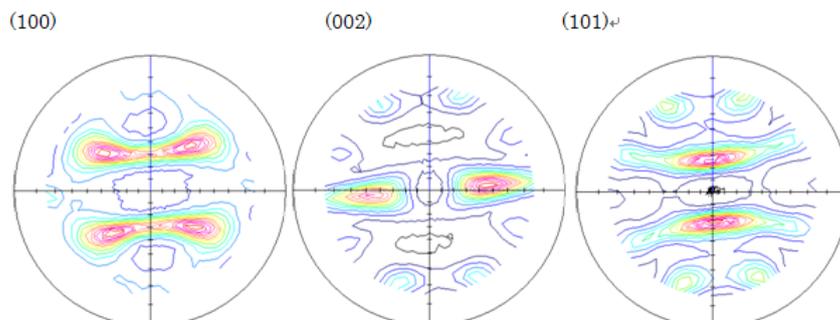
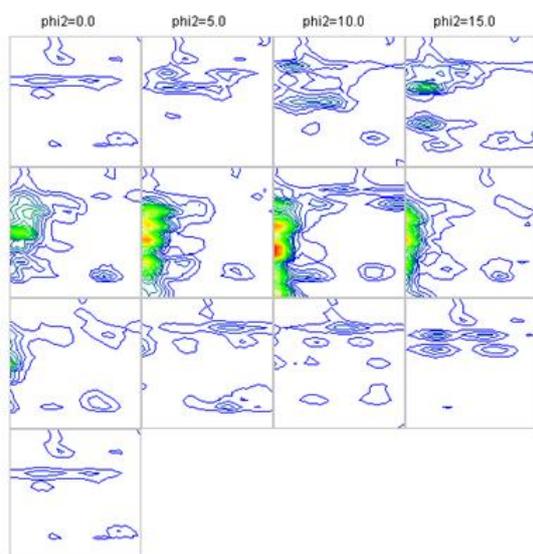


# p o p L Aによる六方晶T iのODF解析と再計算極点図

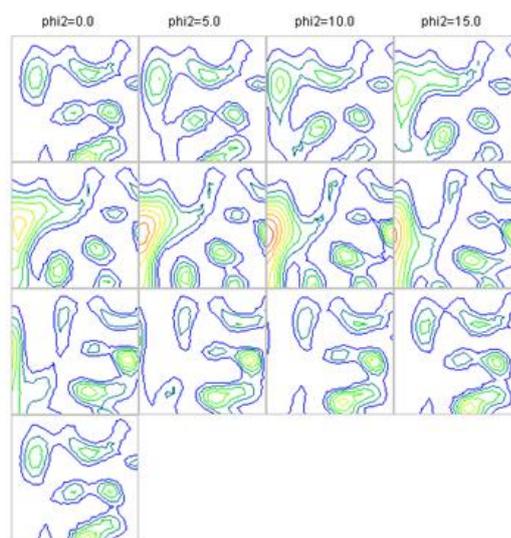
入力データ



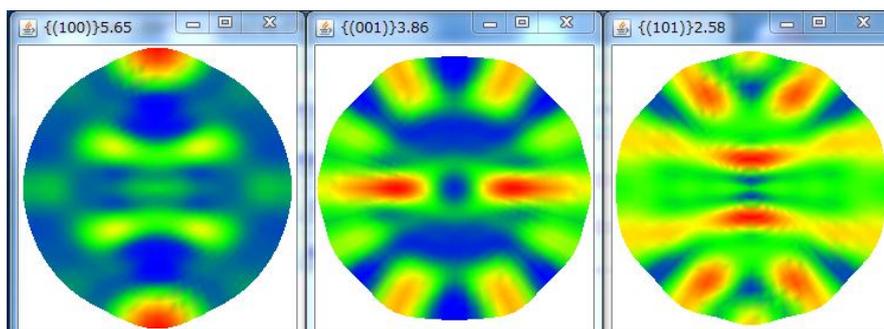
WIMV



Harmonic



Harmonic 再計算極点図



2013年04月05日

*HelperTex Office*

1. 概要
2. 入力データ
3. 測定極点図
4. ASCデータに変換する
5. ODFPoleFigure2 ソフトウェア (CTR パッケージソフトウェア) で正極点データ処理
6. popLA入力ファイルの作成
7. popLA解析
  7. 1 popLAを立ち上げ
  7. 2 入力データをpopLA補正データに変換
  7. 3 WIMV法の準備
  7. 4 六方晶、Tiのパラメータファイル (WIM) の作成
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  7. 7 再計算極点図の表示
  7. 8 Harmonic法解析
  7. 9 六方晶の指定、展開係数の計算
  7. 10 Harmonic法によるODF図の計算
  7. 11 ODFDisplay2 ソフトウェアでODF図の表示
  7. 12 再計算極点図

## 1. 概要

popLAソフトウェアは、Los Alamosで作成されたODFでHarmonicとWIMV法がサポートされているODF解析ソフトウェアであり、DOSベースで動作する。

(WIMVは開発者の名前で、Williams method, Imhof methodをMatthiesとVinelが結合)

リガクRINT2000で測定したTi(六方晶)の解析を行ってみる。

**PFtoODF3ソフトウェア Ver8.11**は、C:\CTR\work\PFtoODF3\popla80.txtファイルが存在すると $\alpha$ 領域を1点外挿する機能が働きます。(0 $\rightarrow$ 75のデータを0 $\rightarrow$ 80に拡張する)

## 2. 入力データ

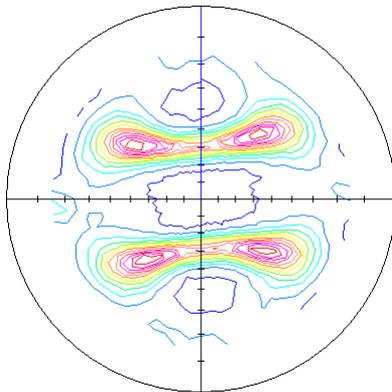
測定装置 リガク製RINT2200+多目的試料台

測定試料 Ti材

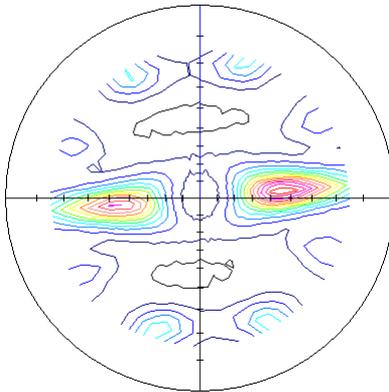
## 3. 測定極点図

Ti(100).raw	28 KB	生データ	2007/01/26 12:53
Ti(101).raw	28 KB	生データ	2007/01/26 14:22
Ti(002).raw	28 KB	生データ	2007/01/26 13:37

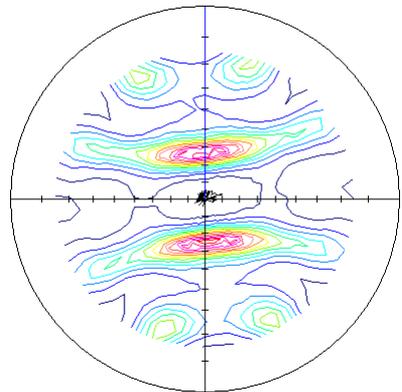
(100)



(002)

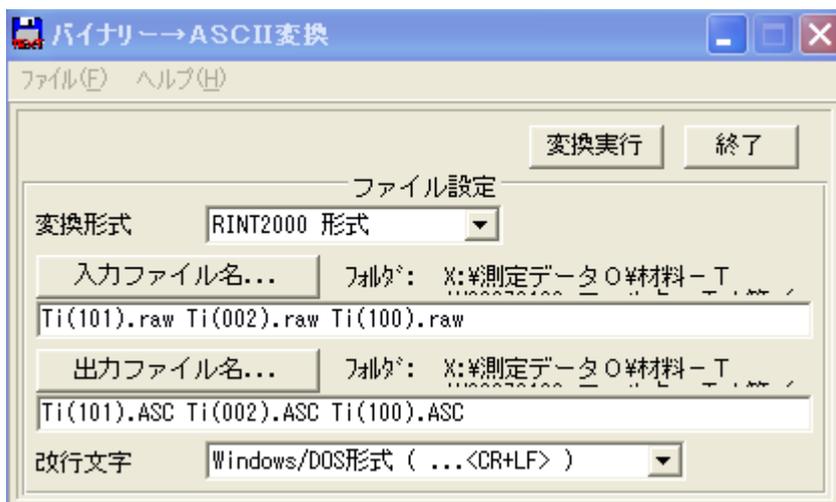


(101)



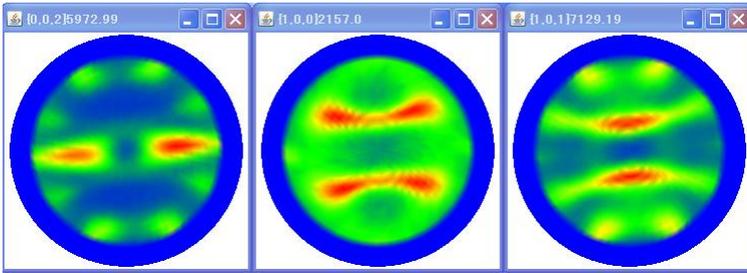
## 4. ASCデータに変換する。

バイナリデータ(raw)をテキストデータ(ASC)にRINT2000付属のバイナリ $\rightarrow$ ASCII変換



Ti(002).ASC	22 KB	RINT2000アスキー	2013/04/05 6:59
Ti(100).ASC	22 KB	RINT2000アスキー	2013/04/05 6:59
Ti(101).ASC	22 KB	RINT2000アスキー	2013/04/05 6:59

