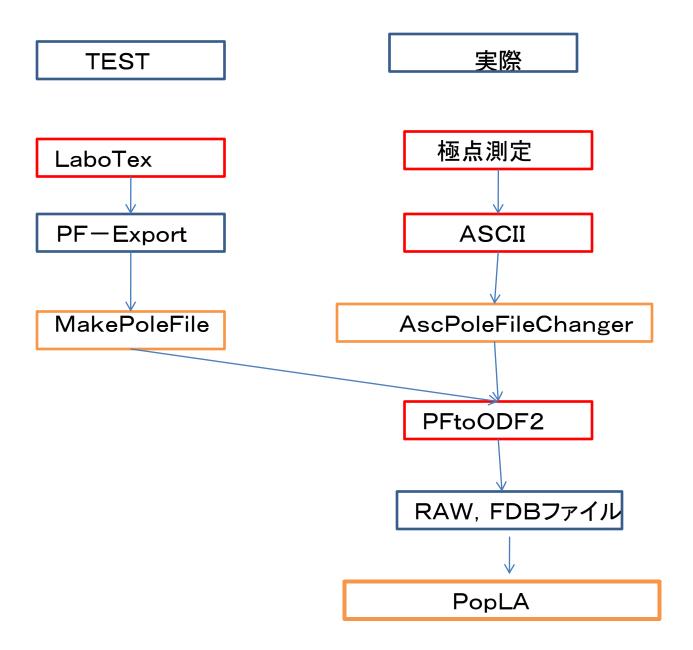
PopLATEST

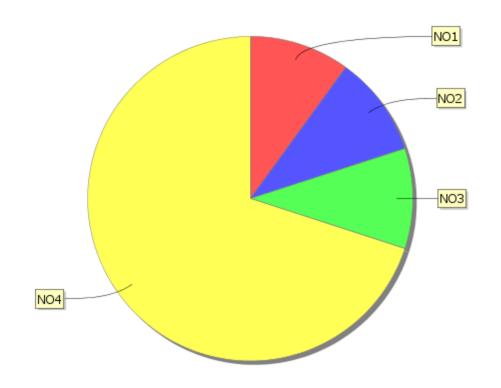
LaboTexでcube, brass, copperをVolumeFraction10%でODF作成し {111}、{200}、{220}極点図をexportし MakePoleFileでTXT2ファイルを作成し、PFtoODF2(Ver. No. 5. 520)でpopLA用RAW,DFBファイルを作成 PopLAでデータの読み込み EPFファイル、HCFファイル、FULファイルを作成した。 Harmonic Analysis で動作確認した。 この事で、 極点図の補正をAscPoleFileChangerで行い PFtoODF2ソフトウエアでRAW, DFBファイルを作成すれば、PopLAの機能が使える事が判明した。

