CubicSymmetry23&43

Yb2O3のODF解析（MTEX，LaboTex）

2021年01月10日

HelperTex Office

１．概要

Ｃｕｂｉｃに関して、ＬａｂｏＴｅｘではＯ－ＣｕｂｉｃとＴ－ＣｕｂｉｃでＯＤＦ解析結果が異なる

Symmetry		Cubic**		Hexagonal		Tetragonal		Trigonal		Ortho-rhombic	Mono-clinic	Triclinic
		O	T	D_6	C_6	D_4	C_4	D_3	C_3	D_2	C_2	C_1
LaboTex structure code		7	6	11	10	5	4	9	8	3	2	1
ϕ_1	triclinic* (C_1)	360°	360°	360°	360°	360°	360°	360°	360°	360°	360°	360°
	monoclinic* (C_2)	180°	180°	180°	180°	180°	180°	180°	180°	180°	180°	180°
	orthorhombic*(D_2)	90°	90°	90°	90°	90°	90°	90°	90°	90°	90°	90°
	axial*	-***	-	-	-	-	-	-	-	-	-	-
Φ		90°	90°	90°	180°	90°	180°	90°	180°	90°	180°	180°
ϕ_2		90°	180°	60°	60°	90°	90°	120°	120°	180°	180°	360°

* - sample symmetry
** - there are three non-linear basic region inside described region
*** - for any ϕ_1 angle

ほとんどのＣｕｂｉｃ材料はＯ－Ｃｕｂｉｃであるが、Ｔ－Ｃｕｂｉｃと考えられる材料である
Ｙｂ２Ｏ３の対応を考えます。

C:¥CTR¥DATA¥EBSDtoLaboTex¥SpaseG.TXT

192	P6/mcc	62	11↓
193	P63/mcm	62	11↓
194	P63/mmc	62	11↓
195	P23	23	6↓
196	F23	23	6↓
197	I23	23	6↓
197	P213	23	6↓
199	I213	23	6↓
200	Pm3	23	6↓
201	Pn3	23	6↓
202	Fm3	23	6↓
203	Fd3	43	7↓
204	Im3	43	7↓
205	Pa3	43	7↓

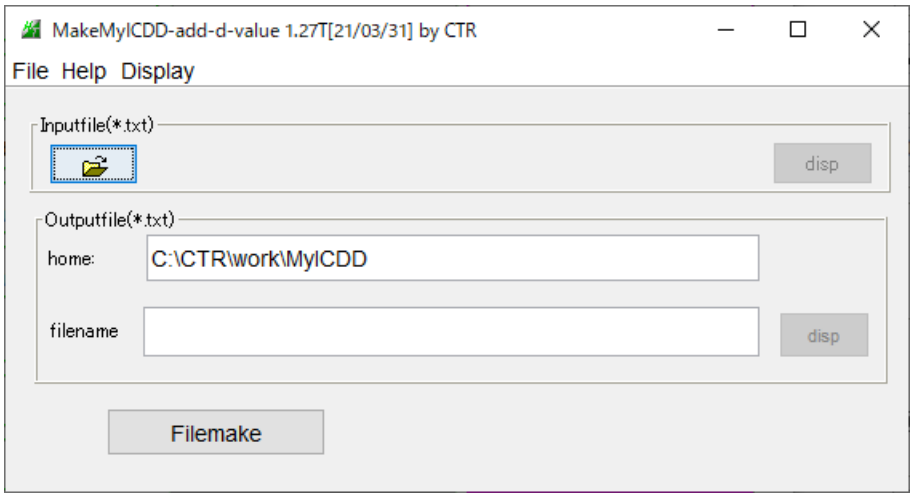
Ｓｙｍｍｅｔｒｙは６でＴ－Ｃｕｂｉｃとして解析を行ってみます。

従来のＤａｔａＢａｓｅには空間群情報が登録されていません。
新規登録方法、修正方法、Ｓｙｍｍｅｔｒｙを利用しているソフトウエアの説明を行った後、
テストデータでシュミレーションを行ってみます。