5. ODFPoleFigure2 ソフトウェア (CTR パッケージソフトウェア) で正極点データ処理

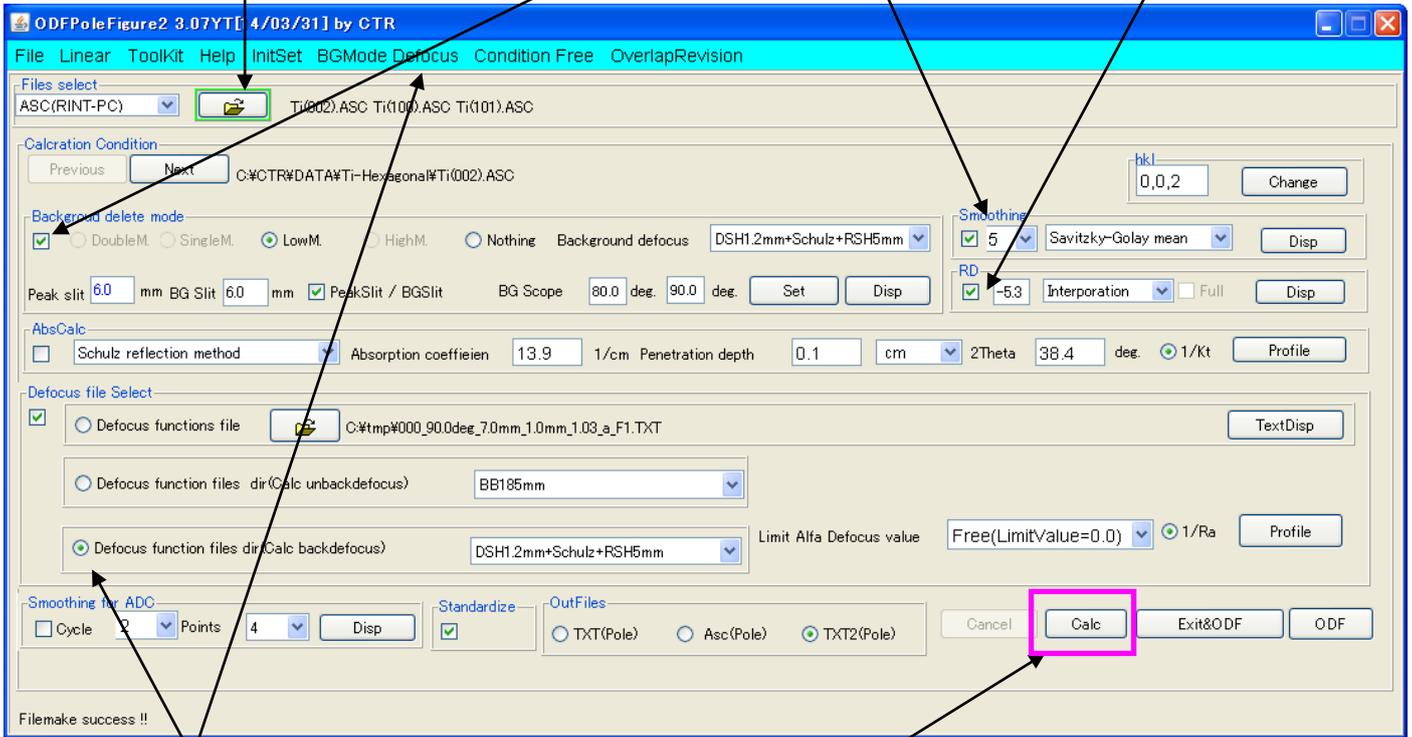


複数のファイルを選択

バックグラウンド補正

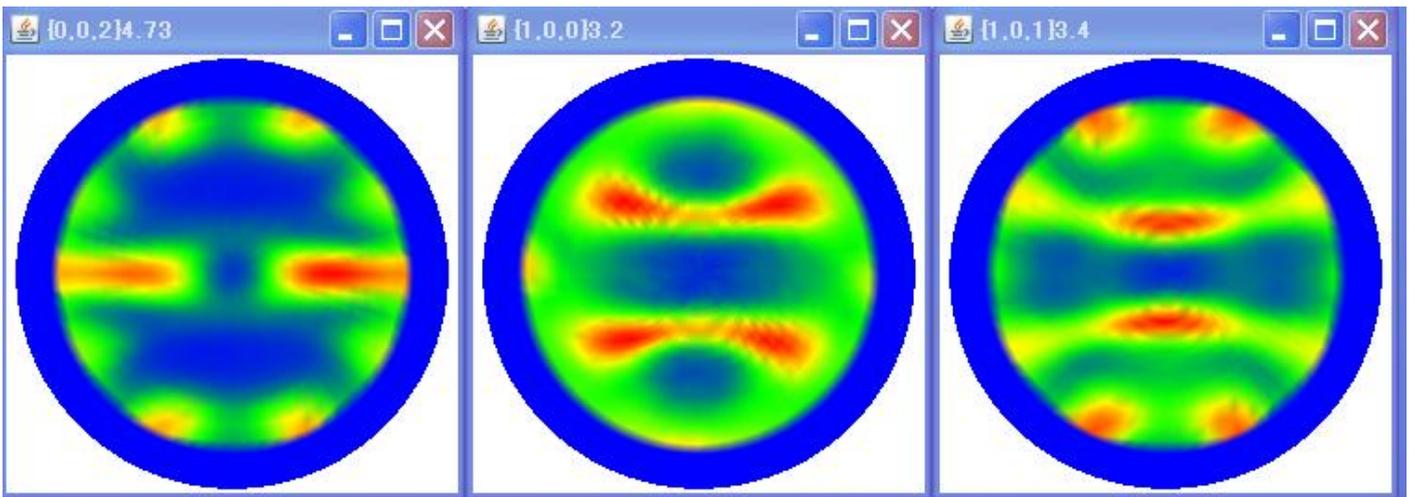
平滑化

RD 補正



Defocus (BG-defocus-mode) を指定

補正計算開始



計算結果ファイル (TXT2)

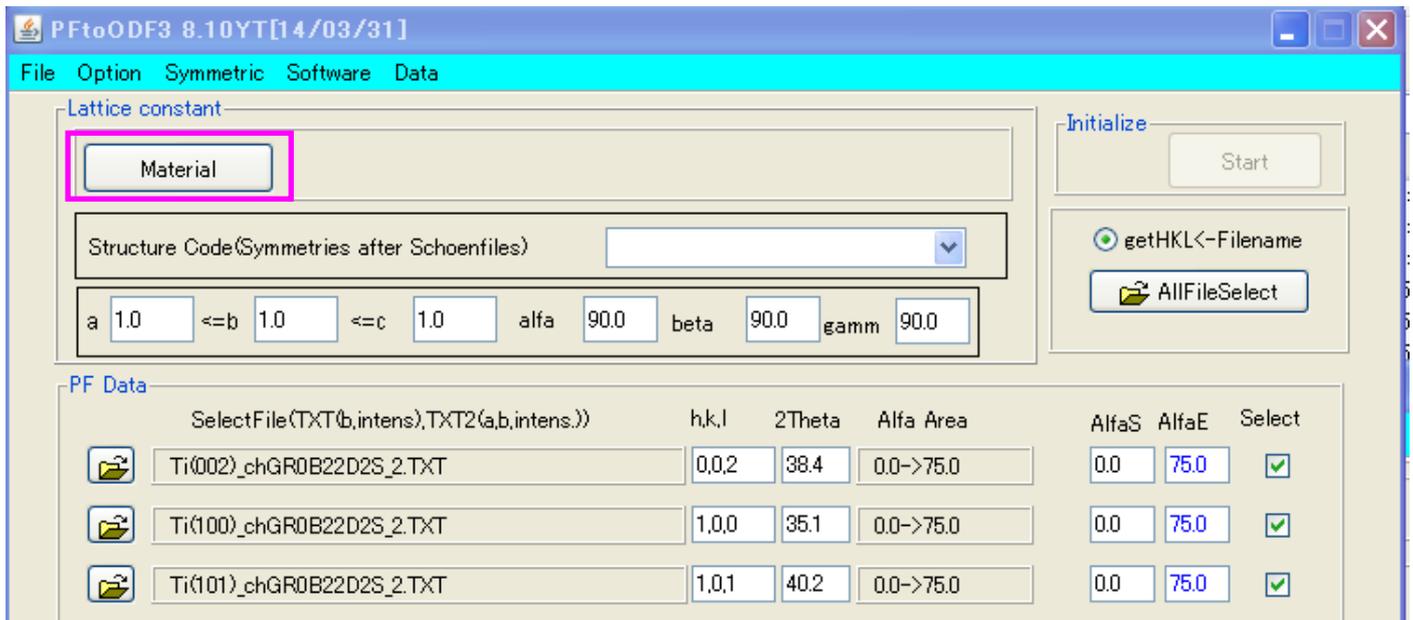
Ti(002)_chGR0B22D2S_2.TXT	22 KB	テキスト文書	2013/04/05 7:11
Ti(100)_chGR0B22D2S_2.TXT	22 KB	テキスト文書	2013/04/05 7:11
Ti(101)_chGR0B22D2S_2.TXT	22 KB	テキスト文書	2013/04/05 7:11

