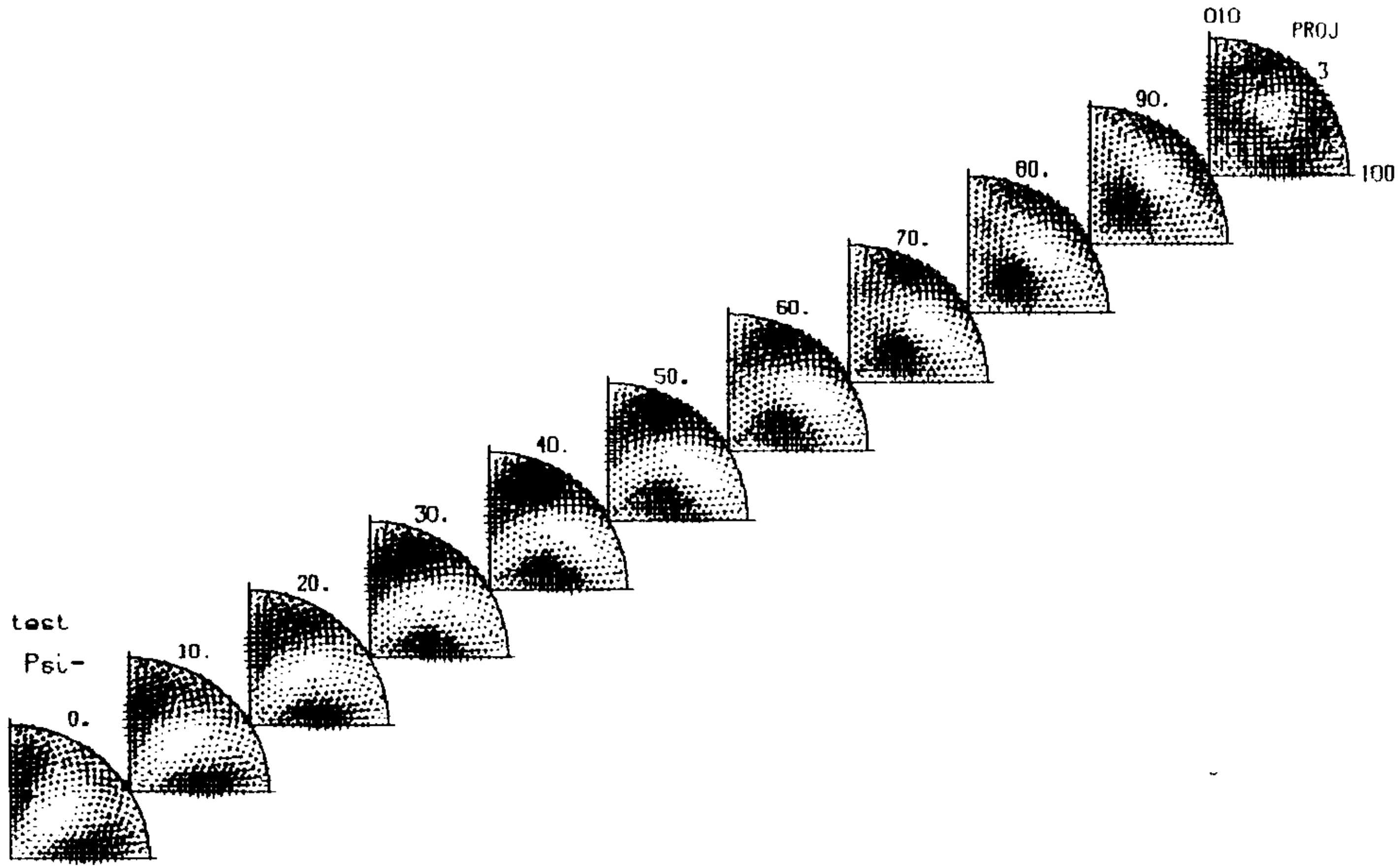
Evm	F11	F12	F13	F21
0.000	1.000	0.000	0.000	0.(

texlat :64x18=1152 or's. (07jul88)
(up to 6 state parameters, f8.2)