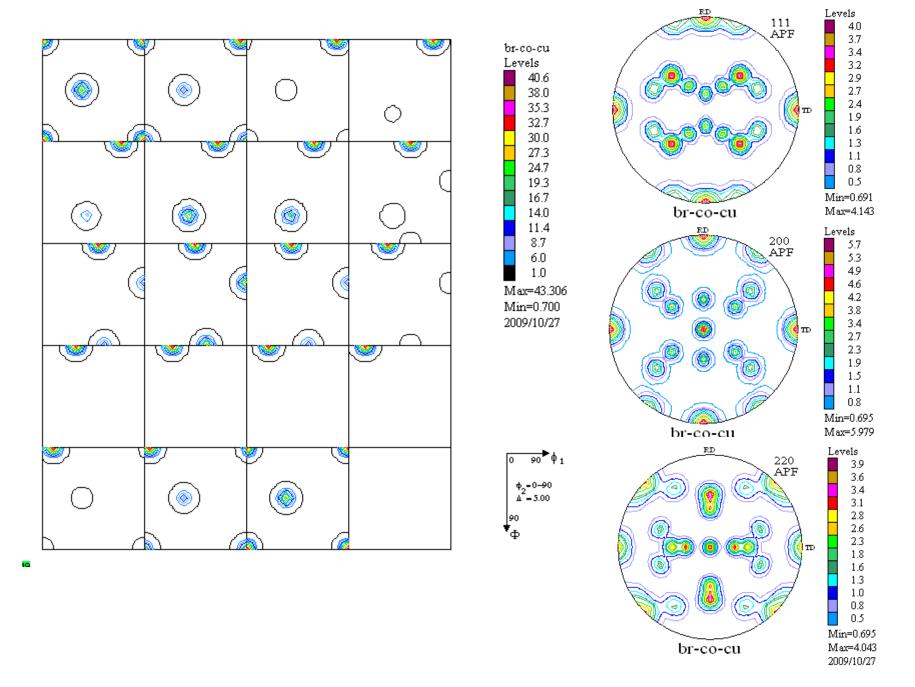
HelperTex 2009年11月07日



TEST結晶方位

File	Help						
	Job	JO B2	Sample : b	r-co-cu			Project : popLA
No.	VF(%)	Phi1 (FWHM)	Phi(FWHM)	Phi2(FWHM)		Orientation	
1:	10.0	10.1	10.0	9.9 {		01	
2:	10.0	10.0	10.0	10.0 {	1	10 K 1 -1 2 >	brass
2: 3:	10.0	10.0	10.0	10.0 {	1	12 K 1 1-1>	copper
4:	69.99	Background \	/olume Fraction				





0.70

0.70

0.70

0.70

35.0 0.70 0.70 0.70 0.70 0.70

0.71

0.70

0.70

0.70

15.0 0.78

20.0 0.70

25.0 0.70

30.0 0.70

0.70

0.70

0.70

0.70

0.70

0.70

0.70

0.70

0.79

0.70

0.70

0.70

0.70

0.70

0.70 0.70

0.70 0.70

0.73 0.75

0.70

0.70

0.70

1.31 1.91 1.40 0.82 0.71

0.70 0.70

0.73 0.71

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0.71

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0.70

0.70

0.78

0.70

0.70

0.70

0.85

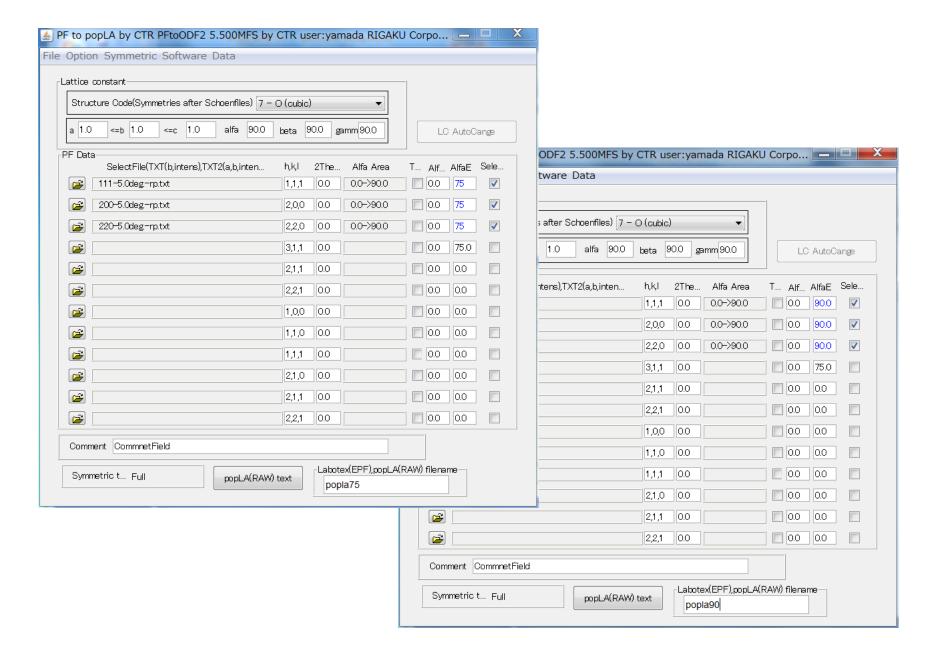
0.70

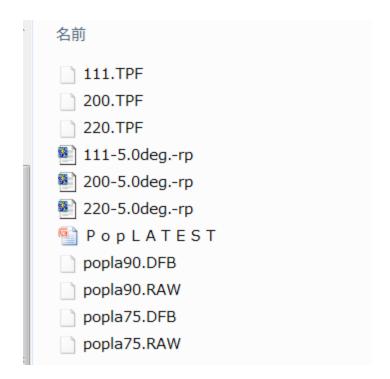
0.70

0.70

0.70

完全極点図からαMax90度,75度としてpopLA用RAWデータ作成





RAWファイル、DFBファイルを C: ¥Xにコピーする。 DOSプロンプトを起動

```
Microsoft Windows [Version 6.1.7600]
Copyright (c) 2009 Microsoft Corporation. All rights reserved.
C:\text{Users}\text{yamada}\text{>cd c:}\text{\text{}}\text{}
c:\text{\text{}}\text{Ympdos}
```