Calc で正極点処理が終了

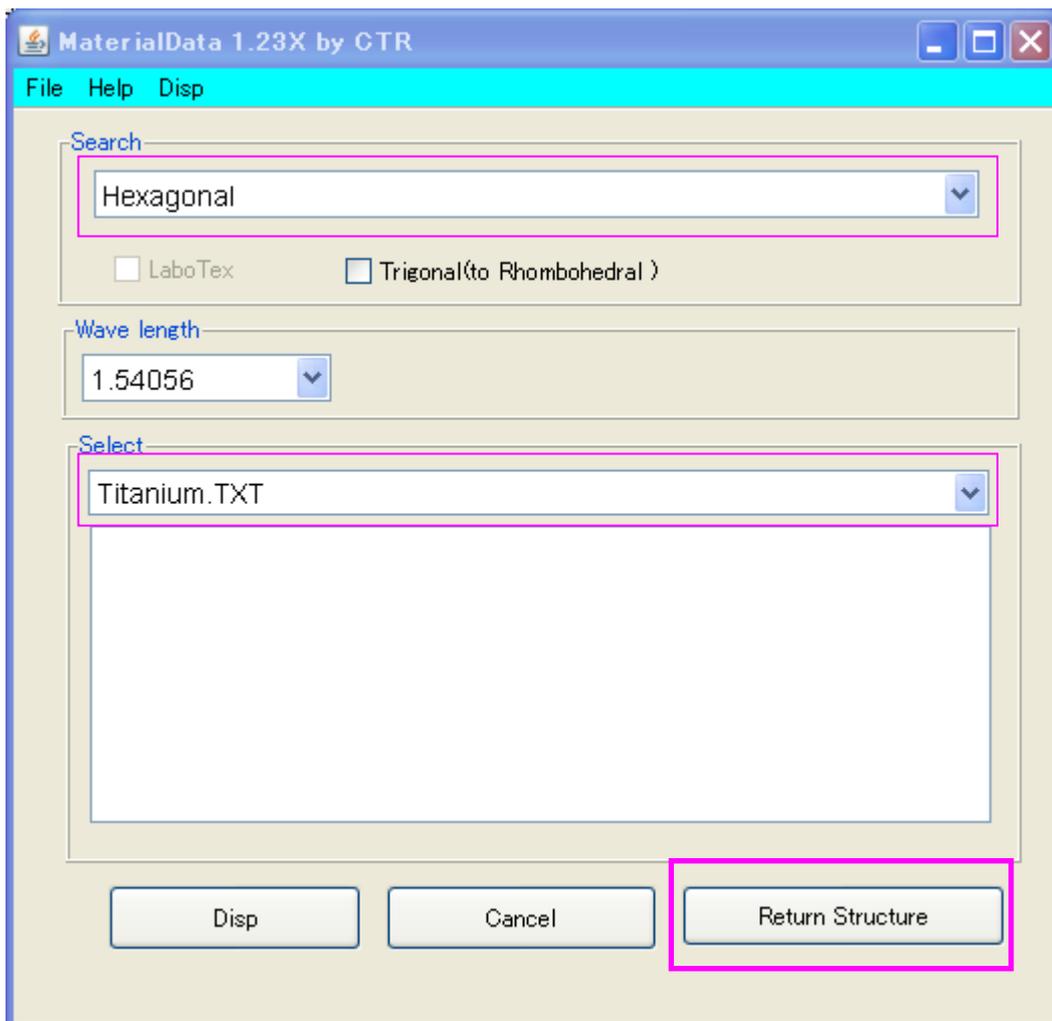
## 6. popLA入力ファイルの作成



ODFをマウスクリックする。

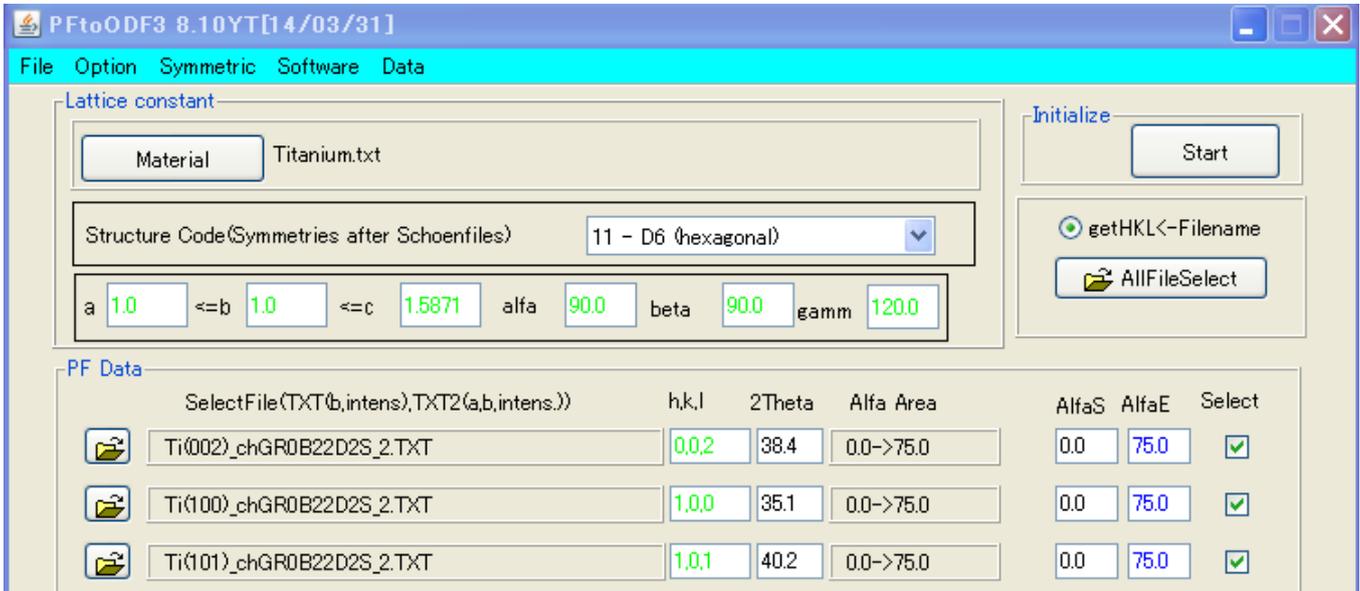


Material をマウスクリック

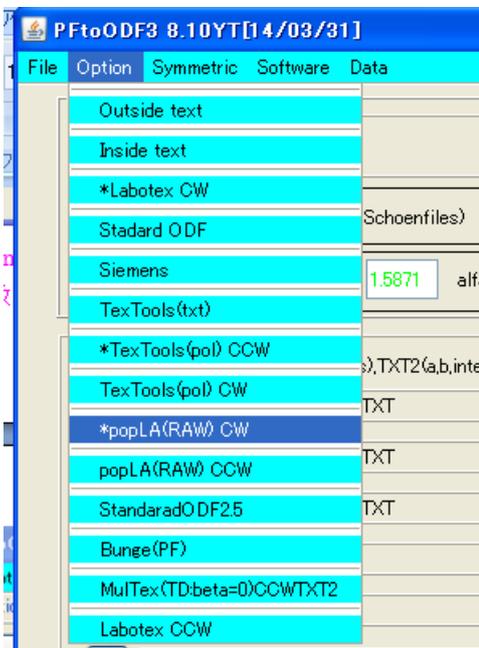


Hexagonal -> Titanium を選択して ReturnStructure をマウスクリック

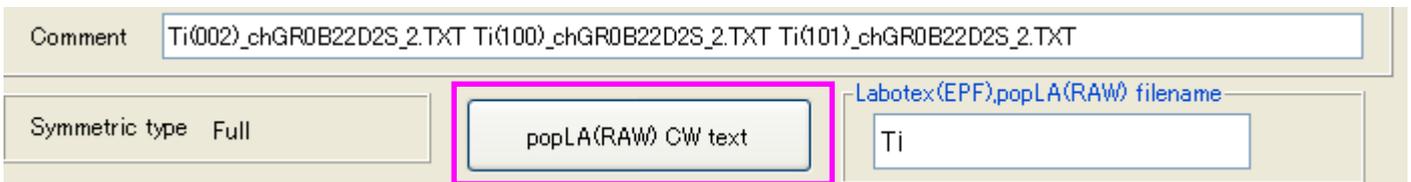
格子定数と軸比が表示され、極点図の指数チェックが行われる。



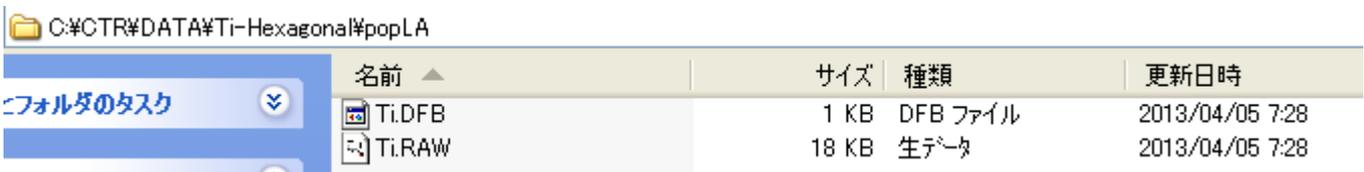
popLA-ODFを選択



ファイル名をTiとしてpopLA入力ファイルを作成



Ti(002)_chGR0B22D2S_2.TXT	22 KB	テキスト文書	2013/04/05 7:11
Ti(100)_chGR0B22D2S_2.TXT	22 KB	テキスト文書	2013/04/05 7:11
Ti(101)_chGR0B22D2S_2.TXT	22 KB	テキスト文書	2013/04/05 7:11
popLA		ファイル フォルダ	2013/04/05 7:28



popLA用入力データ作成完了

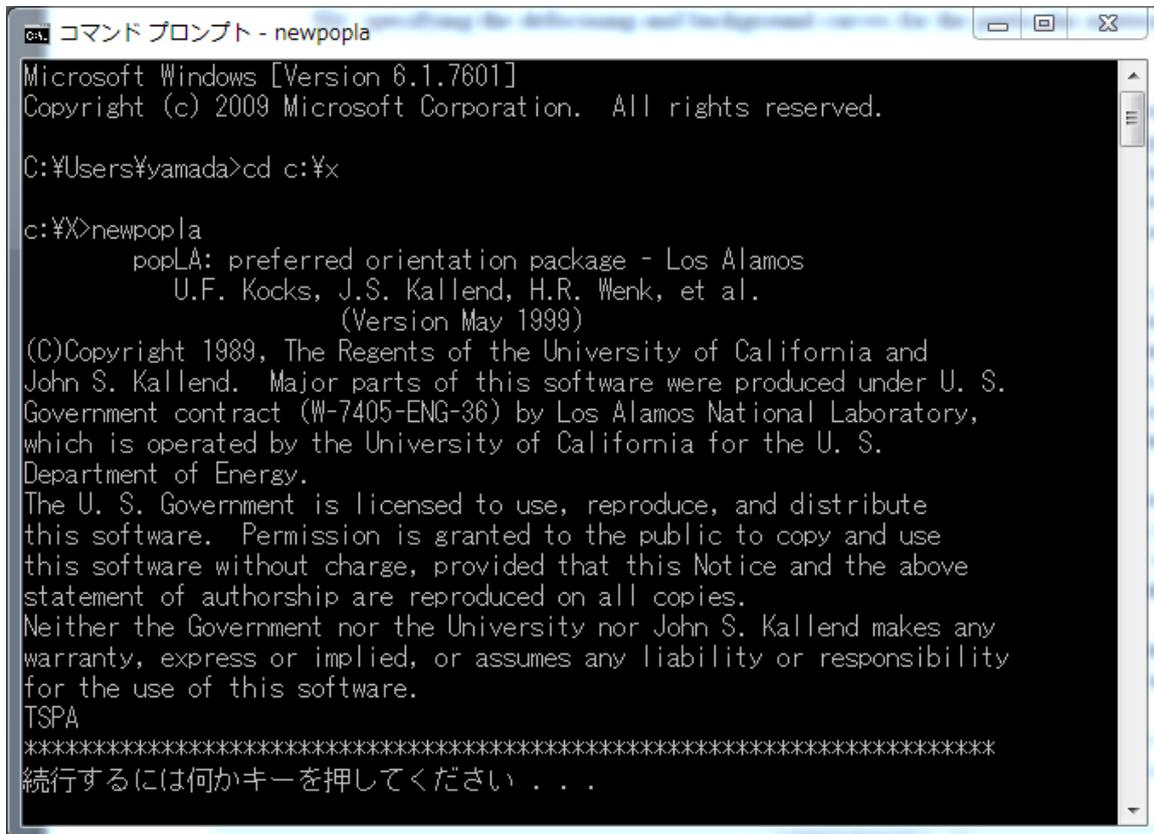
## 7. popLA解析

popLAはDosベースのソフトウェアであるため、Windows-7(32Bit)のDosモードを使う。

popLAはC:\¥Xにインストールされている。

解析を行うデータは、C:\¥XにCopyする。

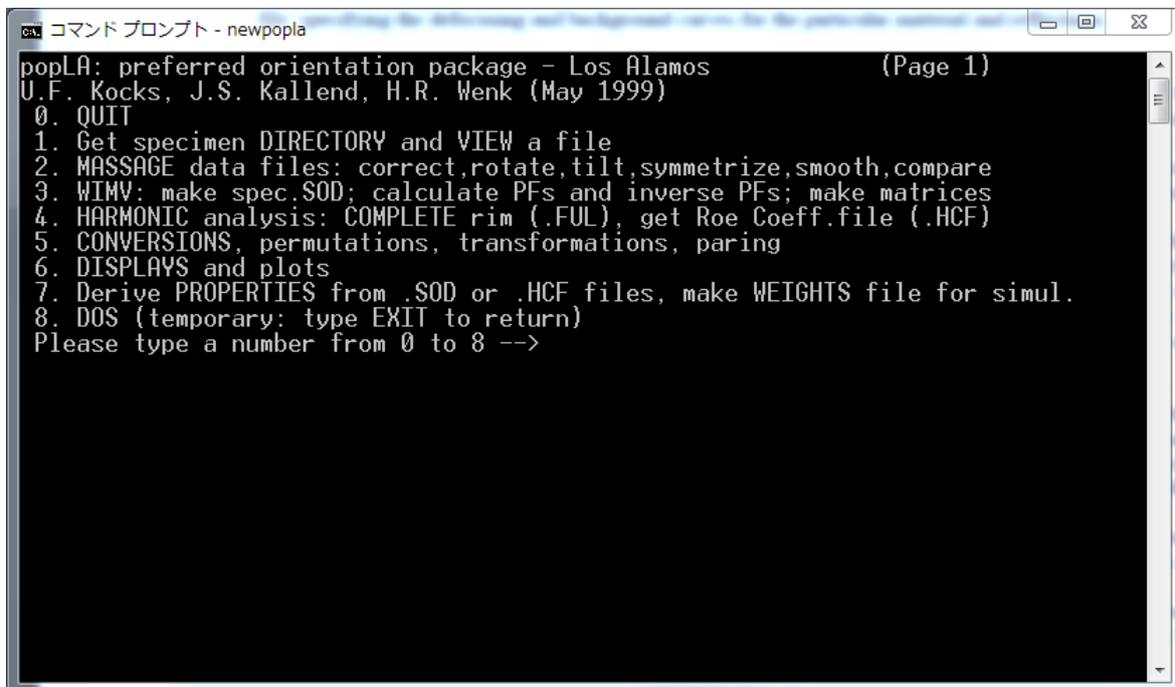
### 7. 1 popLAを立ち上げ



```
ca. コマンドプロンプト - newpopla
Microsoft Windows [Version 6.1.7601]
Copyright (c) 2009 Microsoft Corporation. All rights reserved.

C:\¥Users¥yamada>cd c:\¥x

c:\¥X>newpopla
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
warranty, express or implied, or assumes any liability or responsibility
for the use of this software.
TSPA
*****
続行するには何かキーを押してください . . .
```



```
ca. コマンドプロンプト - newpopla
popLA: preferred orientation package - Los Alamos                (Page 1)
U.F. Kocks, J.S. Kallend, H.R. Wenk (May 1999)
0. QUIT
1. Get specimen DIRECTORY and VIEW a file
2. MESSAGE 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 -->
```