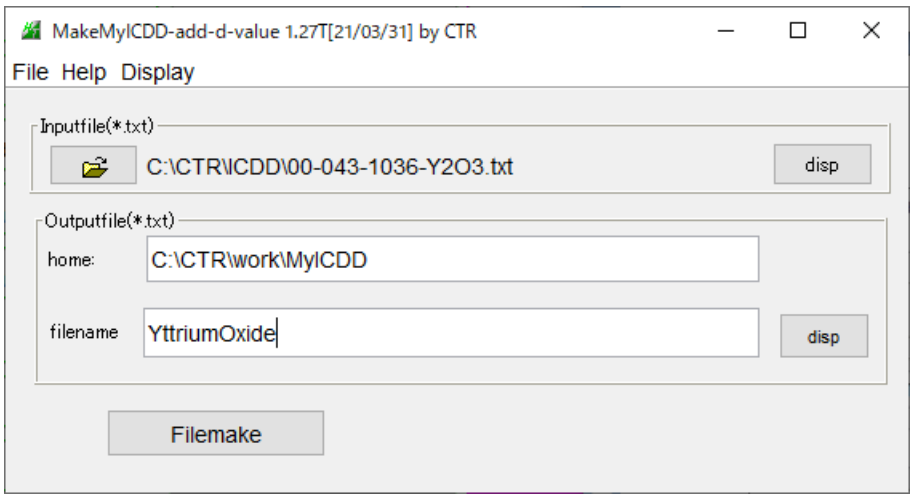
２．Ｓｙｍｍｅｔｒｙコード

２．１　ＭＹＩＣＤＤに登録

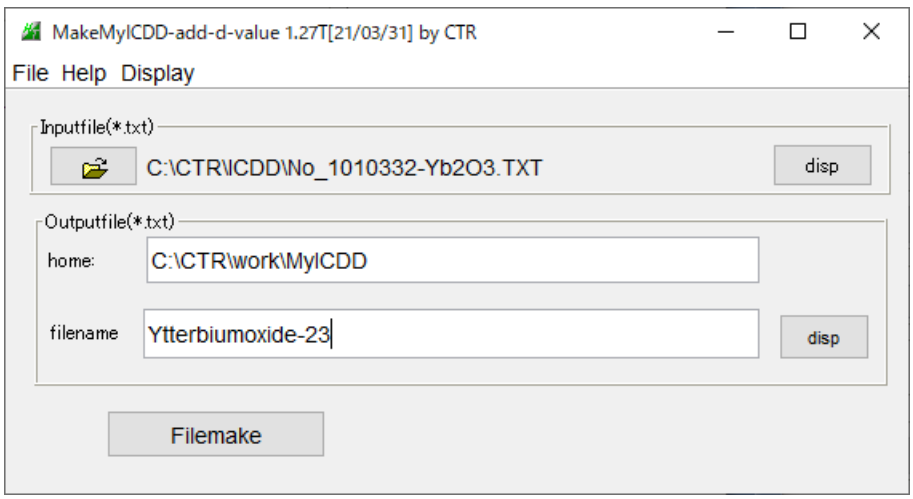
Version1.27 以降、空間群に対応しています。



入力データを選択



C:¥CTR¥work¥MYICDD に登録



登録されたデータ

TextDisplay 1.14S C:¥CTR¥work¥MYICDD¥Ytterbiumoxide-23.TXT

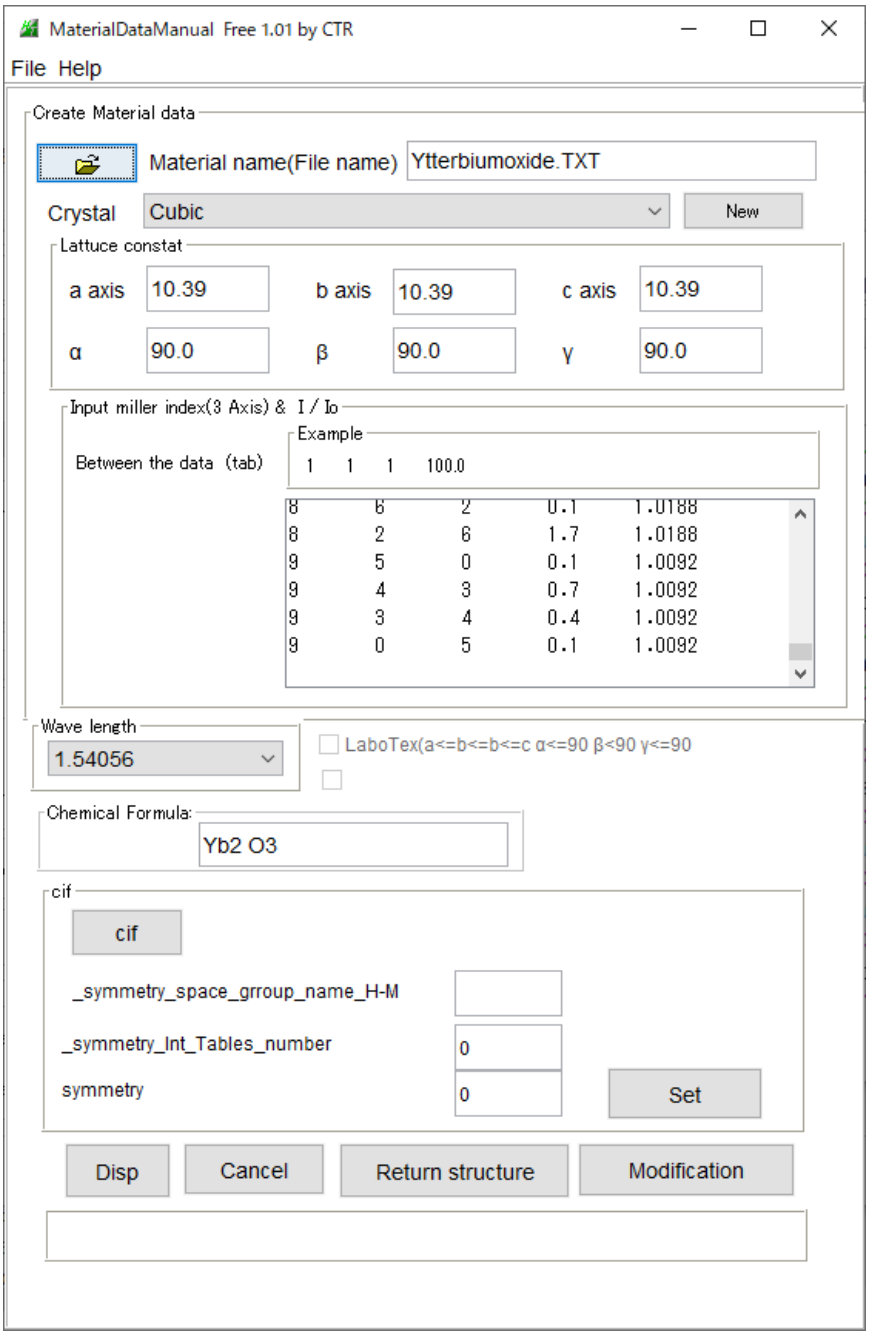
File Help

Ytterbiumoxide-23
0
10.39
10.39
10.39
90.0
90.0
90.0
1.54059
121

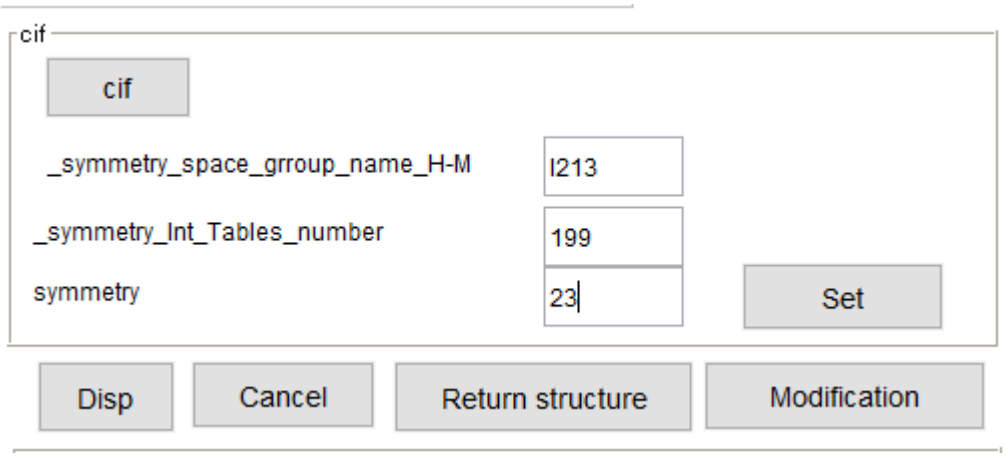
1	1	0	0.3	7.347	12.04
2	0	0	0.1	5.195	17.05
2	1	1	2.6	4.242	20.93
2	2	0	0.0	3.673	24.21
3	1	0	0.3	3.286	27.12
3	0	1	0.1	3.286	27.12
2	2	2	100.0	2.999	29.76
3	2	1	3.9	2.777	32.21
10	0	0	0.3	1.039	95.70
8	6	0	1.0	1.039	95.70
8	0	6	0.0	1.039	95.70
10	1	1	0.3	1.029	96.97
7	7	2	0.2	1.029	96.97
10	2	0	0.5	1.019	98.24
10	0	2	0.5	1.019	98.24
8	6	2	0.1	1.019	98.24
8	2	6	1.7	1.019	98.24
9	5	0	0.1	1.009	99.51
9	4	3	0.7	1.009	99.51
9	3	4	0.4	1.009	99.51
9	0	5	0.1	1.009	99.51

1010332 data_1010332(COD) Ytterbium oxide
_symmetry_space_group_name_H-M 'I213'
_symmetry_Int_Tables_number 199
_Symmetry 23