Kocks:Psi	Theta	phi	weight	texlat weight
2.50	.10	45.00	.10	0.14
7.50	4.00	45.00	.08	0.12
2.50	7.00	45.00	.23	0.39
2.50	10.00	45.00	.18	0.18
7.50	25.00	45.00	.56	0.51
2.50	37.00	45.00	.13	0.08
2.50	48.00	45.00	.09	0.07
7.50	54.74	45.00	.08	0.15
7.50	89.90	5.00	.90	0.5
2.50	89.90	10.00	.95	0.5
7.50	89.90	15.00	.83	0.5
2.50	89.90	20.00	.54	0.5
7.50	89.90	25.00	.24	0.5
2.50	89.90	30.00	.34	0.5
7.50	89.90	35.00	.28	0.5
2.50	89.90	40.00	.10	0.5
7.50	89.90	45.00	.05	0.25
2.50	86.49	47.50	.25	1.0
7.50	86.49	52.50	.44	1.0
2.50	86.49	57.50	.62	1.0
7.50	86.49	62.50	.58	1.0
2.50	86.49	67.50	.61	1.0
7.50	86.49	72.50	.78	1.0
2.50	86.49	77.50	1.48	1.0
7.50	86.49	82.50	.94	0.55
7.50	82.81	10.00	1.50	0.66
2.50	82.81	15.00	1.79	1.0
7.50	82.81	20.00	1.43	1.0
2.50	82.81	25.00	.76	1.0
7.50	82.81	30.00	.68	1.0
2.50	82.81	35.00	.92	1.0
7.50	82.81	40.00	.57	1.0
2.50	82.81	45.00	.19	0.5
7.50	79.36	47.50	.89	1.0
2.50	79.36	52.50	1.00	1.0
7.50	79.36	57.50	1.03	1.0
2.50	79.36	62.50	.66	1.0
7.50	79.36	67.50	.87	1.0
2.50	79.36	72.50	1.11	1.0
7.50	79.36	77.50	1.17	0.65
7.50	75.61	15.00	.50	0.56
[illegible]	75.61	20.00	.75	1.0