### 7. 2 入力データをpopLA補正データに変換

popLAは極点図の中心 $\alpha = 0$ とした場合、 $0 \rightarrow 80$ の入力データを仮定している。

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

```
コマンドプロンプト - newpopla
MESSAGE DATA FILES (mostly PFs) (popLA page 2)
0. Quit
1. Return to Page 1
2. "Make THEORETICAL defocussing & background file: DFB (R. Bolmaro)"
3. DIGEST Raw Data (.RAW), with exper.or theor. .DFB: make .EPF
4. ROTATE PFs or adjust for grid offsets: make .RPF or .JWC
5. TILT PFs around right axis: make .TPF (T. Ozturk) [TO BE REPLACED]
6. SYMMETRIZE PFs: make .QPF or .SPF or .FPF
7. "EXPAND PFs back to full circle (needed for WIMV & harm.): .FPF"
8. SMOOTH PFs or ODs with Gaussian Filter (quad, semi, or full): make .MPF
9. Take DIFFERENCE between 2 files (PFs or ODs): make .DIF
Please type a number from 0 to 9 ==>
```

```
コマンドプロンプト - newpopla
???????? C ?????????????? ????????? Windows-7-32-D0 ???
????????????? ?????????????????? B4DF-7643 ???

c:\X ??????????????????

2009/10/28 03:48 17,674 DEMO.RAW
2013/04/05 07:28 17,499 Ti.RAW
2 ?????????????????? 35,173 ??????
0 ????????????????????? 81,143,500,800 ??????????????????
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)
???????????????????????????????????????????????????????? . . .
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) Ti
```

T i を指定

```
Enter name of raw data file (ext .RAW assumed) Ti
Enter name of correction file (ext .DFB assumed)Ti
```

```

コマンドプロンプト - newpopla

Ti Ti(002)_chGR0B22D2S_2.TXT Ti(100)_chGR
(hkl)=(100) Background= 1 Using correction curve 2
...correcting raw data
...extrapolating outer ring

DATA FAKED beyond .0 degrees
...normalizing. ring(j),ibgx(j)= 0.000000E+00 0
Normalization factor= .641
...writing corrected data to Ti .EPF

Ti Ti(002)_chGR0B22D2S_2.TXT Ti(100)_chGR
(hkl)=(101) Background= 1 Using correction curve 3
...correcting raw data
...extrapolating outer ring

DATA FAKED beyond .0 degrees
...normalizing. ring(j),ibgx(j)= 0.000000E+00 0
Normalization factor= .421
...writing corrected data to Ti .EPF
Stop - Program terminated.

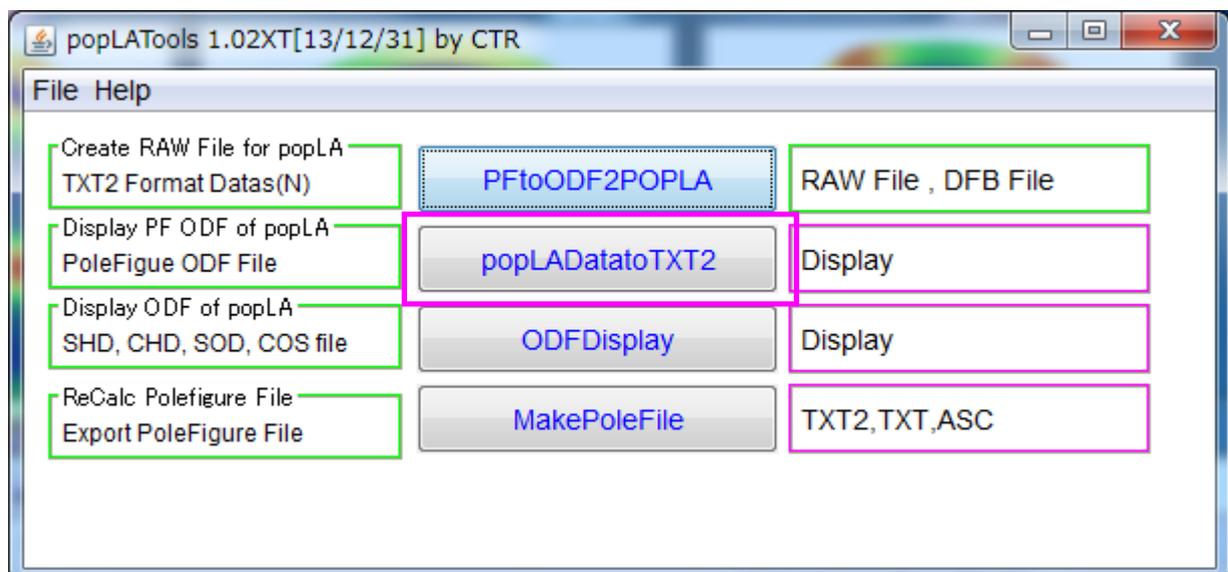
続行するには何かキーを押してください . . .

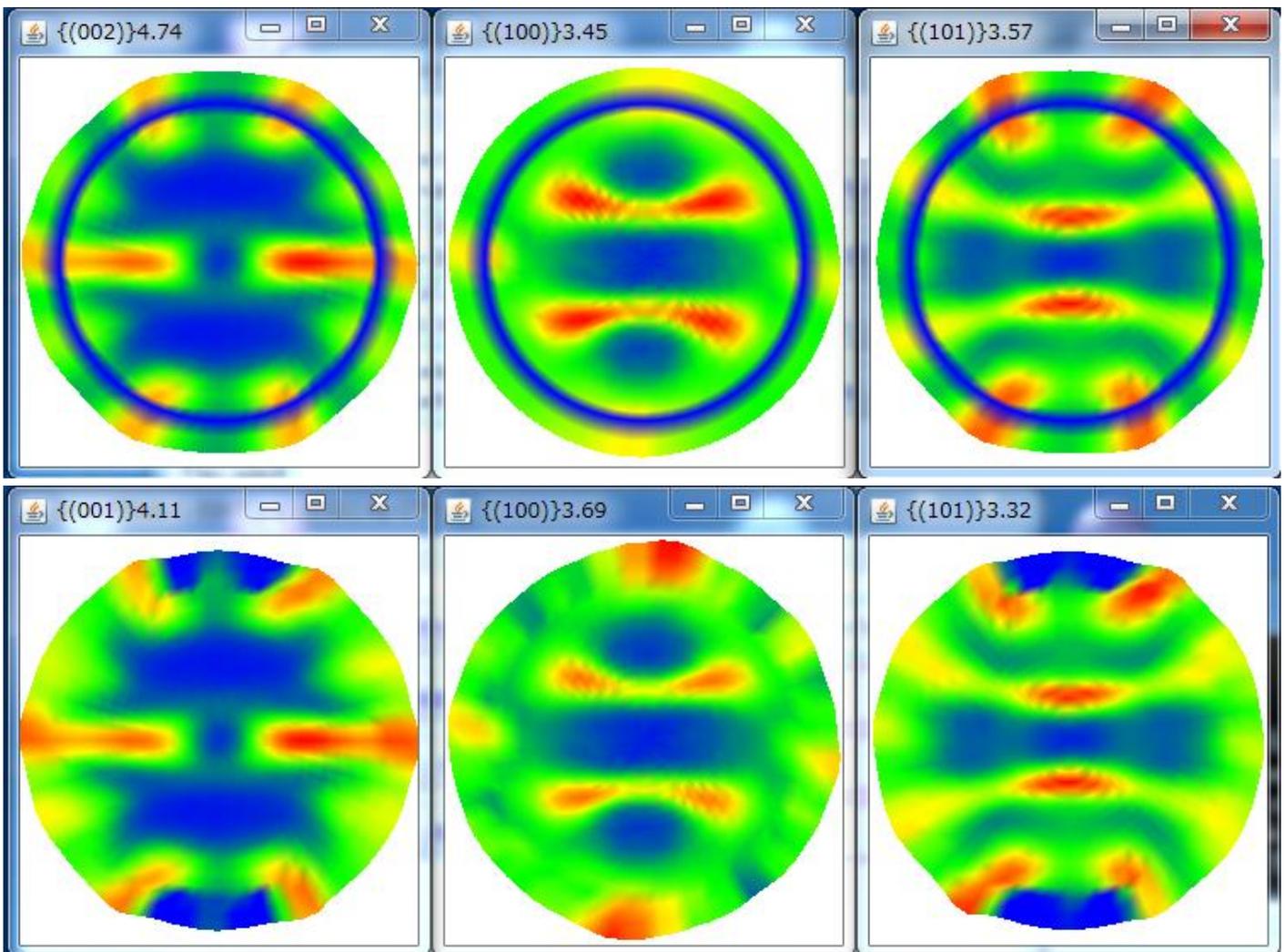
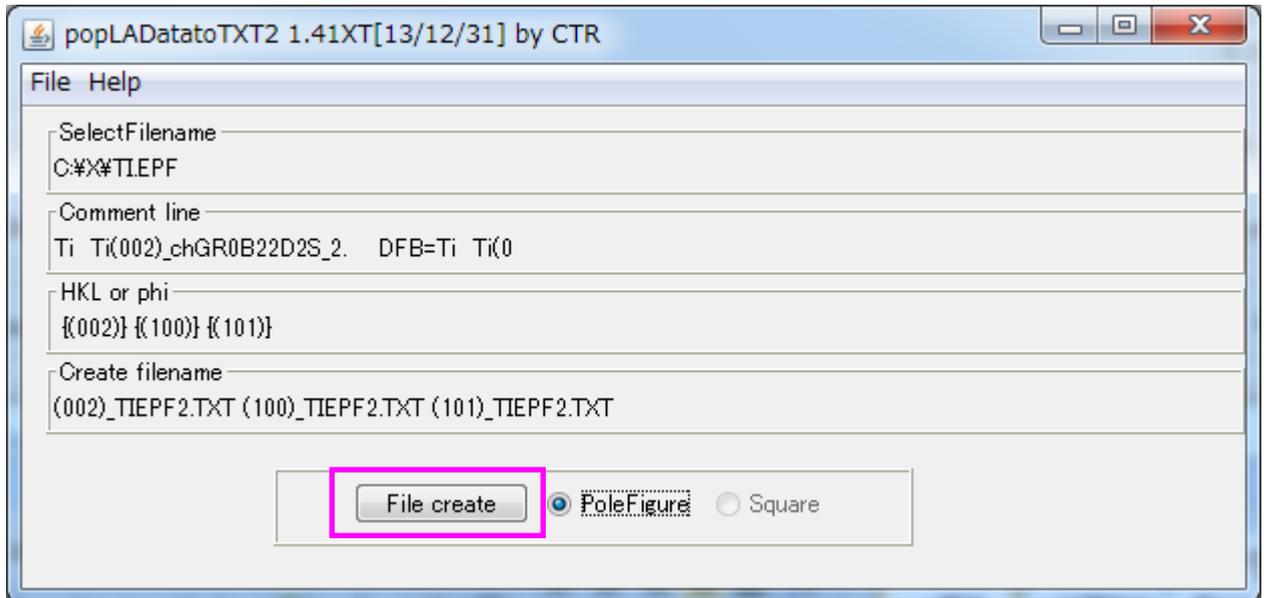
```

T I . E P Fファイルが作成される。

TI	2013/04/05 8:35	Exchange Certifi...	18 KB
TFDEFOCS.DAT	2013/04/05 8:22	DAT ファイル	0 KB
Ti.DFB	2013/04/05 7:28	DFB ファイル	1 KB
Ti.RAW	2013/04/05 7:28	RAW ファイル	18 KB

T i . E P Fファイルを表示 ( p o p L A T o o l s の popLADATatoTXT2 ソフトウェア)