２．２　空間群が登録されていないデータの場合



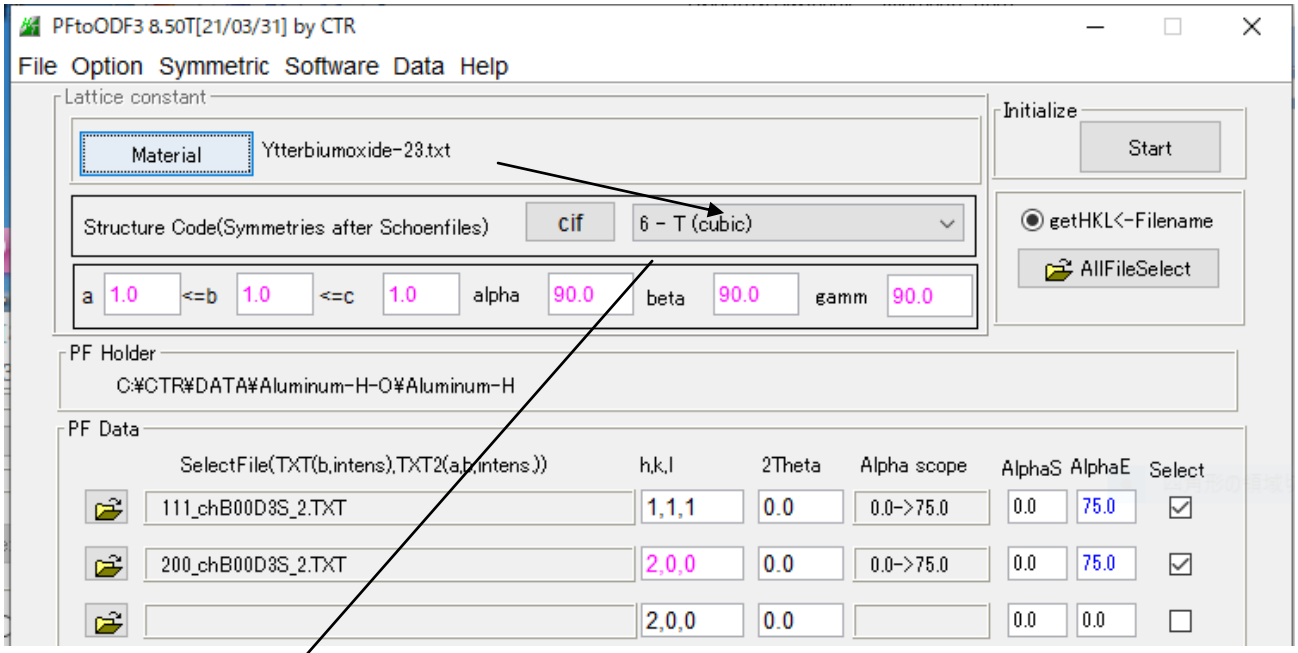
ｃｉｆファイルを選択か直接入力する。

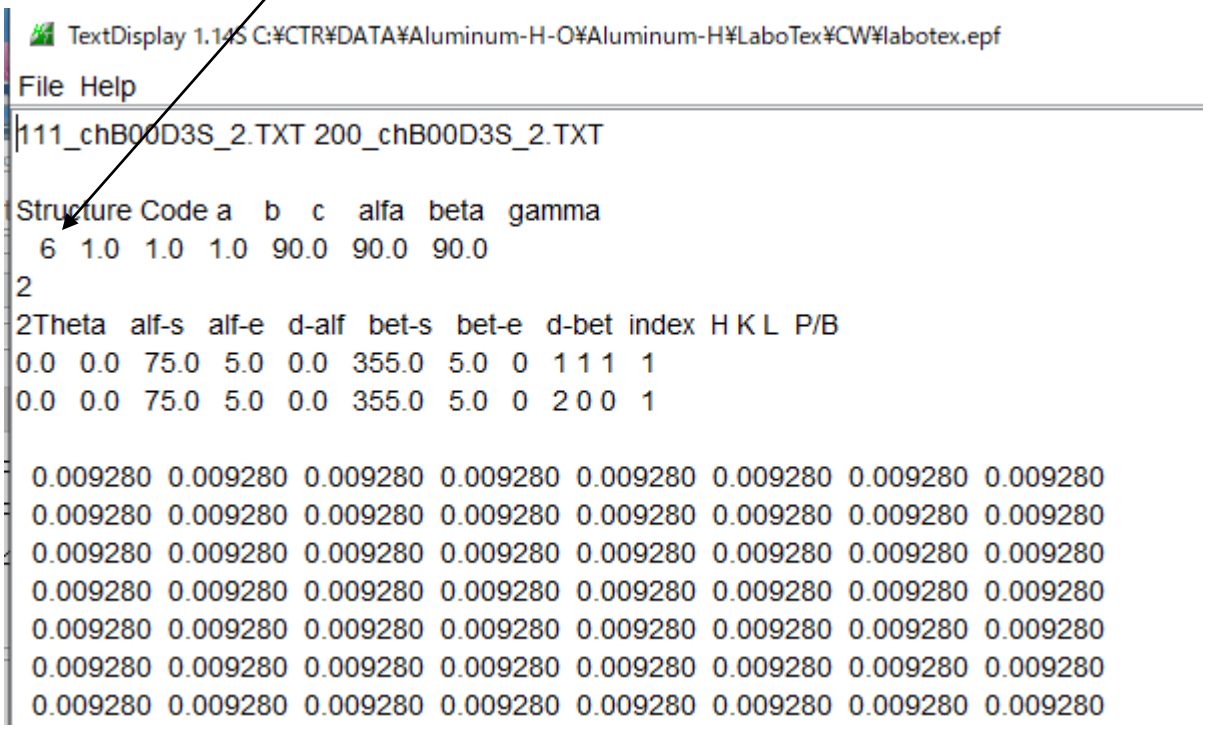


Modification で変更する。　Disp で確認出来ます。

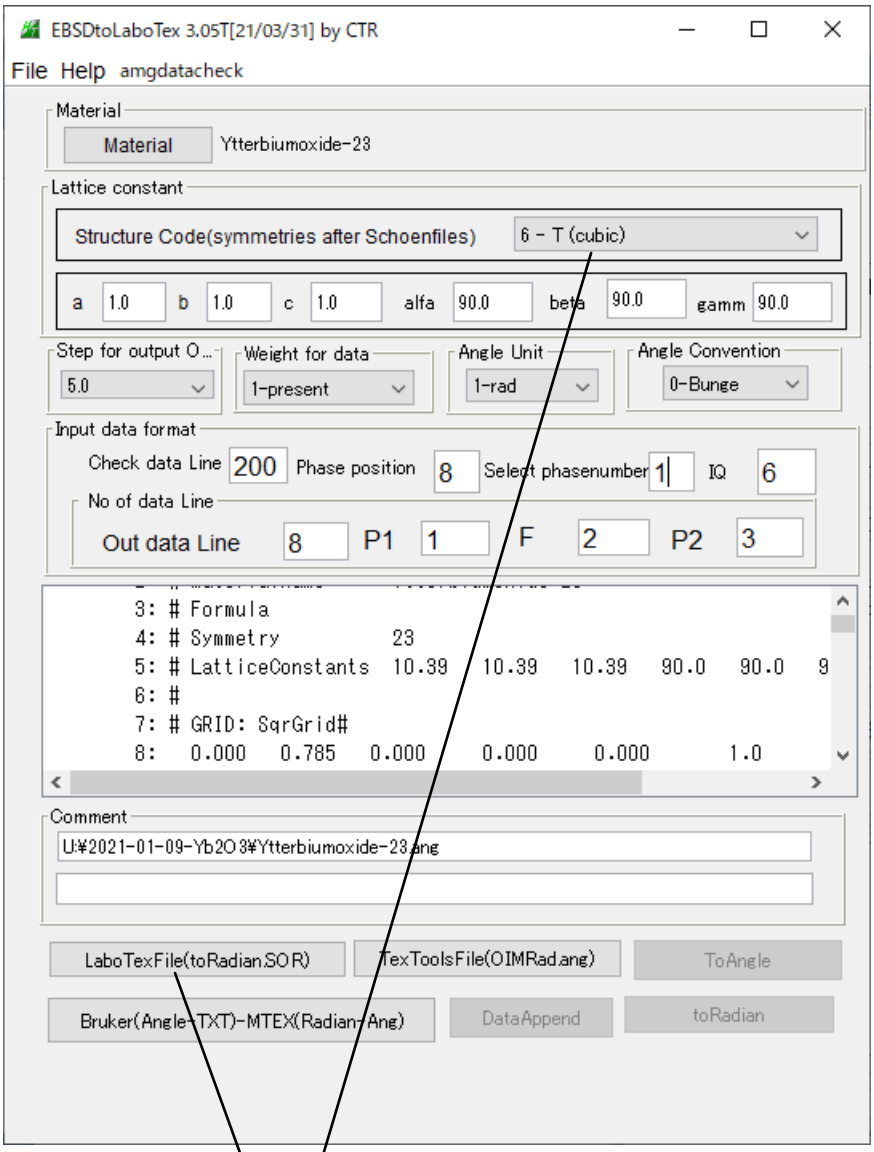
２．３　ＸＲＤ極点図のＬａｂｏＴｅｘ向けＥＰＦデータ作成

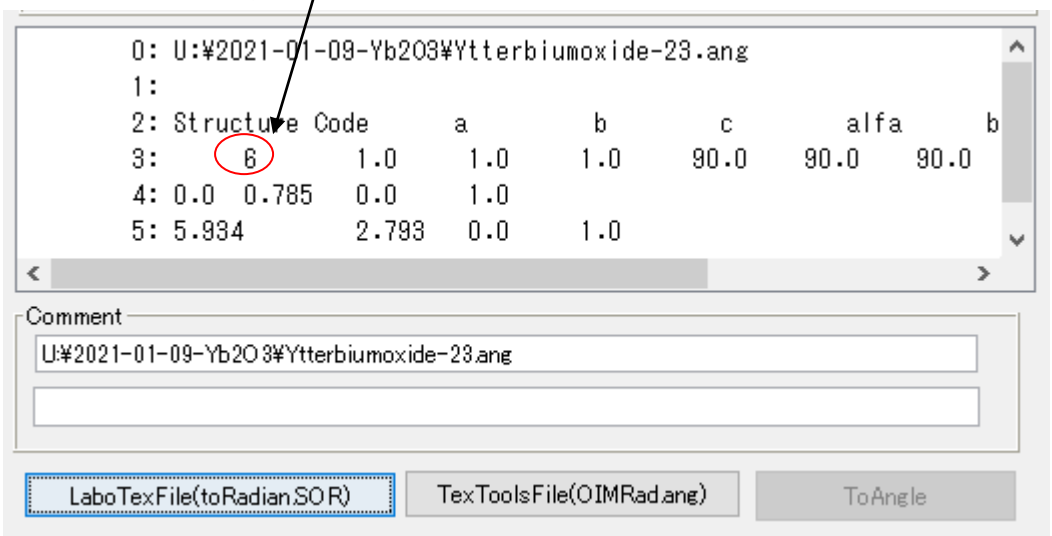