C:\X>newpopla popla90

■ コマンド プロンプト - tmpdos - newpopla popla90 To return to program, type EXIT (from SAME subdirectory) Microsoft(R) Windows DOS (C)Copyright Microsoft Corp 1990–2001. C:\X>newpopla popla90 popLA: preferred orientation package - Los Alamos U.F. Kocks, J.S. Kallend, H.R. Wenk, et al. (Version May 1999) (C)Copyright 1989, The Regents of the University of California and John S. Kallend. Major parts of this software were produced under U. S. Government contract (W-7405-ENG-36) by Los Alamos National Laboratory, which is operated by the University of California for the U. S. Department of Energy. The U. S. Government is licensed to use, reproduce, and distribute this software. Permission is granted to the public to copy and use this software without charge, provided that this Notice and the above statement of authorship are reproduced on all copies. Neither the Government nor the University nor John S. Kallend makes any warrantv. express or implied. or assumes anv liabilitv or responsibilitv for the use of this software. TSPA Press any key to continue . .

```
X
コマンド プロンプト - tmpdos - newpopla popla90
popLA: preferred orientation package - Los Alamos
                                                             (Page 1)
U.F. Kocks, J.S. Kallend, H.R. Wenk (May 1999)
 0. OUIT
1. Get specimen DIRECTORY and VIEW a file
 2. MASSAGE data files: correct,rotate,tilt,symmetrize,smooth,compare
 3. WIMV: make spec.SOD; calculate PFs and inverse PFs; make matrices
 4. HARMONIC analysis: COMPLETE rim (.FUL), get Roe Coeff.file (.HCF)
 5. CONVERSIONS, permutations, transformations, paring
 6. DISPLAYS and plots
 7. Derive PROPERTIES from .SOD or .HCF files, make WEIGHTS file for simul.
 8. DOS (temporary: type EXIT to return)
 Please type a number from 0 to 8 -->
```

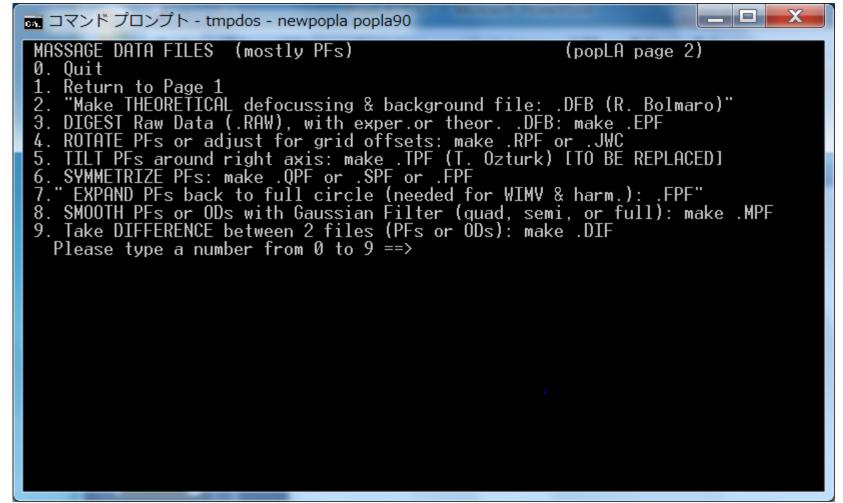
1. Get specimen DIRECTORY and VIEW a file

```
2009/11/01 10:01 614 popla90.DFB
2009/11/01 10:01 17,307 popla90.RAW
2 File(s) 17,921 bytes
0 Dir(s) 89,700,880,384 bytes free
For viewing:
Enter filename: popla90.raw
```

Popla90. Rawとpopla90. DFBの表示

□ □マン	トナ	ロンフ	11-1	tmpdo	s - ne	wpop	la pop	ola90										×
IST		1	200	100	- 11	-01-	:9 1	0:01	♦ P	OPLA	90. R	AW						
opla9		ommne							100									
111	5.0	90.0		.0360		12	1 3	10		1			-		-			
69	69	69	69	69	69	69	69	69	69	69	69	69	69	69	69	69	69	
69	69	69	69	69	69	69	69	69	69	69	69	69	69	69	69	69	69	
69	69	69	69	69	69	69	69	69	69	69	69 69	69	69	69	69	69	69	
69	69	69	69	69	69	69	69	69	69	69	69	69	69	69	69	69	69	
72 71	73	73	73	72	72	72	72 72	72	72 72 72 72 72 71 71	72	72	71	71 72	71	71	71	71	
71	71	71	71	71	71	71	72	72	12	72	72	72	72	72	73	73	73	
72 71 89	73	73	73	72	72	72	72 72	72	72	72 72	72 72	71	71	71	71 73	71	71 72	
71	71	71	71	71	71	71	72	72	72	72	72	72	72	72	73	73	72	
89	90	92	92	86	79	76	74	72	71	70	69	69	69	69	69	69	69	
69	69	69	69	69	69	69	69	70	11	72	74	76	79	86	92	92	90	
89	90	92	92	86	79	76	74	72	71	70	69	69	69	69	69	69	69	
69	69	69	69	69	69	69	69	70	71	72	74	76	79	86	92	92	89	
220	206	175	149	128	104	86	78	75	73	71 75	71	71	71	71	71	71	71	
71	71	71	71	71	71	71	71	71	73	75	78	86	104	128	149	175	206	
220	206	175	149	128	104	86	78	75	73 73 73 73 73	71	71	71	71	71	71	71	71	
71	71	71	71	71	71	71	71	71	73	75	78	86	104	128	149	175	220	
276	254	213	170	129	98	82	74	71	70	69	69	69	69	69	69	69	69	
69	69	69	69	69	69	69	69	69	70	71	74	82	98	129	170	213	254	
276	254	213	170	129	98	82	74	71	70	69	69	69	69	69	69	69	69	
69	69	69	69	69	69	69	69	69	70	71	74	82	98	129	170	213	276	
173	164	140	111	93	85	82	81	79	76	74	72	71	71	70	70	70	70	