上段：0 → 75 のデータから 80 → 90 のデータが Create されている。

下段：80 のデータを外挿した場合、

本来、defocus 補正を行う処理が含まれているが、既に、ODFPoleFigure2 ソフトウェアで処理しているので、defocus 補正データはすべて 1.0 として処理を行った。

### 7. 3 WIMV法の準備

```
コマンドプロンプト - newpopla
popLA: preferred orientation package - Los Alamos (Page 1)
U.F. Kocks, J.S. Kallend, H.R. Wenk (May 1999)
0. QUIT
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 -->
```

### 7. 4 六方晶、Tiのパラメータファイル (WIM) の作成

一度作成すれば、後からTi解析時に使用可能

```
コマンドプロンプト - newpopla
WIMV Analysis (popLA page 3)
0. Quit
1. Return to Page 1
WIMV: make .SOD and recal. pole figures .WPF -- for:
2. cubic, tetra-, hexagonal crystals; sample diad: up to 3 PFs, 13 poles
3. trigonal cry., gen'l. sample sym., or higher: up to 7 PFs, 25 poles
4. orthorhombic crystals; gen'l. sample sym.: up to 7 PFs, 25 poles
Recalculate POLE FIGURES (even non-measured ones): make .APF -
5. using .WIM matrix for the desired PFs (up to 3, 13 poles)
6. using .BWM or .WM3 matrix for the desired PFs (up to 7, 25 poles)
7. Calculate INVERSE pole figures from .SOD: .WIP
   (So far assumes tetragonal crystal symmetry)
8. Make WIMV pointer matrix for new crystal structure and set of PFs
9. Make WIMV pointer matrix for any INVERSE pole figures: make .WMI
Please type a number from 0 to 9 -->
```

```
コマンドプロンプト - newpopla
2. up to 3 PFs, 13 poles, tetrag. crystal sym., sample diad: make .WIM
3. up to 7 PFs, 25 poles, trig. crystal symmetry: make .BWM
4. for orthorhombic version: make .WM3 (7/25/ortho/triclinic)
Please type 2, 3, or 4 -->
```

```
コマンドプロンプト - newpopla
Generate WIMV matrix
Please enter a NAME for this matrix (8 CHARS MAX) TI
Enter crystal system code
3. CUBIC
4. TETRAGONAL
6. HEXAGONAL
==> 6

Please enter C/A for this material: 1.5871
How many pole figures (max=3)? 3

Please enter 3 set(s) POLE FIGURE INDICES
[3 index only, i.e. h k l from (h k * l) ]
[use lowest form, e.g. 0 0 1 , NOT 0 0 2 ]

1 0 0
0 0 1
1 0 1

..Locating the poles
..Total multiplicity 10

..Making the matrix
..Correcting for pole distribution

Output to TI .WIM
```

 TI.WIM	2013/04/05 9:42	WIM ファイル	5 KB
 TI	2013/04/05 8:35	Exchange Certifi...	18 KB
 TFDEFOCS.DAT	2013/04/05 8:22	DAT ファイル	0 KB
 Ti.DFB	2013/04/05 7:28	DFB ファイル	1 KB
 Ti.RAW	2013/04/05 7:28	RAW ファイル	18 KB

7. 5 WIMV法解析

```

コマンドプロンプト - newpopla
WIMV Analysis (popLA page 3)
0. Quit
1. Return to Page 1
WIMV: make .SOD and recalc. pole figures .WPF -- for:
2. cubic, tetra-,hexagonal crystals; sample diad: up to 3 PFs, 13 poles
3. trigonal cry.,gen'l.sample sym.,or higher: up to 7 PFs, 25 poles
4. orthorhombic crystals; gen'l.sample sym.: up to 7 PFs, 25 poles
Recalculate POLE FIGURES (even non-measured ones): make .APF -
5. using .WIM matrix for the desired PFs (up to 3, 13 poles)
6. using .BWM or .WM3 matrix for the desired PFs (up to 7, 25 poles)
7. Calculate INVERSE pole figures from .SOD: .WIP
   (So far assumes tetragonal crystal symmetry)
8. Make WIMV pointer matrix for new crystal structure and set of PFs
9. Make WIMV pointer matrix for any INVERSE pole figures: make .WMI
Please type a number from 0 to 9 -->

```

```

ODF ANALYSIS - WIMV ALGORITHM
COPYRIGHT (C) 1987,1988 JOHN S. KALLEND

*** Version September 1993 ***

Enter the name of the wimv matrix (? .WIM)
[Default is CUBIC] ==> TI
Name of data file (default extension .epf): TI

Sample Symmetry is:

0. Orthorhombic
1. Diad on Z

Enter 0 or 1 ==> 0

Ti Ti(002)_chGR0B22D2S_2.
002 5.0 75.0 5.0360.0 1 1 2-1 3 100 0
100 5.0 75.0 5.0360.0 1 1 2-1 3 100 0
101 5.0 75.0 5.0360.0 1 1 2-1 3 100 0
The minimum pole figure intensity is .10
Do you wish to raise the Fon? N

```

```

Continue? Y
Iteration 59 in progress
Texture Strength (m.r.d.): 2.7
Iteration 59 estimated OD error (%) = 1.4
Continue? Y

```

Continue? Nで打ち切る

```

Continue? Y
Iteration 59 in progress
Texture Strength (m.r.d.): 2.7
Iteration 59 estimated OD error (%) = 1.4

Continue? n

Normalization factor: 1.04

In output file, angles increase from 0 in nomenclature of
1. Kocks (need this one for WEIGHTS)
2. Roe/Matthies
3. Bunge (rotates plot +90 deg.)

Enter 1,2, or 3 ==> 3
Making file TI .SOD
Recalculated PF file name: TI .WPF
続行するには何かキーを押してください . . .

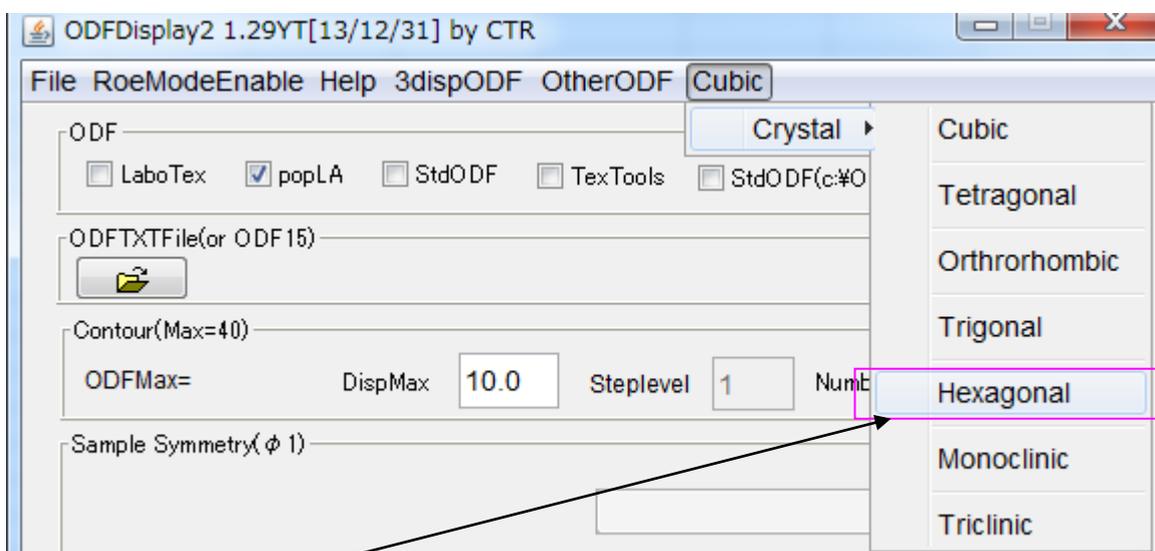
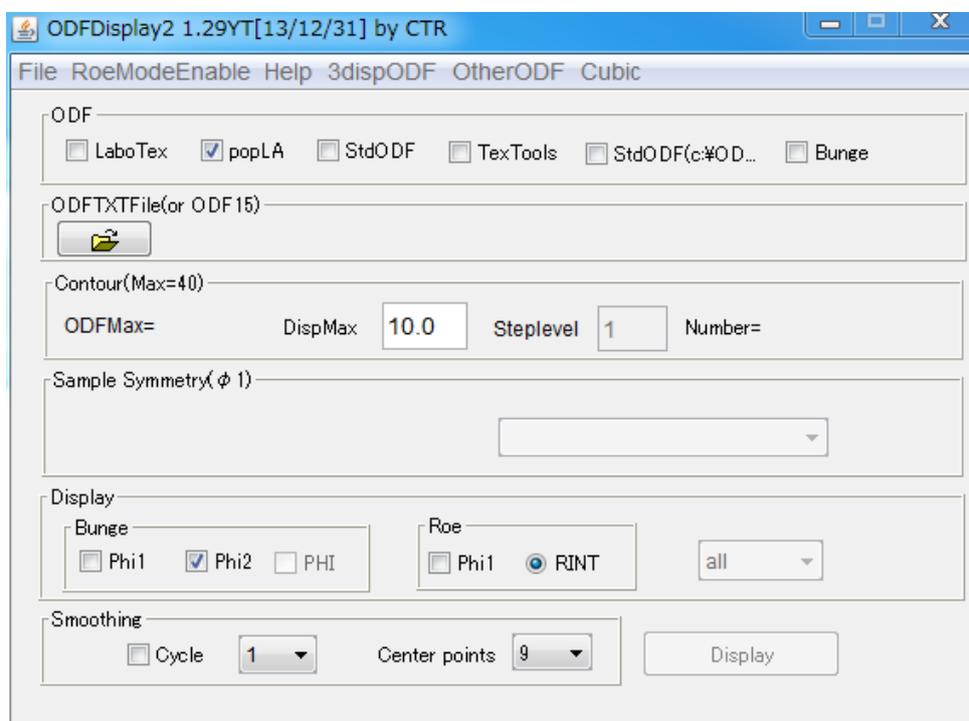
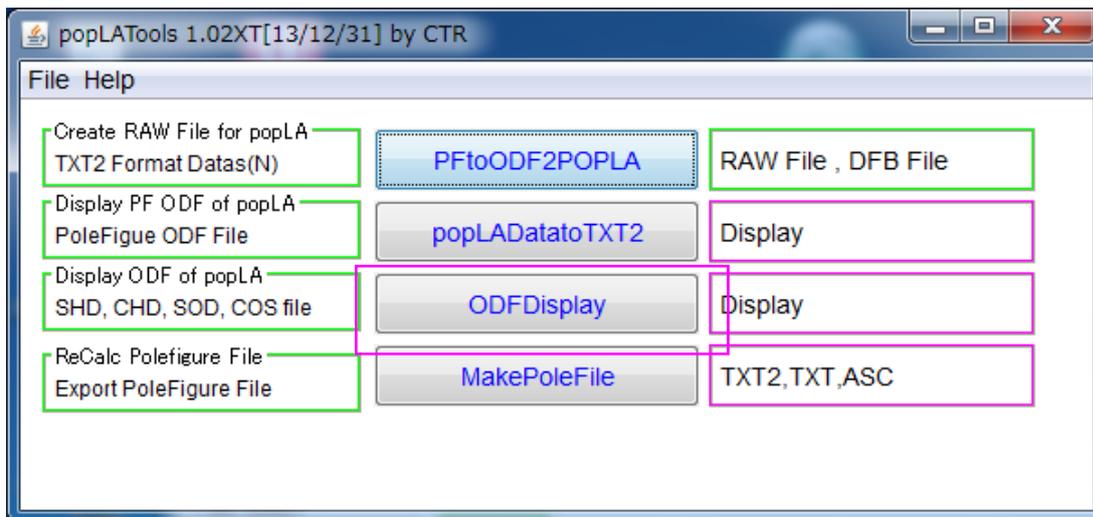
```

<b>.SOD</b>	“Sample Orientation Distribution” – Distribution of sample orientations with respect to crystal axes.
<b>.WPF</b>	“WIMV Pole Figure” – Pole figure recalculated from WIMV-derived orientation distribution.