空間群を登録すると、Ｃｉｆファイル指定は必要ありません。



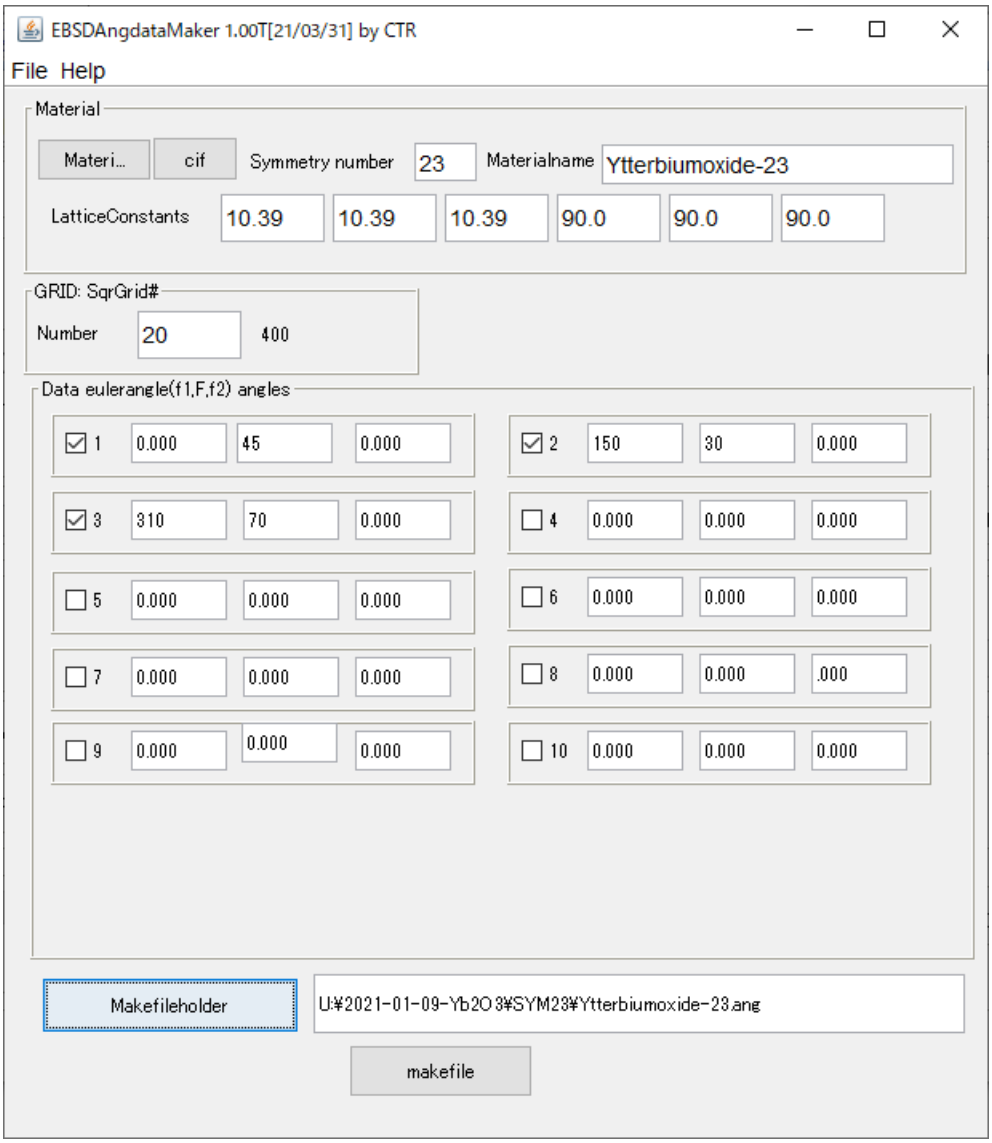


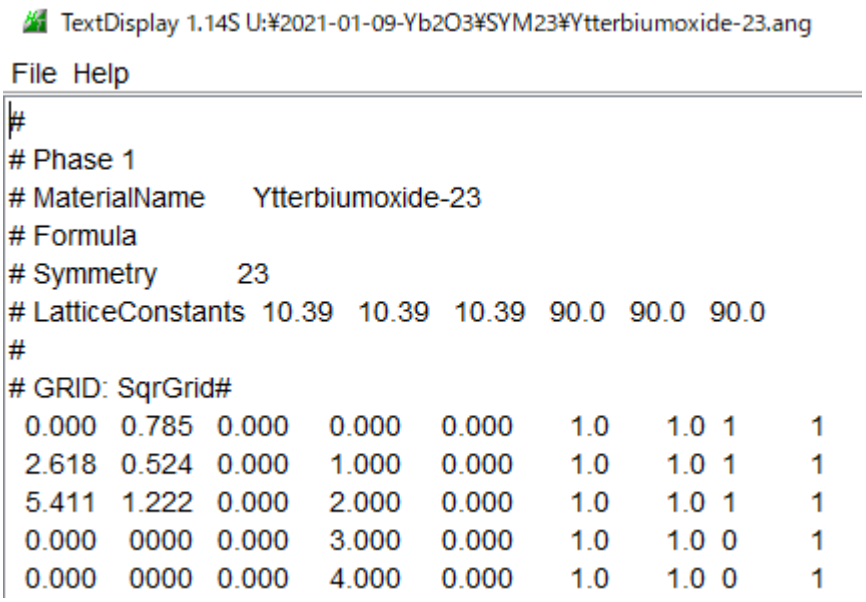
２．４　ＥＢＳＤデータからＬａｂｏＴｅｘ入力のＳＯＲファイル作成



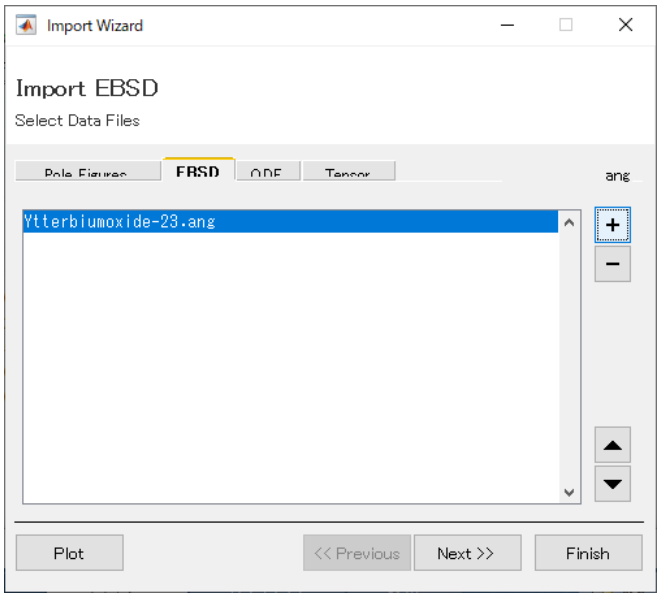


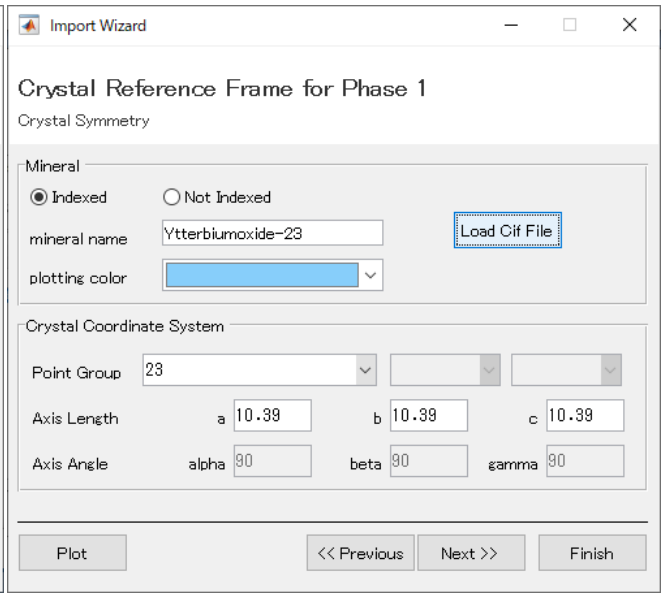
３．Ｙｂ２Ｏ３、Ｓｙｍｍｅｔｒｙ（２３）のＥＢＳＤデータ作成

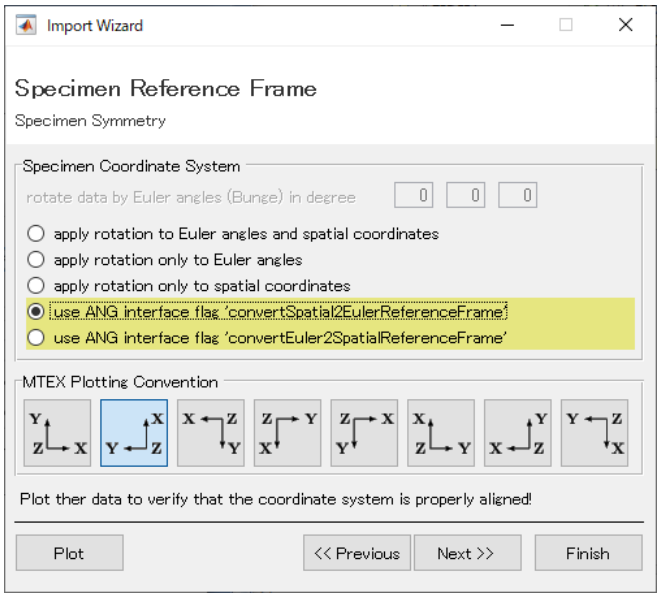