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



EPFファイルの作成

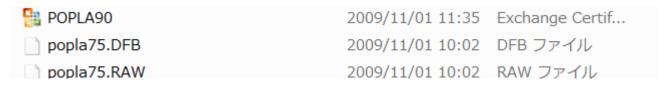
3. DIGEST Raw Data (.RAW), with exper.or theor. .DFB: make .EPF

```
コマンドプロンプト - tmpdos - newpopla popla90
Volume in drive C is Windows-7
 Volume Serial Number is F6C4-42D9
Directory of c:\X
2009/10/28 04:36
                           17.674 DEMO.RAW
2009/11/01 10:02
                       17.307 popla75.RAW
2009/11/01 10:01
                  17,307 popla90.RAW
              3 File(s)
                               52,288 bytes
              0 Dir(s) 89.700.638.720 bytes free
ECHO is off.
Note: If your data are on a SCINTAG .RR file: use DA5READ to make .RAW
     If they are on a PHILIPS .RAW file, use UNPHIL to make our .RAW
     If they are on an Aachen pole figure file, use AC2LA to make .EPF
     If they are on a RIGAKU .PFG file: use RIG2LA to make our .RAW
         (but you must have a PWD subdirectory into which it puts it:
          compliments of RIGAKU/USA.)
     All of these are in the compacted file XCONVERT.EXE
     (BREAK now to do any of the above..., else RETURN)
Press any key to continue . . .
```

Returnで

```
■ コマンドプロンプト - tmpdos - newpopla popla90
Directory of c:\X
2009/10/28 04:36
                           17.674 DEMO.RAW
2009/11/01 10:02
                        17.307 popla75.RAW
52,288 bytes
              3 File(s)
              0 Dir(s) 89.700.638.720 bytes free
ECHO is off.
Note: If your data are on a SCINTAG .RR file: use DA5READ to make .RAW
     If they are on a PHILIPS .RAW file, use UNPHIL to make our .RAW
     If they are on an Aachen pole figure file, use AC2LA to make .EPF
     If they are on a RIGAKU .PFG file: use RIG2LA to make our .RAW
         (but you must have a PWD subdirectory into which it puts it:
          compliments of RIGAKU/USA.)
     All of these are in the compacted file XCONVERT.EXE
     (BREAK now to do any of the above..., else RETURN)
Press any key to continue . . .
Empirical Defocussing Correction
Note: the sample is assumed to have rotated counter-clockwise
Data will be sequenced clockwise in .EPF
Enter name of raw data file (ext .RAW assumed) popla90
Enter name of correction file (ext .DFB assumed)popla90
```

```
Enter name of raw data file (ext .RAW assumed) popla90
Enter name of correction file (ext .DFB assumed)popla90
oopla90 CommnetField
(hkl)=(111) Background= - 1 Using correction curve 1
 ..correcting raw data
   ...normalizing. Normalization factor= 1.009
     ...writing corrected data to popla90
                                                  .EPF
oopla90 CommnetField
(hkl)=(200) Background= - 1 Using correction curve 2
 ..correcting raw data
   ...normalizing. Normalization factor= 1.006
     ...writing corrected data to popla90
                                                  .EPF
oopla90 CommnetField
(hkl)=(220) Background= - 1 Using correction curve 3
 ..correcting raw data
   ...normalizing. Normalization factor= 1.007
     ...writing corrected data to popla90
                                                  .EPF
Stop - Program terminated.
```