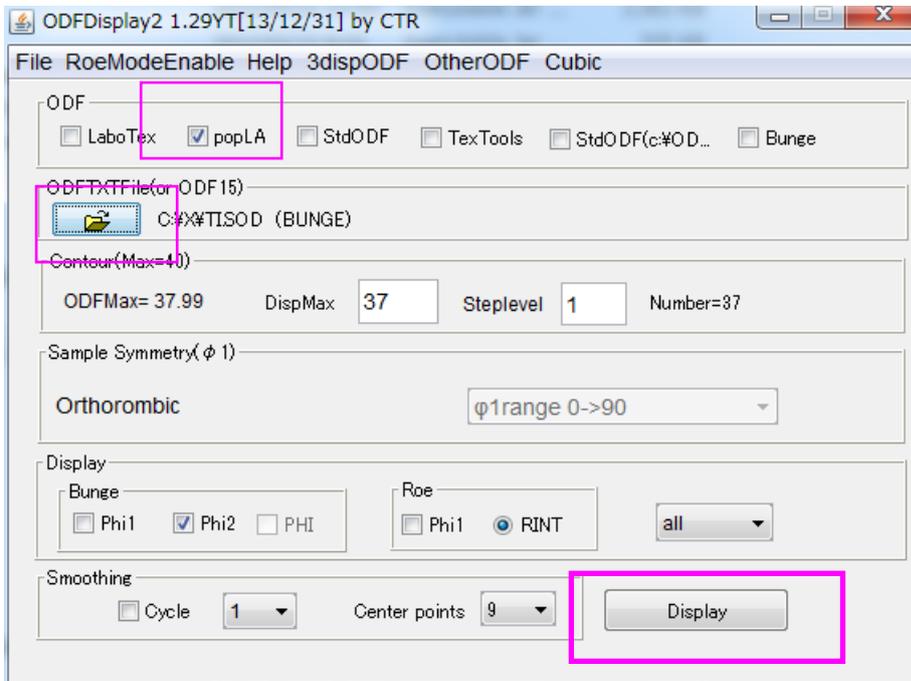
ODF 計算と再計算極点図が計算されている。

TI.SOD	2013/04/05 9:54	SOD ファイル	33 KB
TI.WPF	2013/04/05 9:54	WPF ファイル	5 KB
TI.WIM	2013/04/05 9:42	WIM ファイル	5 KB
TI	2013/04/05 8:35	Exchange Certifi...	18 KB
TFDEFOCS.DAT	2013/04/05 8:22	DAT ファイル	0 KB
Ti.DFB	2013/04/05 7:28	DFB ファイル	1 KB
Ti.RAW	2013/04/05 7:28	RAW ファイル	18 KB

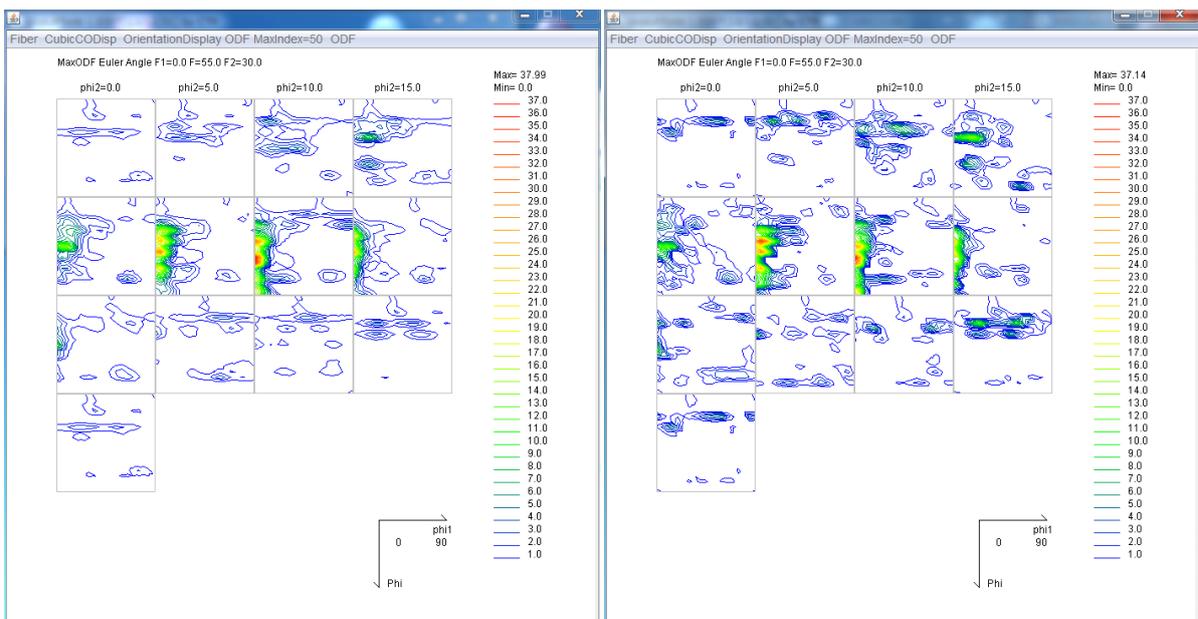
7. 6 ODF図の表示 ODFDisplay2 ソフトウェア (CTR パッケージ)



Hexagonal;を指定



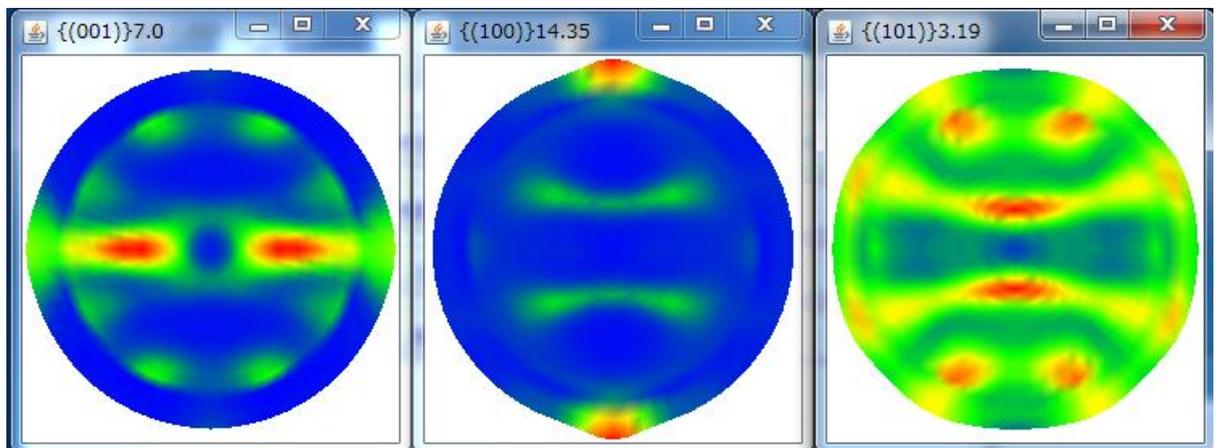
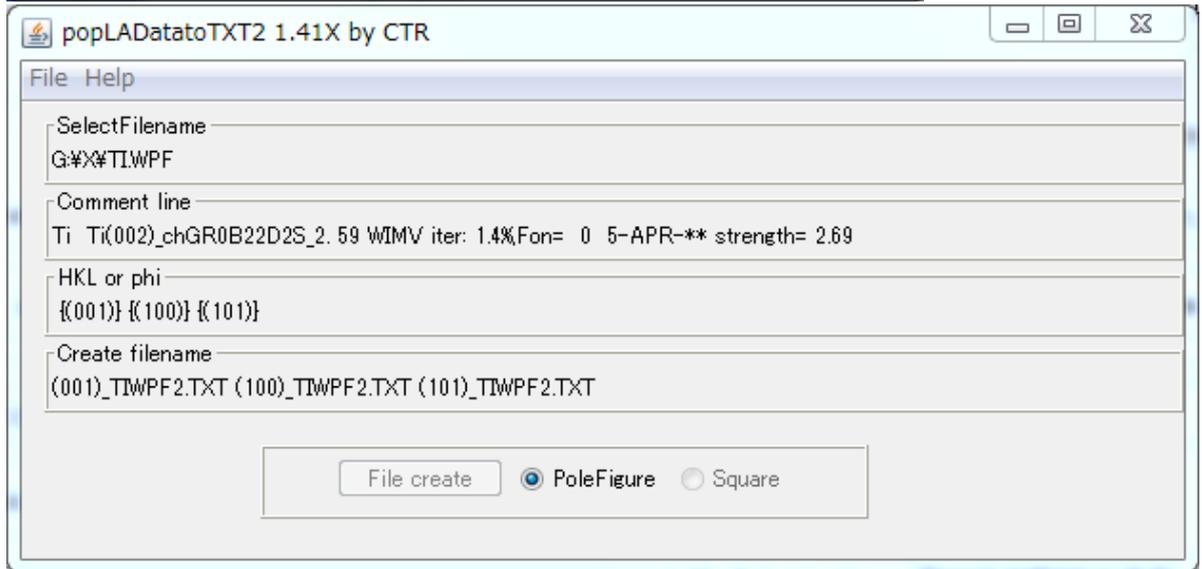
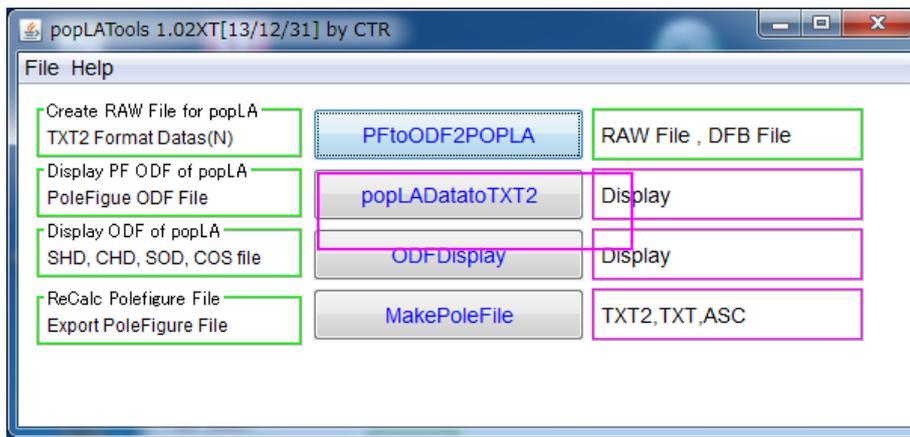
popLA で、Ti.SOD を選択で、ODFMax=37.99 を示す。Disp で ODF 図が表示