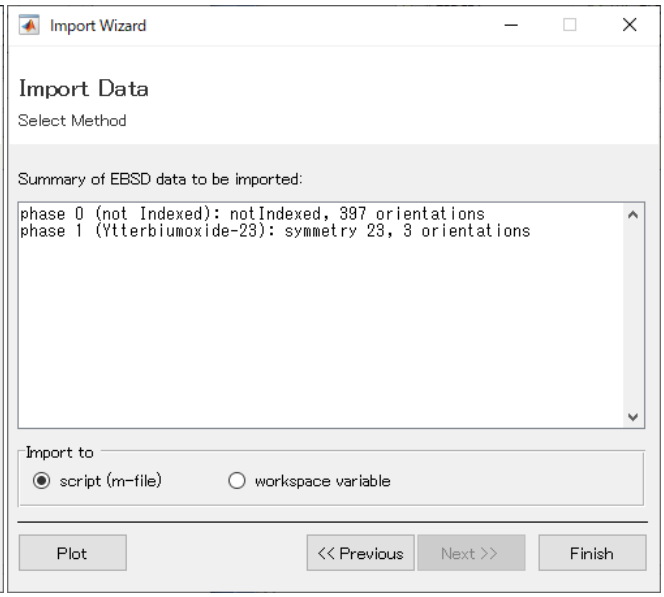


３．１　ＭＴＥＸの解析

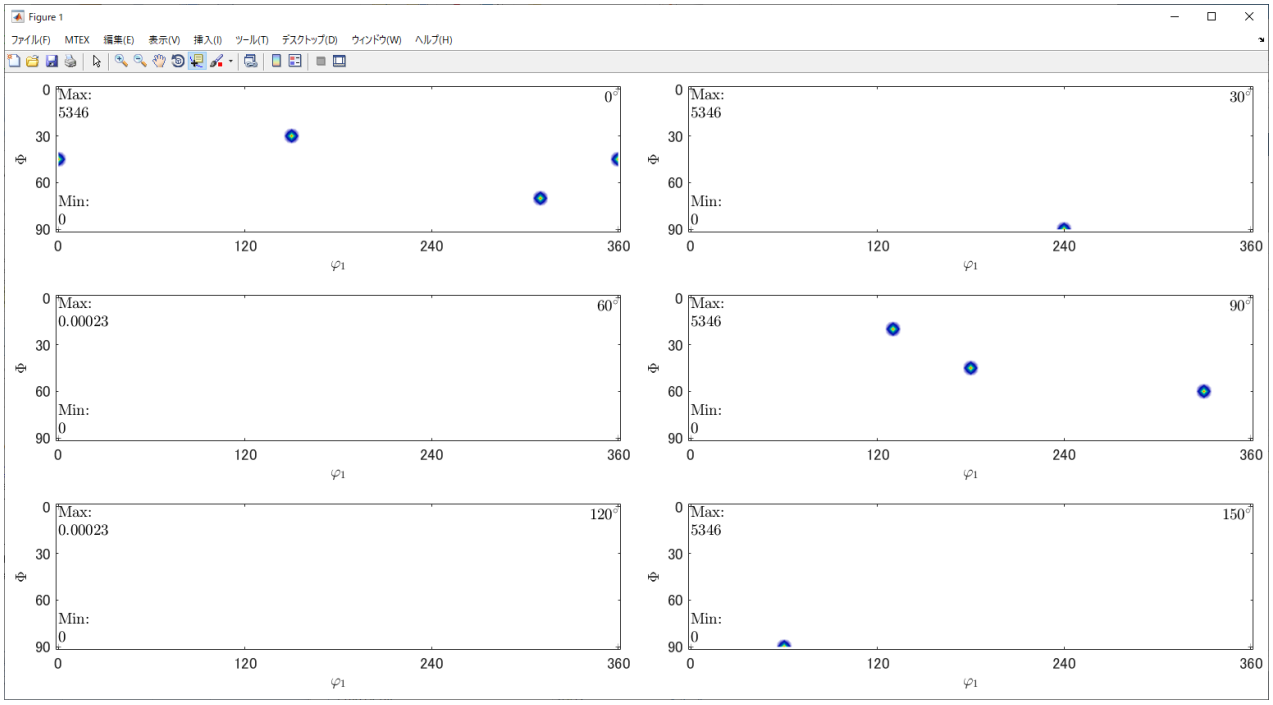






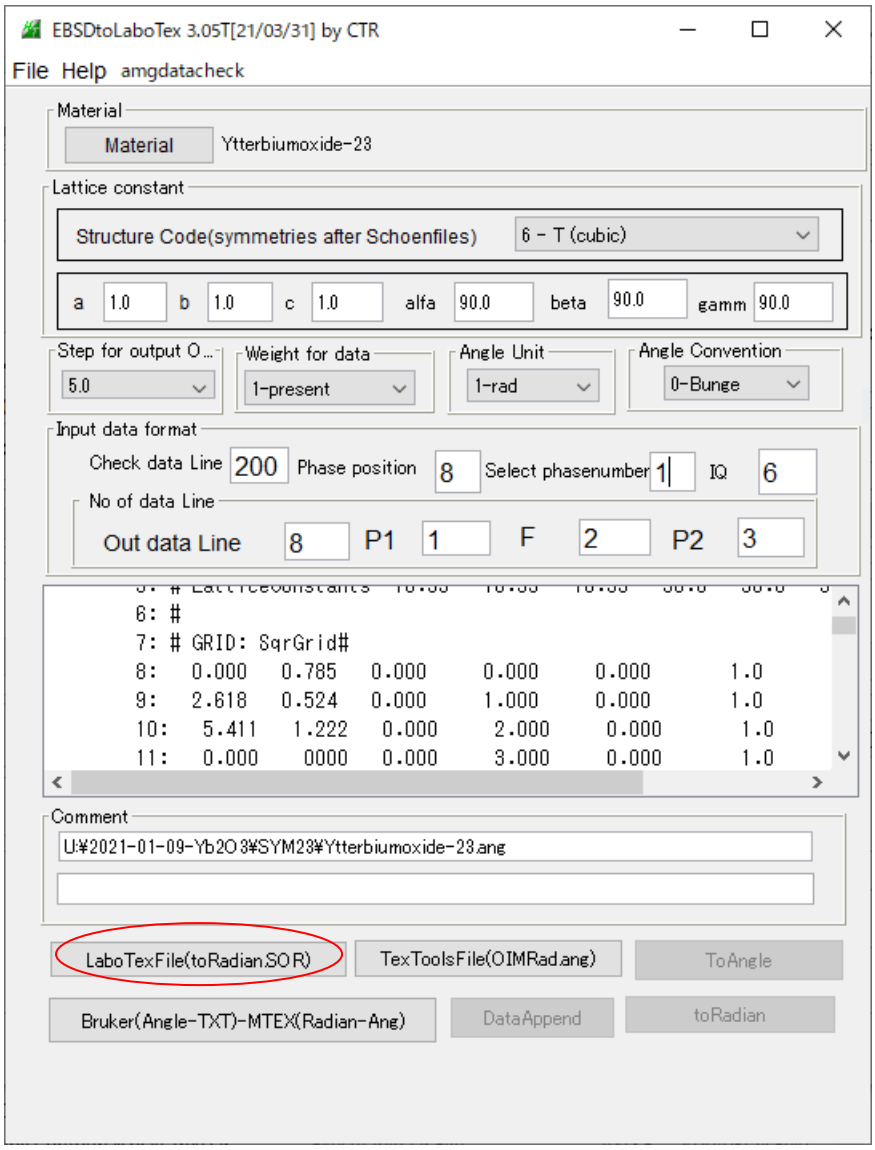


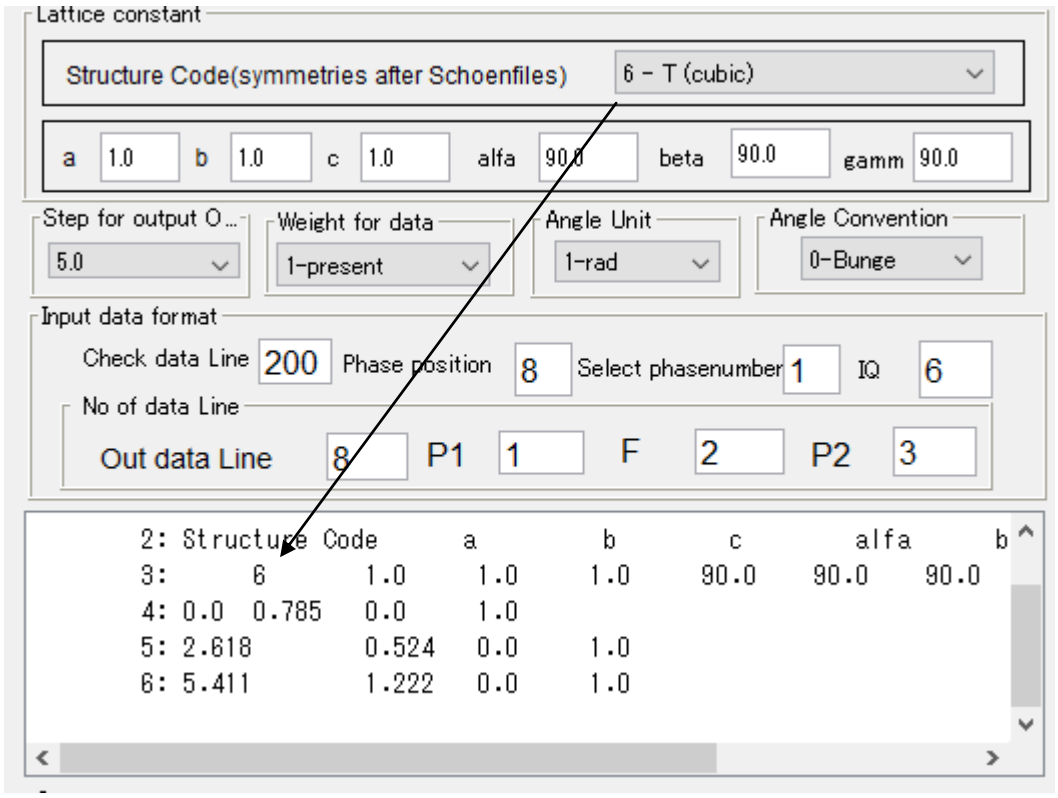
odf = calcDensity(ebsd('Ytterbiumoxide-23').orientations,'halfwidth',2*degree)