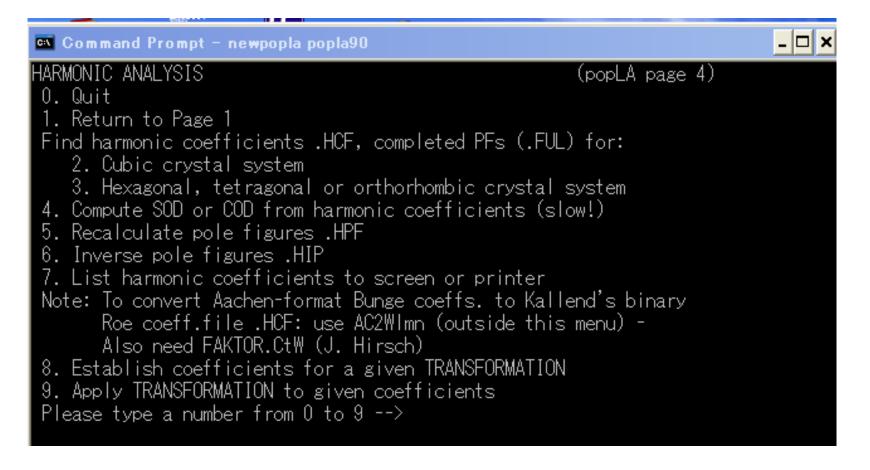
Popla90のEPFファイルが作成された。

```
2009/11/01 10:01 614 popla90.DFB
2009/11/01 11:35 17,607 POPLA90.EPF
2009/11/01 10:01 17,307 popla90.RAW
3 File(s) 35,528 bytes
0 Dir(s) 89,700,618,240 bytes free
For viewing:
Enter filename: popla90.epf
```

EPFファイルの確認

Cal Cor				- ne			pla90											_ 🗆 ×
LIST		1				1-07	7-:9	22:4	3 4	POPL	A90.	.EPF						
popla9	90 C	ommr	netFi	ield			DFB:	=popl	a90									
(111)	5.0	80.	0 5	5.036		1 1		3 1	00	- 1								
68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	
68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	
68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	
68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	68	69
71	71	72	72	71	71	-71	- 71	71	71	71	-71	70	70	70	70	70	70	
70	70	70	70	70	70	70	- 71	71	71	- 71	-71	-71	71	71	72	72	72	
71	72	72	72	71	71	-71	- 71	71	71	- 71	-71	70	70	70	70	70	70	
70	70	70	70	70	70	70	- 71	71	-71	- 71	-71	-71	-71	71	72	72	72	71
88	88	91	91	85	78	75	73	71	70	69	68	68	68	68	68	68	68	
68	68	68	68	68	68	68	68	69	70	- 71	73	75	78	85	91	91	89	
88	89	91	91	85	78	75	73	71	70	69	68	68	68	68	68	68	68	
68	68	68	68	68	68	68	68	69	70	- 71	73	75	78	85	91	91	89	75
220	220	175	149	128	103	85	- 77	74	72	70	70	70	70	70	70	70	70	
70	70	70	70	70	70	70	70	70	72	74	-77	85	103	128	149	175	206	
220	206	175	149	128	103	85	- 77	74	72	70	70	70	70	70	70	70	70	
70	70	70	70	70	70	70	70	70	72	74	-77	85	103	128	149	175	206	99
277	277	213	170	129	97	81	73	70	69	68	68	68	68	68	68	68	68	
68	68	68	68	68	68	68	68	68	69	70	73	81	97	129	170	213	255	
277	255	213	170	129	97	81	73	70	69	68	68	68	68	68	68	68	68	
68	68	68	68	68	68	68	68	68	69	70	73	81	97	129	170	213	255	105
173	173	140	110	92	84	81	80	78	75	73	71	70	70	69	69	69	69	

Page1から 4. HARMONIC analysis: ĆOMPLETE rim (.FUL), get Roe Coeff.file (.HCF)



Find harmonic coefficients .HCF, completed PFs (.FUL) for:

2. Cubic crystal system

3. Hexagonal, tetragonal or orthorhombic crystal system

Harmonic Pole Figure Analysis (Cubic)

Program (C) 1968–1987 by John Kallend. All rights reserved

Enter name of data file (default .epf): popla90

1popla90 CommnetField 3 Pole figures read in.