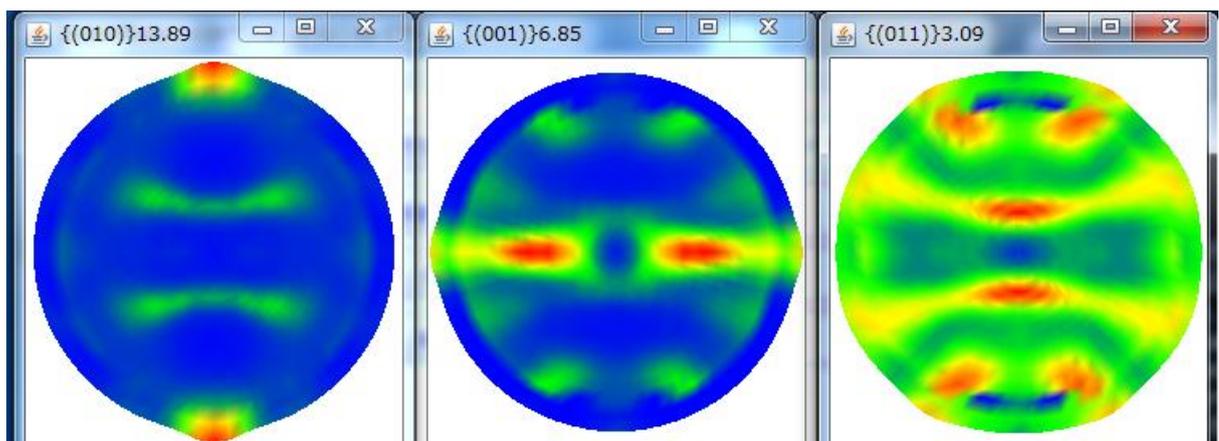
$\alpha=80$  データを外挿した場合

ODF 結晶方位密度の最大値は、 $\phi 1 = 0$ 、 $\Phi = 55$ 、 $\phi 2 = 30$  と表示

7. 7 再計算極点図の表示



$\alpha = 80$  を外挿した場合



## 7. 8 Harmonic解析

```
コマンドプロンプト - newpopla
popLA: preferred orientation package - Los Alamos (Page 1)
U.F. Kocks, J.S. Kallend, H.R. Wenk (May 1999)
0. QUIT
1. Get specimen DIRECTORY and VIEW a file
2. MESSAGE data files: correct,rotate,tilt,symmetrize,smooth,compare
3. WTMV: 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 -->
```

### 7. 9 六方晶の指定、展開係数の計算

```
コマンドプロンプト - newpopla
HARMONIC ANALYSIS (popLA page 4)
0. Quit
1. Return to Page 1
Find harmonic coefficients .HCF, 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 .HIP
7. List harmonic coefficients to screen or printer
Note: To convert Aachen-format Bunge coeffs. to Kallend's binary
Roe coeff.file .HCF: use AC2Wlmn (outside this menu) -
Also need FAKTOR.CtW (J. Hirsch)
8. Establish coefficients for a given TRANSFORMATION
9. Apply TRANSFORMATION to given coefficients
Please type a number from 0 to 9 -->
```

入力ファイルの指定

```
コマンドプロンプト - newpopla
Pole figure analysis to find Wlmn, non cubic
Harmonic method.
Program (C) John Kallend 1971,1982
Enter the data file name [default .EPF]: Ti
```

パラメータ指定

```
コマンドプロンプト - newpopla
ODF Analysis for Ti
Enter CRYSTAL SYSTEM code
2=ORTHORHOMBIC,4=TETRAGONAL,6=HEXAGONAL

Enter 2, 4, or 6 ==> 6

Enter C/A ratio ==> 1.5871

Please enter sample symmetry:
0. Orthorhombic
1. Mirror perpendicular to Z (monoclinic)

Enter 0 or 1 ==> 0

Error analysis output to:
1. Printer
2. Screen

Enter 1 or 2 ==> 2
```

結果が表示される。

```
コマンドプロンプト - newpopla
100 Reflection. Truncation error = .17 NORMLN 1.002
101 Reflection. Truncation error = .16 NORMLN 1.012
Insufficient data for least squares fit at 12th order
Severity = 1.97. Generated to L = 16

EXPERIMENTAL ERRORS: 1. Polefigures
  L      MEAN      002      100      101
  0      .76E-08    .93E-08    .18E-08    .11E-07
  2      .98E-02    .76E-02    .14E-01    .87E-02
  4      .54E-02    .31E-02    .80E-02    .43E-02
  6      .20E-02    .14E-02    .13E-02    .31E-02
  8      .37E-02    .74E-03    .47E-02    .45E-02
  10     .19E-02    .73E-03    .15E-02    .29E-02
  12     .49E-09    .24E-09    .78E-09    .26E-09
  14     .13E-09    .12E-09    .15E-09    .15E-09
  16     .23E-09    .19E-09    .20E-09    .31E-09
  ALL    .22E+00    .14E+00    .30E+00    .23E+00

2. Estimated exptl. error in ODF = .5

RE-ESTIMATING MISSING PARTS OF POLEFIGURES

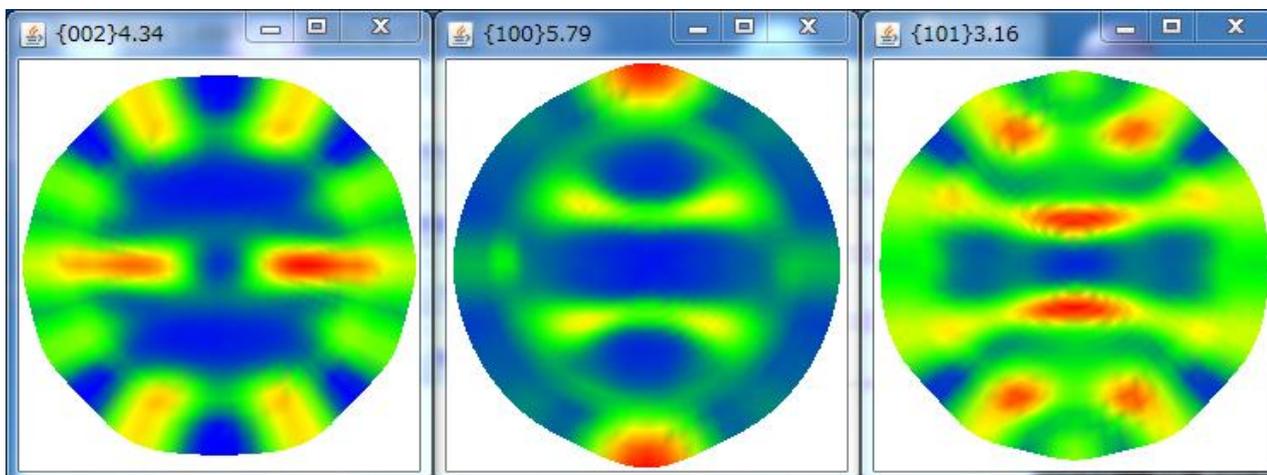
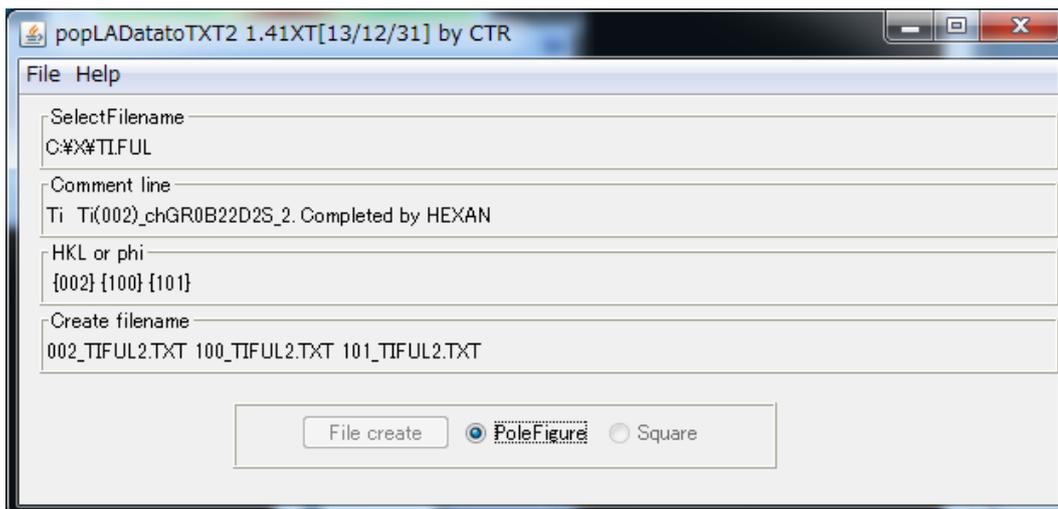
Print out Wlmn ? N
Completed polefigures to Ti .FUL
続行するには何かキーを押してください . . .
```

計算された極点図

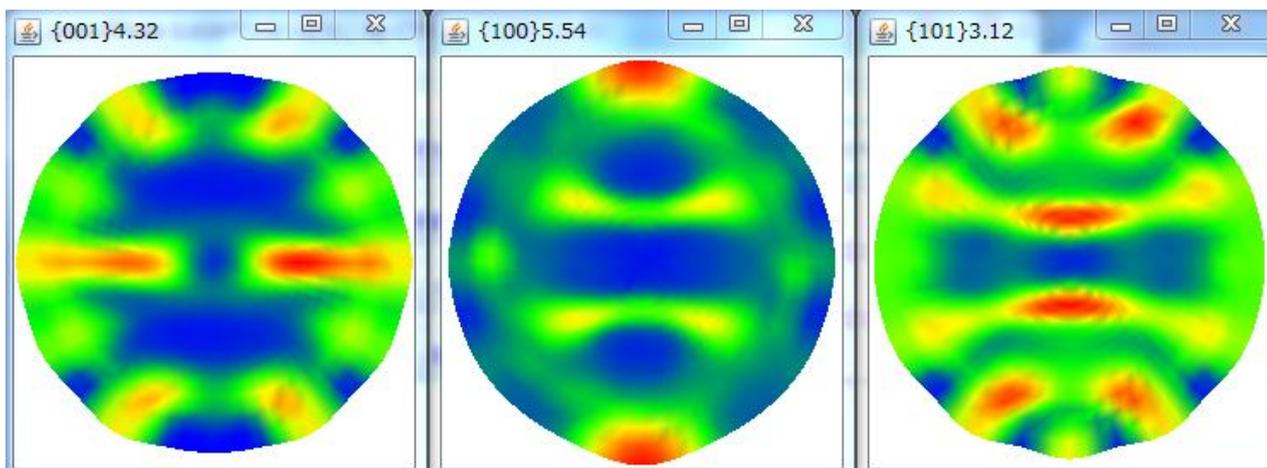
 TI.FUL	2013/04/05 14:36	FUL ファイル	17 KB
 TI.HCF	2013/04/05 14:36	HCF ファイル	1 KB

.FUL	“Full Pole Figure” – Complete pole figure, with high angle intensities, as determined by harmonic analysis; renormalized.
.HCF	“Harmonic Coefficients File” – A list of coefficient for the harmonic series expansion of the Orientation Distribution Function (ODF) according to Roe. Not a density file for plotting.