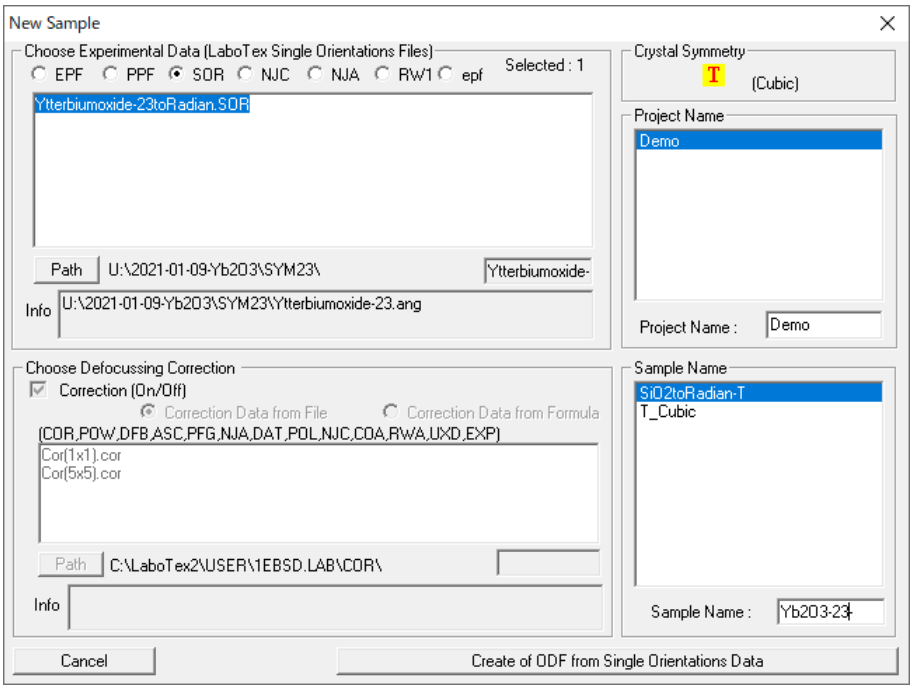
３．２　ＬａｂｏＴｅｘの解析

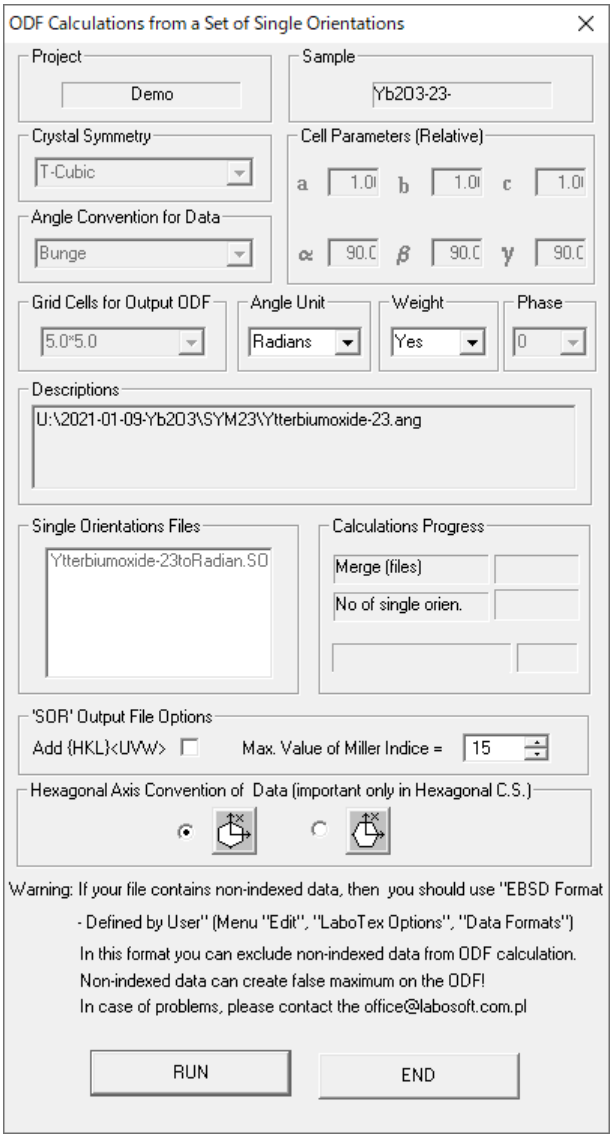
ＬａｂｏＴｅｘ入力ＳＯＲデータ作成

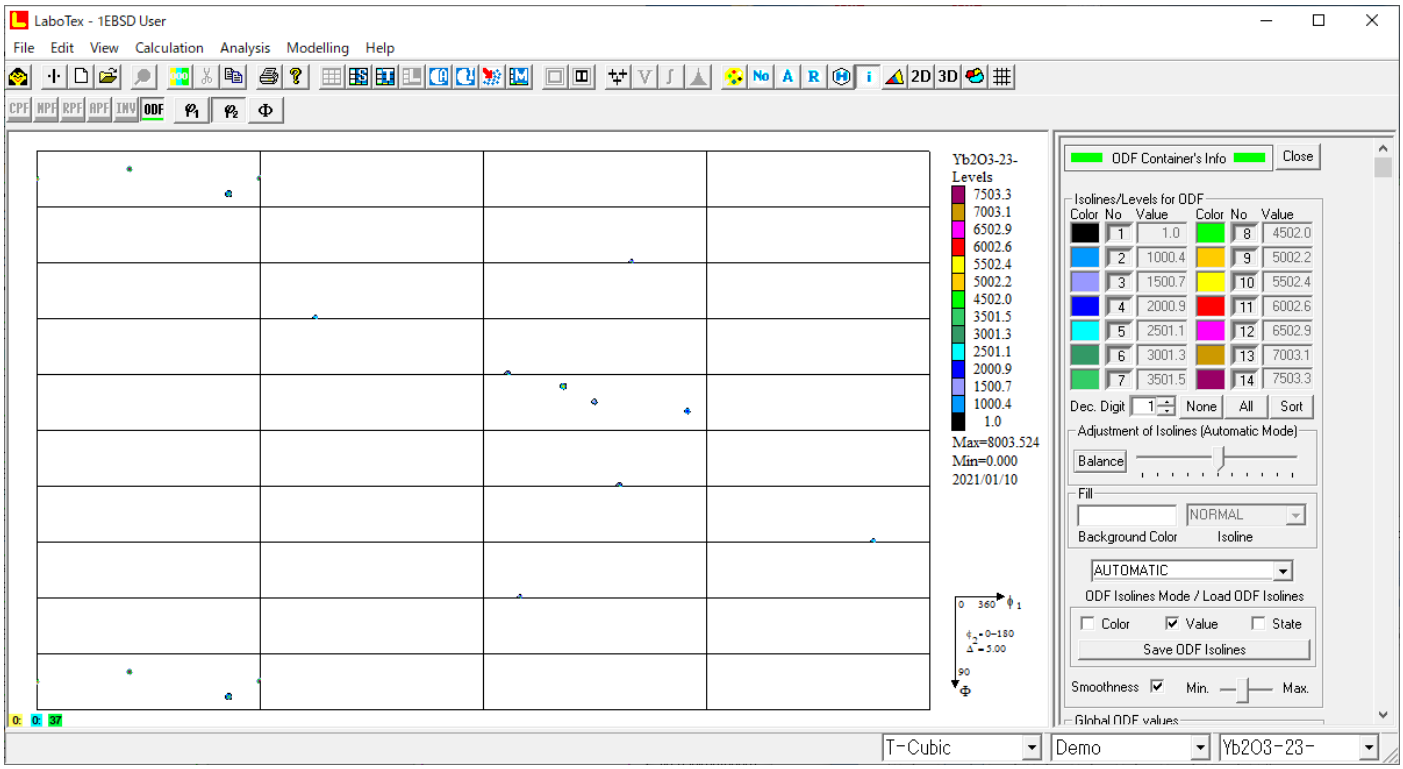


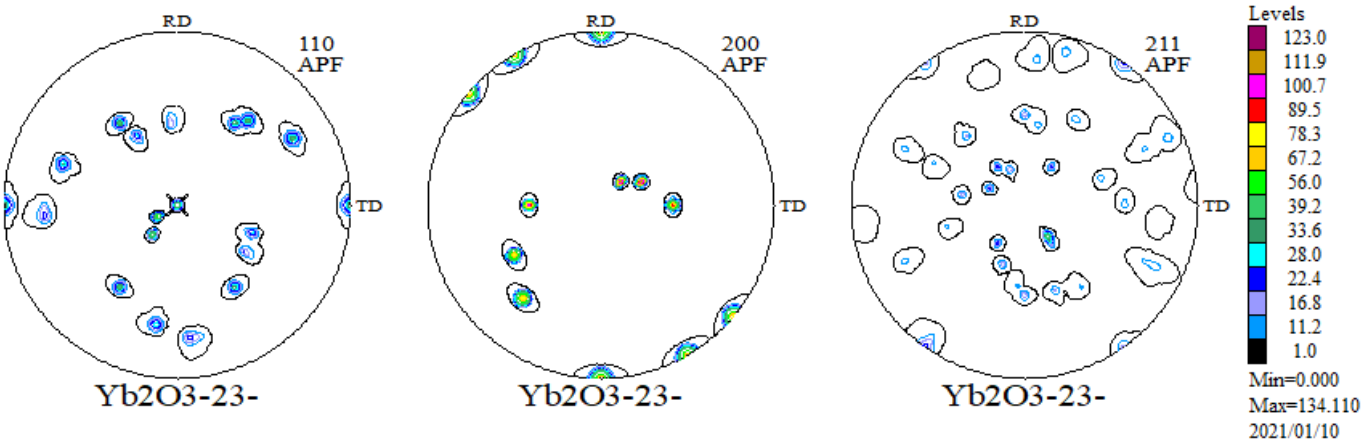


ＬａｂｏＴｅｘに読み込み





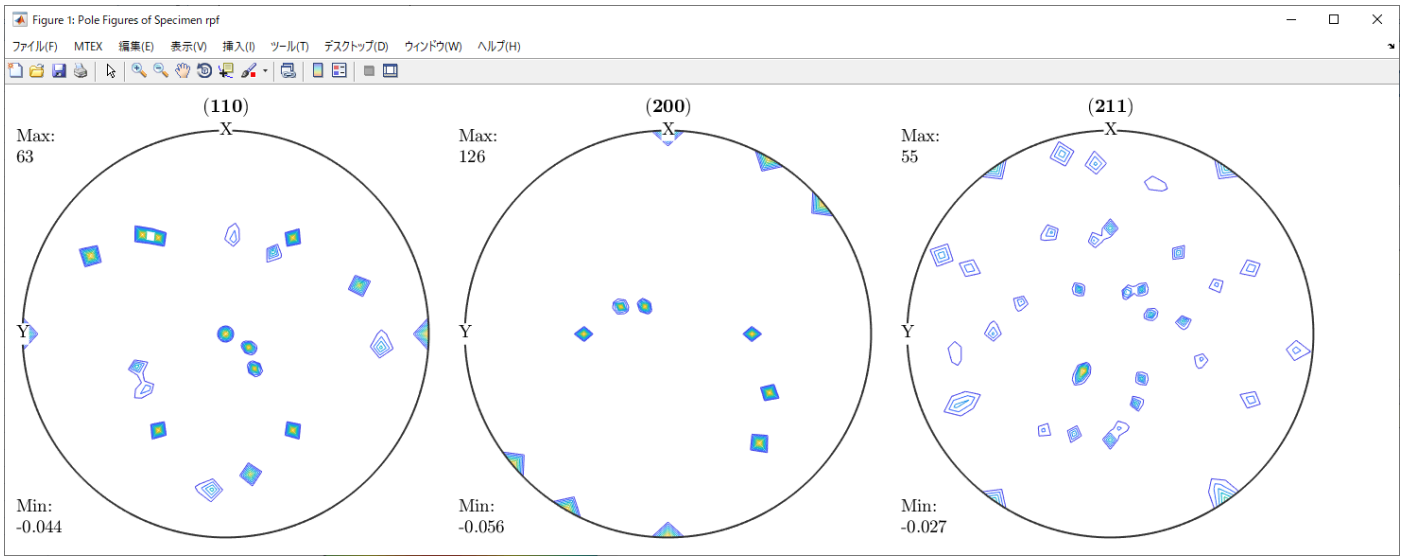




ＭＴＥＸとＯＤＦ図は一致

３．３　ＭＴＥＸＯＤＦ後のＰＦデータＥｘｐｏｒｔしＸＲＤ極点図として

```
cs=ebsd('Ytterbiumoxide-23').CS
h={Miller(1,1,0,cs),Miller(2,0,0,cs),Miller(2,1,1,cs)}
rpf=calcPoleFigure(odf,h)
plot(rpf,'contour','projection','eangle')
```