How many iterations on missing parts? 4

CUBIC ODF ANALYSIS FOR popla90

1-NOV-**

Sample symmetry:

- 0. Orthorhombic
- 1. Mirror <u>perpendicular to Z</u>

Enter \emptyset or $1=>\emptyset$

Error output to:

- 1. printer
- 2. screen

Enter 1 or $2 \Longrightarrow 2$

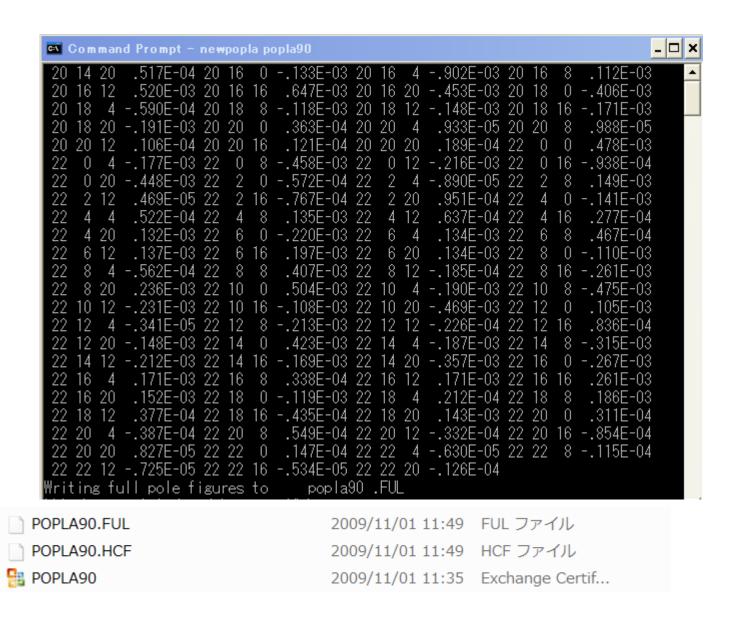
200 Reflection. Trunc. error = .18 Normalization = .10E+01 220 Reflection. Trunc. error = .16 Normalization = .10E+01 Severity = 1.142. Generated to I = 22

ERROR ESTIMATES: 1. Polefigures

L	MEAN	111	200	220
0	.223E-06	.225E-06	.225E-06	.218E-06
2	.258E-03	.810E-04	.327E-03	.292E-03
4	.438E-03	.510E-03	.488E-03	.279E-03
6	.391E-03	.341E-03	.428E-03	.398E-03
8	.748E-03	.431E-03	.113E-02	.466E-03
10	.875E-03	.113E-02	.718E-03	.704E-03
12	.265E-03	.371E-03	.773E-04	.260E-03
14	.836E-03	.653E-03	.113E-02	.628E-03
16	.423E-03	.871E-04	.324E-03	.652E-03
18	.528E-03	.762E-03	.296E-03	.411E-03
20	.153E-03	.149E-03	.949E-04	.198E-03
22	.419E-03	.365E-04	.324E-03	.648E-03
ALL	.562E-01	.546E-01	.597E-01	.540E-01

2. Estimated avg. error in ODF .21 RE-ESTIMATING MISSING PARTS OF POLEFIGURES

Writing harmonic coefficients to popla90 .HCF Print out Wlmn coefficients?Y



FULとHCFファイルが作成される。

同様にpopla75を調べると

```
Command Prompt - newpopla popla75
                                                                      _ | 🗆 | × |
                                                    .10E+01
200 Reflection. Trunc. error = .18 Normalization =
                                                    .10E+01
Severity =  1.130. Generated to I = 22
 ERROR ESTIMATES: 1. Polefigures
                  MEAN
                                          200
                                                      220
                 .220E-06
                                        .225E-06
                                                   .218E-06
                            .218E-06
                 .309E-03
                          .188E-03
                                        .280E-04
                                                   .500E-03
    4
6
8
                            .149E-03
                 .298E-03
                                        .465E-03
                                                   .167E-03
                            .419E-03
                                        .246E-03
                 .368E-03
                                                   .411E-03
                 .722E-03
                          .520E-03
                                        .974E-03
                                                   .585E-03
    10
                 .974E-03
                          .128E-02
                                        .811E-03
                                                   .739E-03
    12
                 .246E-03
                           .344E-03
                                        .717E-04
                                                   .242E-03
    14
                 .870E-03
                            .731E-03
                                        .118E-02
                                                   .578E-03
    16
                 .496E-03
                           .102E-03
                                        .379E-03
                                                   .764E-03
    18
                                                   .394E-03
                 .506E-03
                          .729E-03
                                        .284E-03
   20
                          .151E-03
                                        .963E-04
                                                   .201E-03
                 .155E-03
   22
                 .352E-03
                            .306E-04
                                        .272E-03
                                                   .544E-03
   ALL
                 .571E-01
                            .578E-01
                                        .591E-01
                                                   .544E-01
2. Estimated avg. error in ODF .22
RE-ESTIMATING MISSING PARTS OF POLEFIGURES
Writing harmonic coefficients to popla75 .HCF
Print out Wlmn coefficients?Y
```