表示



$\alpha = 80$  を外挿した場合



## 7. 10 Harmonic法によるODF図の計算

```
コマンドプロンプト - newpopla
HARMONIC ANALYSIS (popLA page 4)
0. Quit
1. Return to Page 1
Find harmonic coefficients .HCF, 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 .HIP
7. List harmonic coefficients to screen or printer
Note: To convert Aachen-format Bunge coeffs. to Kallend's binary
      Roe coeff.file .HCF: use AC2Wlmn (outside this menu) -
      Also need FAKTOR.CtW (J. Hirsch)
8. Establish coefficients for a given TRANSFORMATION
9. Apply TRANSFORMATION to given coefficients

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

```
Calculate ODF from Harmonic Coefficients
Program by John Kallend (c) 1968 - 1988

What is the specimen name (.HCF Assumed)? Ti
ENTER OUTPUT FORMAT REQUIRED
1. COD sections every 10 degrees, ROE angles only
2. SOD or COD every 5 degrees

==> 2
```

```
Average values of Wlmn for different orders of l

      1      Avg. Wlmn
      2      .28E-02
      4      .26E-02
      6      .30E-02
      8      .21E-02
     10      .86E-03
     12      .17E-02
     14      .34E-03
     16      .14E-02

Default = CALCULATE TO L = 16, OK ? Y
```

```
CALCULATIONS FINISHED
MAX. VALUE = 9.78 MIN. VALUE = -5.71

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
```

```

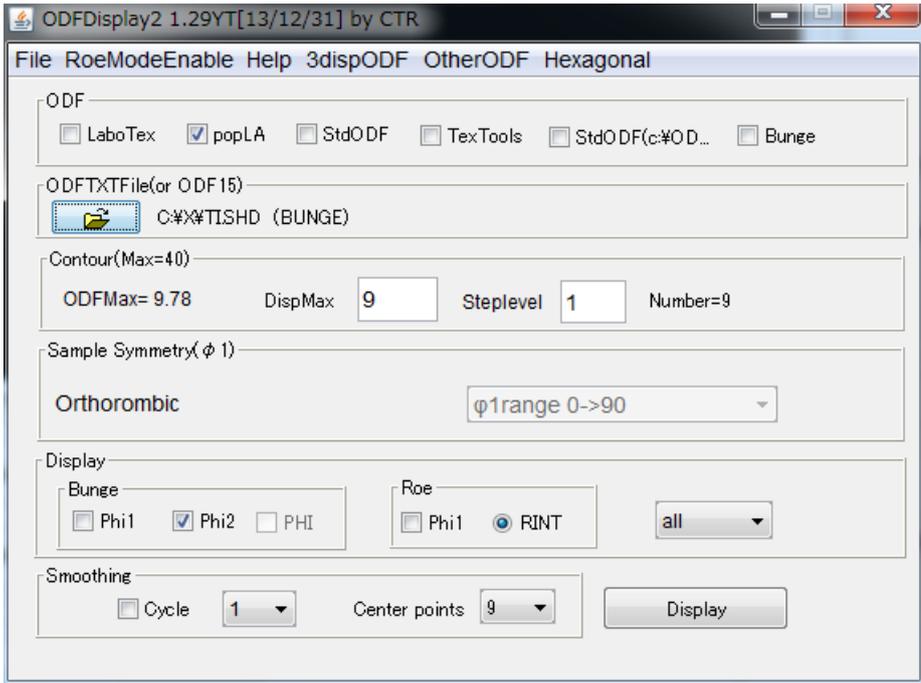
Enter 1,2, or 3 ==> 3
Making file Ti .SHD
続行するには何かキーを押してください . . .

```

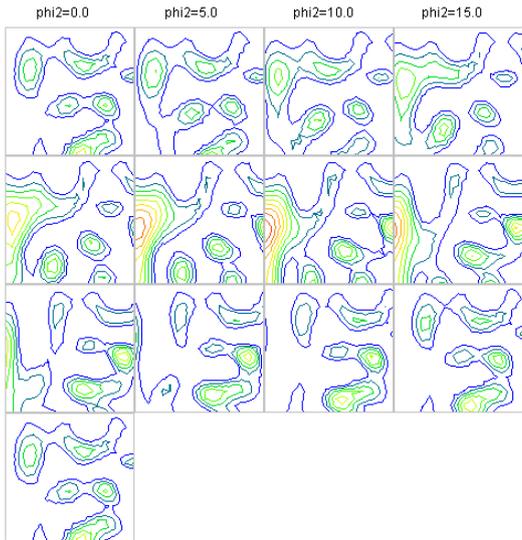
TI.SHD	2013/04/05 14:52	SHD ファイル	32 KB
TI.FUL	2013/04/05 14:36	FUL ファイル	17 KB
TI.HCF	2013/04/05 14:36	HCF ファイル	1 KB

.SHD	Projection along y of .SHD. .SOD derived from harmonic analysis.
------	---------------------------------------------------------------------

7. 1 1 ODFDisplay2 ソフトウェアでODF図の表示

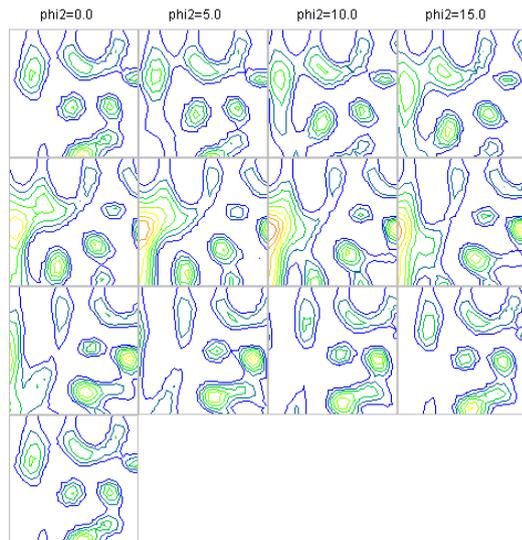


MaxODF Euler Angle F1=0.0 F=55.0 F2=30.0

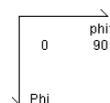
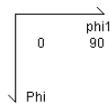


Max= 9.77  
Min= 0.0  
9.0  
8.0  
7.0  
6.0  
5.0  
4.0  
3.0  
2.0  
1.0

MaxODF Euler Angle F1=0.0 F=50.0 F2=30.0



Max= 10.07  
Min= 0.0  
10.0  
9.0  
8.0  
7.0  
6.0  
5.0  
4.0  
3.0  
2.0  
1.0



$\alpha = 80$  を外挿した場合

7. 1 2 再計算極点図

```

コマンド プロンプト - newpopla
HARMONIC ANALYSIS (popLA page 4)
0. Quit
1. Return to Page 1
Find harmonic coefficients .HCF, 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 .HIP
7. List harmonic coefficients to screen or printer
Note: To convert Aachen-format Bunge coeffs. to Kallend's binary
      Roe coeff.file .HCF: use AC2Wlmn (outside this menu) -
      Also need FAKTOR.CtW (J. Hirsch)
8. Establish coefficients for a given TRANSFORMATION
9. Apply TRANSFORMATION to given coefficients

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

```

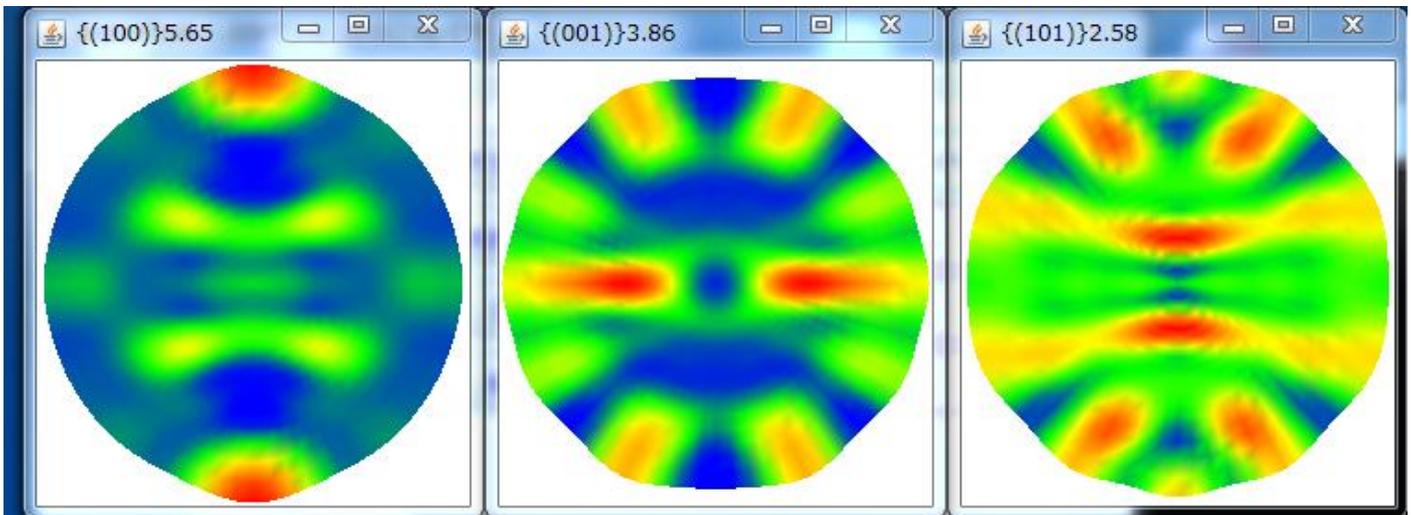
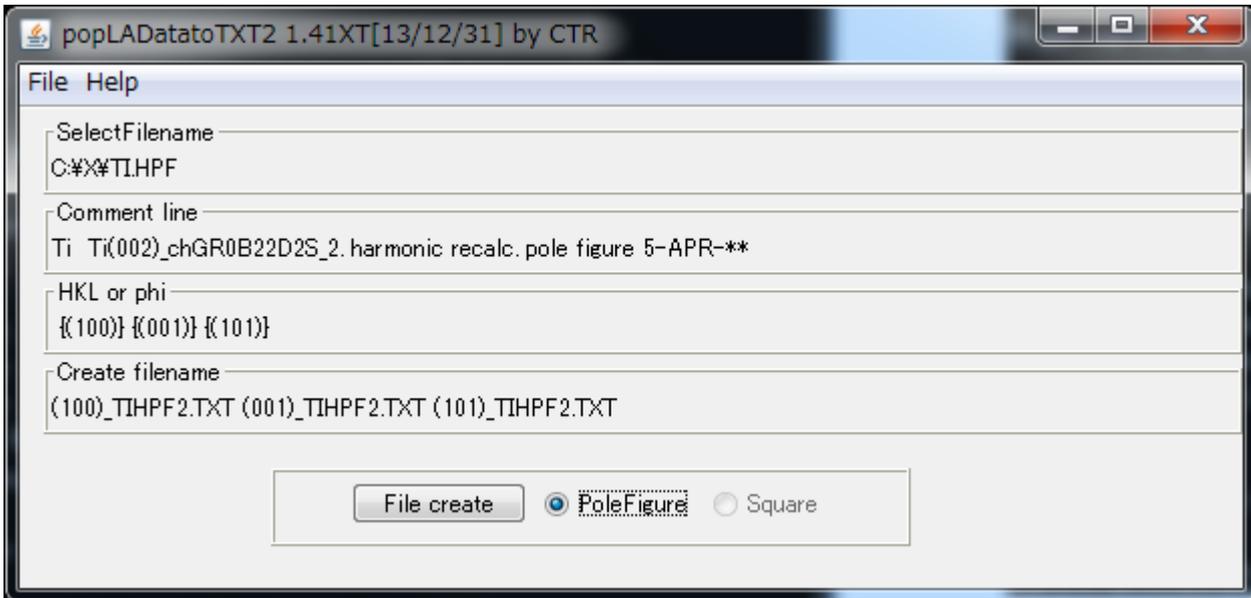
Recalculate Pole Figures (Harmonic Method)
Program by John Kallend

What is the specimen name (.HCF Assumed)? TI
How many PFs are required? 3
Enter Miller indices of polefigures required
e.g. 1 1 1, 2 0 0, 1 1 0 etc.
What are the indices of PF 1? 1 0 0
What are the indices of PF 2? 0 0 1
What are the indices of PF 3? 1 0 1
101 Working on L=16
Output to
Ti .HPF
Stop - Program terminated.

続行するには何かキーを押してください . . .
  
```

TI.HPF	2013/04/05 14:58	HPF ファイル	5 KB
TI.SHD	2013/04/05 14:52	SHD ファイル	32 KB
TI.FUL	2013/04/05 14:36	FUL ファイル	17 KB
TI.HCF	2013/04/05 14:36	HCF ファイル	1 KB

HPF	“Harmonic Pole Figure” – Pole figure recalculated from harmonic coefficients.
-----	-------------------------------------------------------------------------------



$\alpha = 80$  を外挿した場合