mscr11.lat (w/inv)_

89/05/10

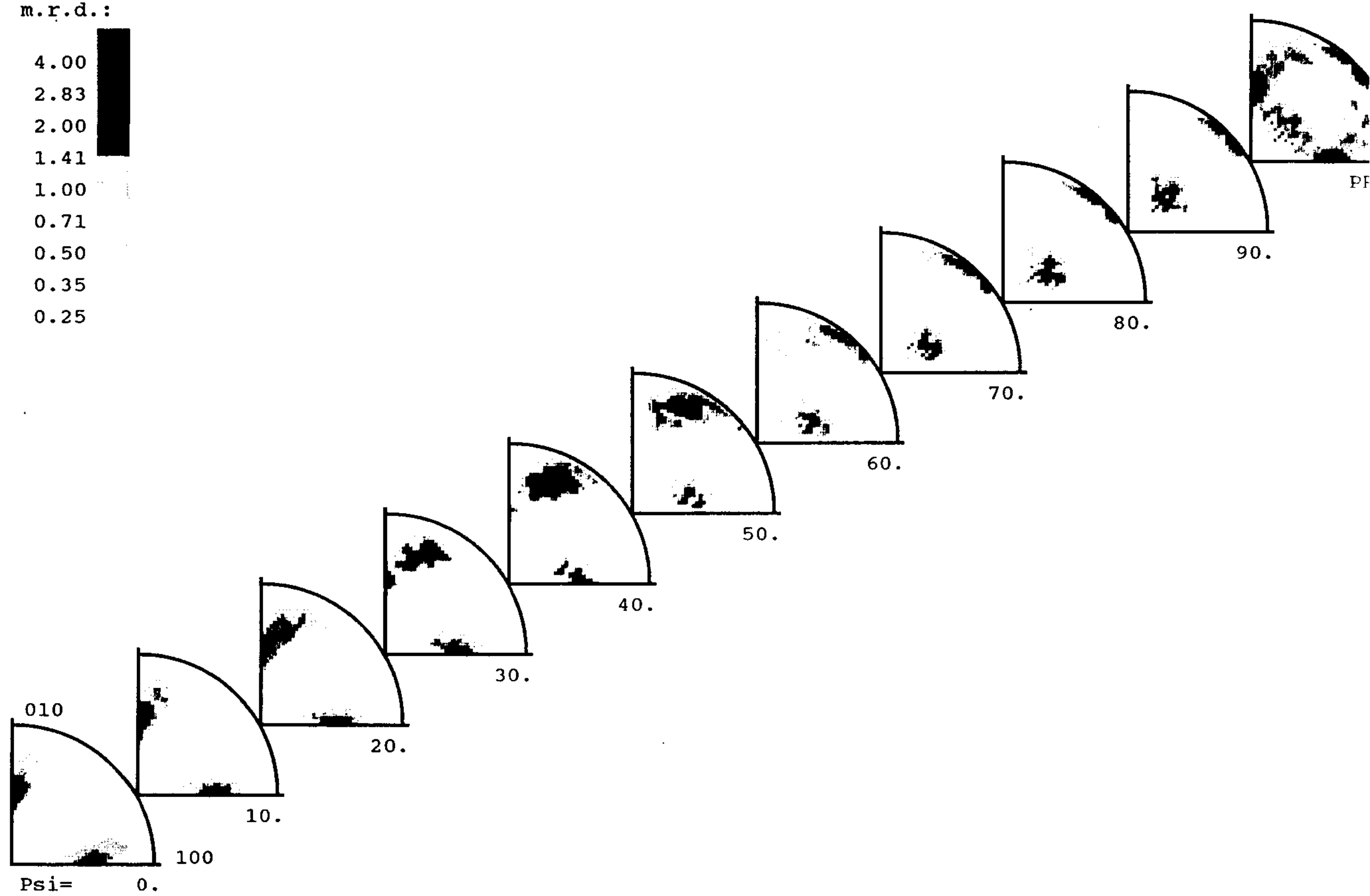


test .WTS file from its SOD and texlat3 10-MAY-89 (F from simul.)

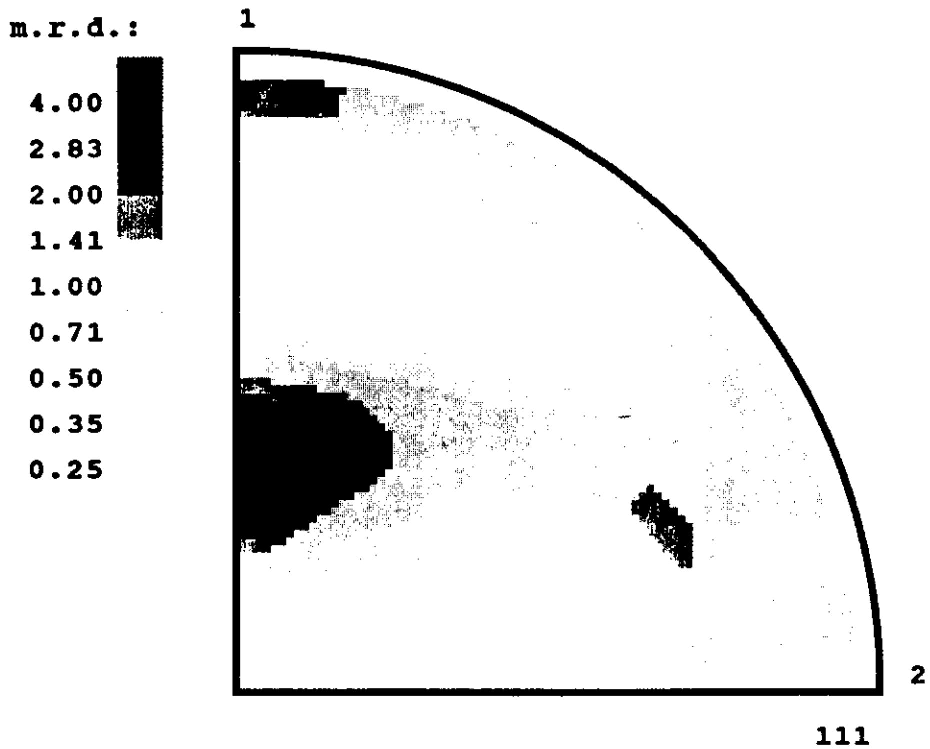
SODK Psi= min= 1; max= 1330; median= 29

m.r.d.:

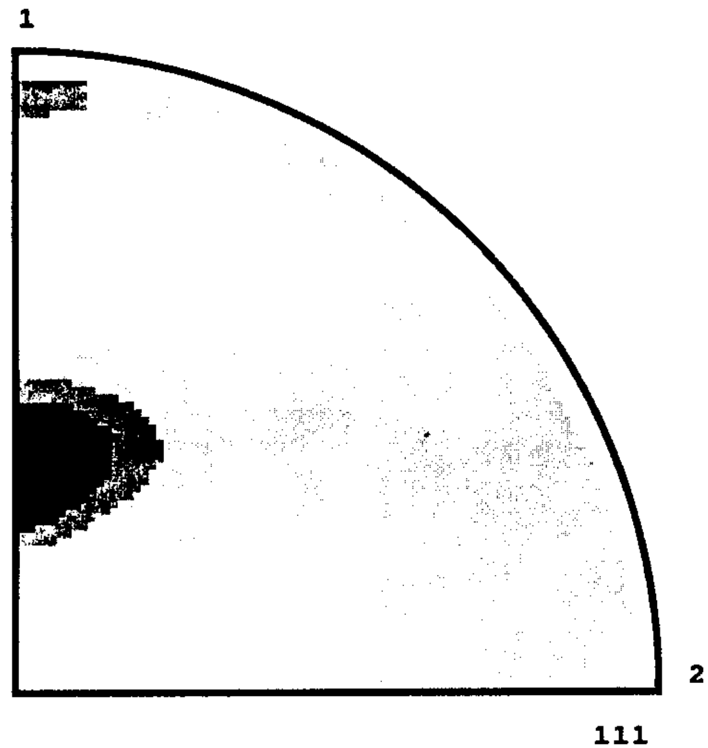
4.00
2.83
2.00
1.41
1.00
0.71
0.50
0.35
0.25