Command Prompt - newpopla popla75	_	□×
	03 20 16 4970E-03 20 16 8 .117E-03 03 20 16 20491E-03 20 18 0431E-03 03 20 18 12151E-03 20 18 16174E-03 04 20 20 4333E-05 20 20 8 .750E-05 04 20 20 20 .746E-05 22 0 0 .479E-03 03 22 0 12230E-03 22 0 16149E-03 04 22 2 4113E-04 22 2 8 .148E-03 04 22 2 2 0 .930E-04 22 4 0938E-04 03 22 4 12 .373E-04 22 4 16290E-05 03 22 6 4 .130E-03 22 6 8 .675E-04 03 22 6 4 .130E-03 22 8 0117E-03 03 22 8 12137E-04 22 8 16253E-03 03 22 10 4181E-03 22 10 8410E-03 03 22 10 4181E-03 22 10 8410E-03 03 22 12 12 .159E-04 22 12 16 .106E-03 03 22 14 4174E-03 22 14 8252E-03 03 22 14 20304E-03 22 16 0229E-03 04 22 18 4 .849E-05 22 18 8 .146E-03 04 22 18 4 .849E-05 22 18 8 .146E-03 04 22 18 20 .107E-03 22 20 0 .373E-04 04 22 20 12360E-04 22 20 16865E-04	
POPLA75.FUL	2009/11/01 11:53 FUL ファイル	1
POPLA75.HCF	2009/11/01 11:53 HCF ファイル	
POPLA75	2009/11/01 11:52 Exchange Certif	1
POPLA90.FUL	2009/11/01 11:49 FUL ファイル	1
POPLA90.HCF	2009/11/01 11:49 HCF ファイル	

2009/11/01 11:35 Exchange Certif...

18 KE

POPLA90

```
4. Compute SOD or COD from harmonic coefficients (slow!)
 Directory of c:\X
2009/09/25 13:39
                               2.129 CNULL.HCF
                               2.129 POPLA75.HCF
2009/11/04
           10:12
2009/11/04
           10:04
                                2,129 POPLA90.HCF
                3 File(s)
                                    6,387 bytes
                0 Dir(s) 88,450,461,696 bytes free
Calculate ODF from Harmonic Coefficients
  Program by John Kallend (c) 1968 - 1988
What is the specimen nam Average values of Wlmn for different orders of I
ENTER OUTPUT FORMAT REQU
                                          Avg. Wimn
1. COD sections every 10
                                           .00E+00
2. SOD or COD every 5 de
                                           .42E-03
3. COD sections at low i
                                           .12E-02
                                           .12E-02
                                 10
                                           .52E-03
                                           .94E-03
                                 14
                                           .23E-03
                                 16
                                           .49E-03
                                 18
                                           .26E-03
```

.29E-03

Default = CALCULATE TO L = 22, OK ? Y

20

```
CALCULATIONS FINISHED

MAX. VALUE = 14.25 MIN. VALUE = -3.57

Choose output format:

1. as SOD (will be called .SHD)

2. as COD (will be called .CHD)

Enter 1 or 2 ==> 1

In output file, angles increase from 0 in nomenclature of

1. Kocks

2. Roe/Matthies

3. Bunge

Enter 1,2, or 3 ==> 3

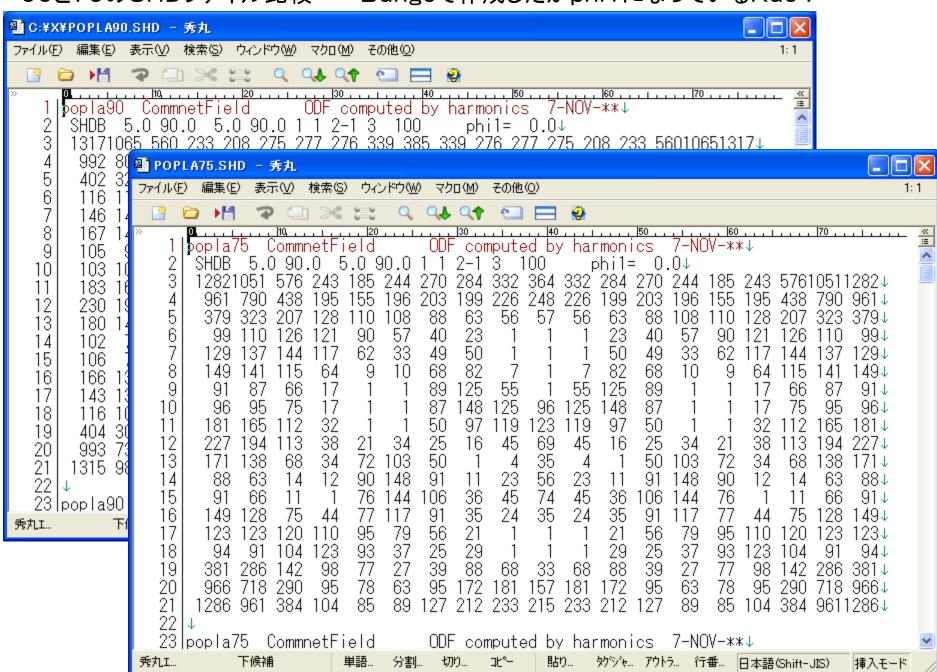
Making file popla90 .SHD

Press any key to continue . . .
```

同様にpopla75も処理する。

POPLA75.SHD	2009/11/04 10:17
POPLA90.SHD	2009/11/04 10:15

90と75のSHDファイル比較 Bungeで作成したがphi1になっているRue?