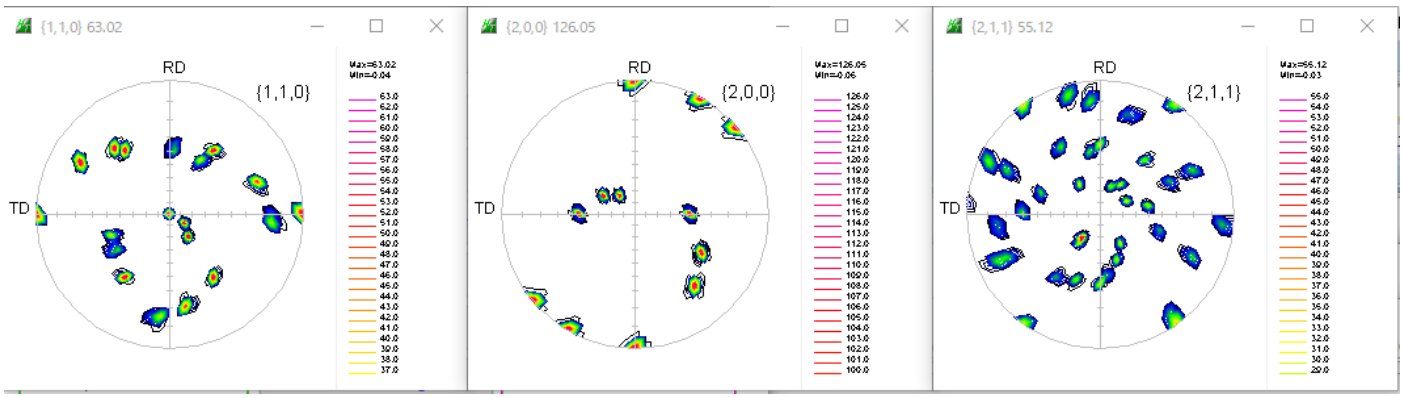


極点図のＴＤ方向はＬａｂｏＴｅｘに対し１８０度回転している。

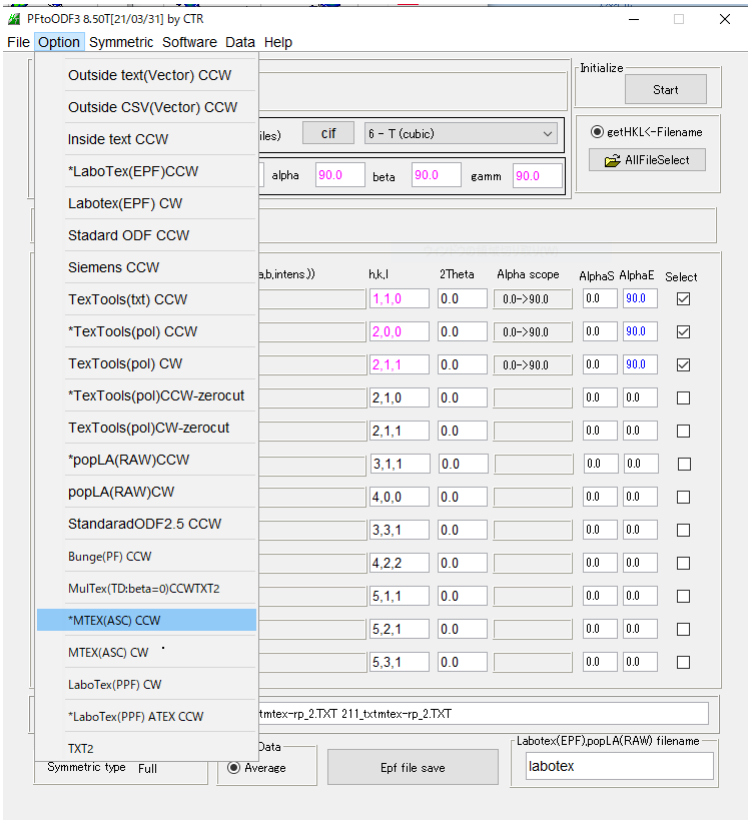
ＭＴＥＸ－ＣＣＷ　　一般的

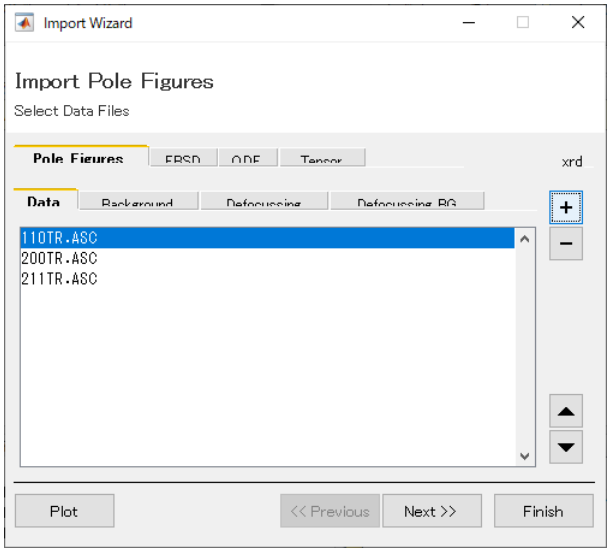
ＬａｂｏＴｅｘ－ＣＷ

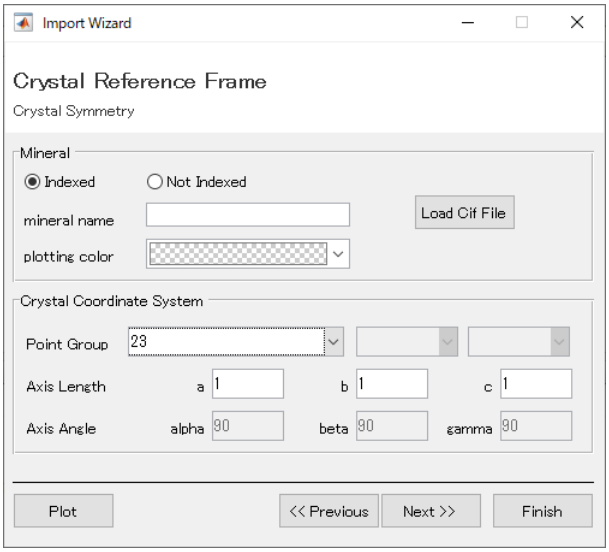
再計算極点図をＥｘｐｏｒｔ

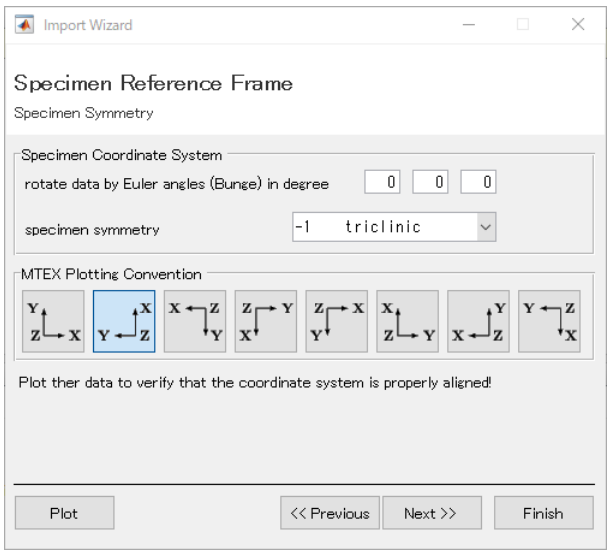


３．３．１　ＭＴＥＸ解析

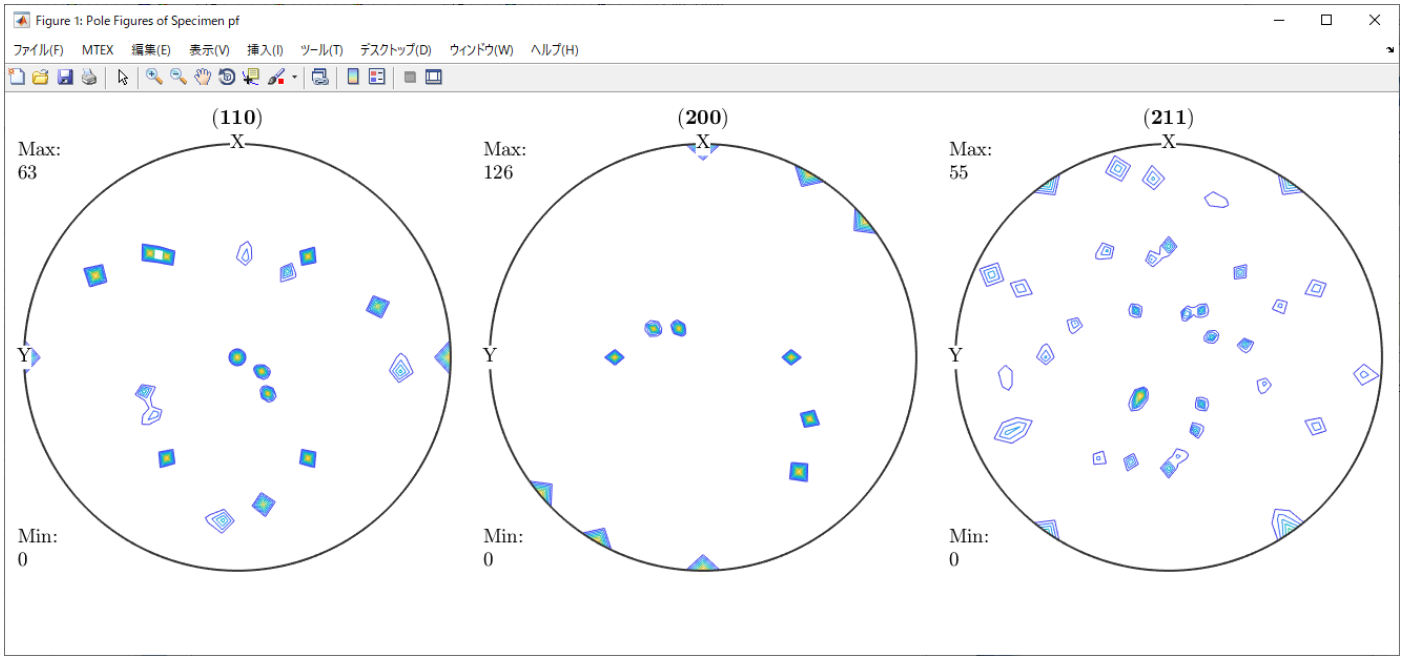

PFtoODF3 8.50T[21/03/31] by CTR
File Option Symmetric Software Data Help
Outside text(Vector) CCW
Outside CSV(Vector) CCW
Inside text CCW
*LaboTex(EPF)CCW
Labotex(EPF) CW
Stadard ODF CCW
Siemens CCW
TexTools(txt) CCW
*TexTools(pol) CCW
TexTools(pol) CW
*TexTools(pol)CCW-zerocut
TexTools(pol)CW-zerocut
*popLA(RAW)CCW
popLA(RAW)CW
StandaradODF2.5 CCW
Bunge(PF) CCW
MulTex(TD:beta=0)CCWTXT2
*MTEX(ASC) CCW
MTEX(ASC) CW
LaboTex(PPF) CW
*LaboTex(PPF) ATEX CCW
TXT2
Initialize
Start
cif
6 - T (cubic)
getHKL<-Filename
AllFileSelect
alpha 90.0 beta 90.0 gamm 90.0