MSCR11 8/3/88 , Rot. 3.5 degs.
pole figures min= 1; max= 345

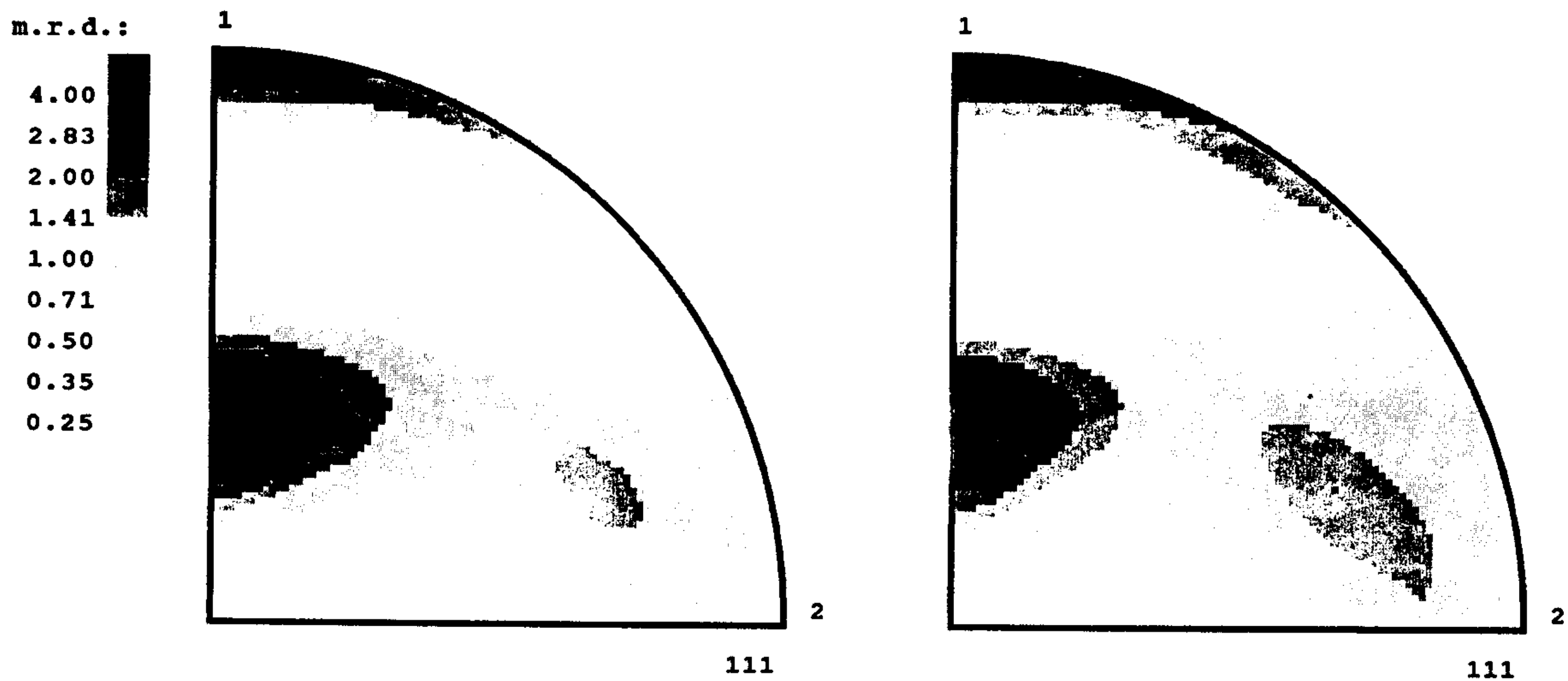


MSCR11 8/3/88 , Rot. 3.5 degs., Smoot
min= 1; max= 313; median= 0



MSCR11 8/3/88 Recalculated by WIMV 2-MA MSCR11 8/3/88 recalc. pole figure 3-

pole figures min= 2; max= 538 min= 0; max= 494; median= 100



title

this is a TEXOUT file produced by orz

```
t5ro120      texout LApp52 88/08/30
  Evm       F11      F12      F13      F21      F22      F23      F31      F32      F33
  2.000     5.550    0.000   -0.006    0.000    1.000   -0.004    0.000    0.000    0.174
Kocks:Psi   Theta     phi     ,gr.wt.,  tau,     har;               4taup
     0.21   26.60    45.14     0.05    81.05     3.54
     8.12   33.39   -39.83     1.00    82.87     3.54
   -33.66   24.42   -57.16     1.00    82.55     3.54
    33.45   36.33   -25.39     1.00    81.53     3.54
    39.34   35.24   -18.04     1.00    82.37     3.54
    55.37   40.71   -10.99     1.00    80.00     3.54
    56.63   60.90    18.56     1.00    85.62     3.54
    32.39   36.33   -18.52     1.00    86.41     3.54
    55.72   62.81    20.24     1.00    85.07     3.54
   161.85   33.23  -147.53     0.58    85.62     3.54
  -170.77   84.73  -157.84     0.73    81.52     3.54
    37.55  104.58   147.65     1.10    81.79     3.54
  -135.13   71.98  -153.46     0.85    85.62     3.54
   157.46   35.69  -152.57     0.86    87.01     3.54
    87.83   65.92     1.26     0.97    80.20     3.54
   132.87   36.91    17.68     1.10    80.07     3.54
   141.74   76.02   147.64     0.38    83.47     3.54
  -111.17   51.81  -170.65     0.48    79.82     3.54
  -162.67   33.47   146.37     1.08    84.68     3.54
   -63.74   51.96   -10.71     0.38    82.00     3.54
   -61.58   61.89  -110.76     0.94    86.43     3.54
   -54.48  111.50    23.34     0.72    82.53     3.54
   128.38   66.72    67.14     0.50    85.99     3.54
   -57.46   61.78  -110.23     1.01    84.38     3.54
   -51.42   70.21   -25.23     0.60    88.38     3.54
  -119.55   58.50    16.13     0.48    83.28     3.54
    19.07   33.30  -122.52     1.36    84.36     3.54
   -46.78   36.94  -102.44     0.47    79.96     3.54
   -44.52   72.34  -118.54     0.46    86.11     3.54
```

current grain shape

Euler angles (changed by rotation)

current CRSS

potential further state parameters

256 grains, weighted by initial texture (stay)
(texran0)