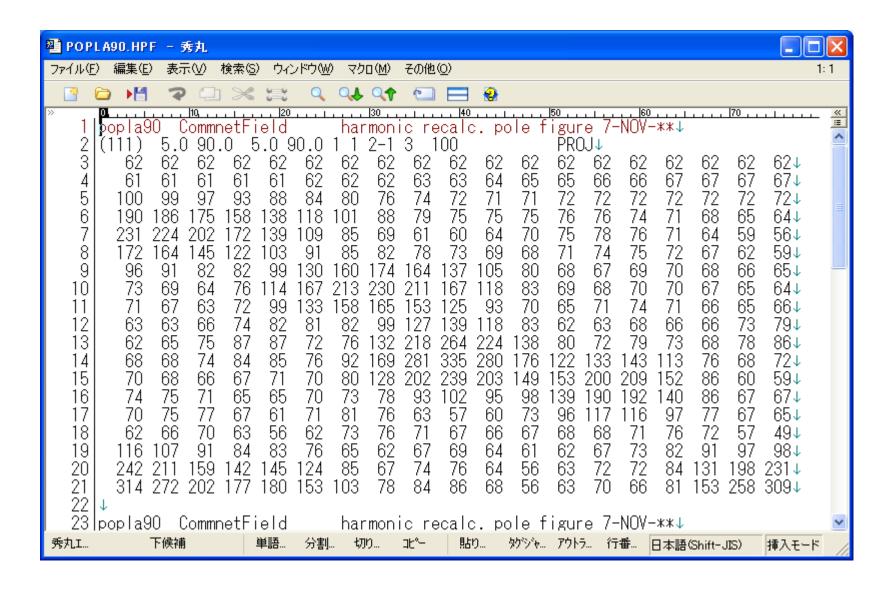
5. Recalculate pole figures .HPF

```
_ - X
■ コマンド プロンプト - tmpdos - newpopla popla90
 Volume Serial Number is 308D-8899
 Directory of c:\X
2009/09/25 13:39
                             2.129 CNULL HCF
2009/11/04 10:12
2009/11/04
          10:04
                              2.129 POPLA90.HCF
               3 File(s)
                                  6.387 bytes
               0 Dir(s) 88.450.424.832 butes free
Recalculate Pole Figures (Harmonic Method)
 Program by John Kallend
What is the specimen name (.HCF Assumed)? popla90
How many PFs are required? 3
Enter Miller indices of polefigures required
e.g. 111, 200,110 etc.
What are the indices of PF 1? 1 1 1
What are the indices of PF 2? 2 0 0
What are the indices of PF 3? 2 2 0
```

```
220 Working on L=22
Output to
popla90 .HPF
Stop – Program terminated.
Press any key to continue . . .
```

POPLA75.HPF	2009/11/04 10:29
POPLA90.HPF	2009/11/04 10:27
POPLA75.SHD	2009/11/04 10:17
POPLA90.SHD	2009/11/04 10:15

複数の再極点図が作成される。



逆極点図作成

```
_ D X
■ コマンド プロンプト - tmpdos - newpopla popla90
                                2,129 POPLA90.HCF
2009/11/04 10:04
                3 File(s)
                                    6,387 bytes
                0 Dir(s) 88,450,297,856 bytes free
Inverse Pole Figure (Harmonic Method)
  Program by John Kallend
What is the specimen name (.HCF Assumed)? popla90
How many IPFs are required? 3
Enter IPF required using pseudo cubic Miller indices
e.g. ND = 0 0 1. TD = 0 1 0. RD = 1 0 0 etc.
WHAT ARE THE "INDICES" OF IPF 1? 0 0 1
WHAT ARE THE "INDICES" OF IPF 2? 0 1 0
WHAT ARE THE "INDICES" OF IPF 3? 1 0 0
1 0 0 working on L= 22
Output to popla90 .HIP
Stop – Program terminated.
Press any key to continue . . .
```

POPLA75.HIP 2009/11/04 10:35 POPLA90.HIP 2009/11/04 10:34