h,k,l 2Theta Alpha scope AlphaS AlphaE Select
Symmetric type Full
Average
Epf file save
Labotex(EPF),popLA(RAW) filename
labotex


Import Wizard
Import Pole Figures
Select Data Files
Pole Figures
EBSD
ODF
Tensor
xrd
Data
Background
Defocussing
Defocussing BG
110TR.ASC
200TR.ASC
211TR.ASC
Plot
<< Previous
Next >>
Finish

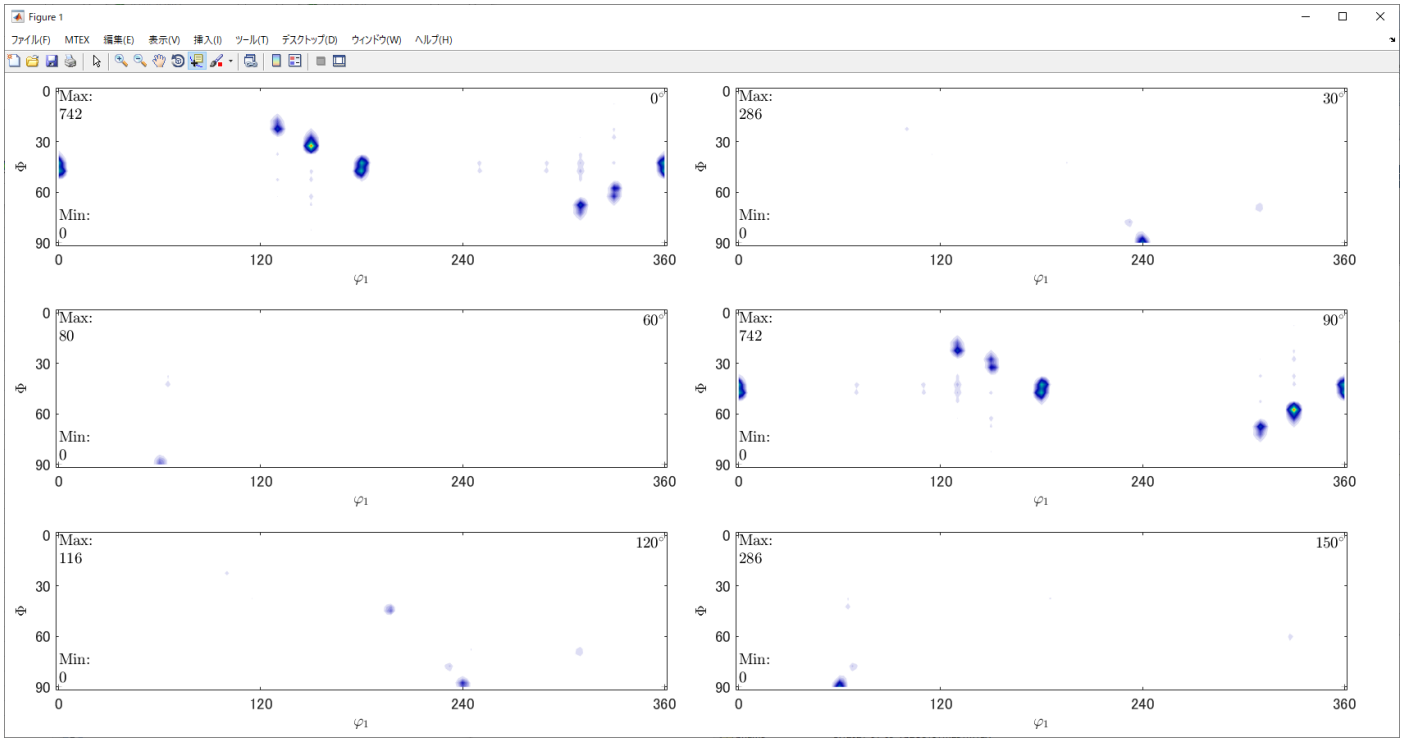

Import Wizard
Crystal Reference Frame
Crystal Symmetry
Mineral
Indexed
Not Indexed
mineral name
plotting color
Load Cif File
Crystal Coordinate System
Point Group 23
Axis Length a 1 b 1 c 1
Axis Angle alpha 90 beta 90 gamma 90
Plot
<< Previous
Next >>
Finish


Import Wizard
Specimen Reference Frame
Specimen Symmetry
Specimen Coordinate System
rotate data by Euler angles (Bunge) in degree 0 0 0
specimen symmetry -1 triclinic
MTEX Plotting Convention
Plot ther data to verify that the coordinate system is properly aligned!
Plot
<< Previous
Next >>
Finish

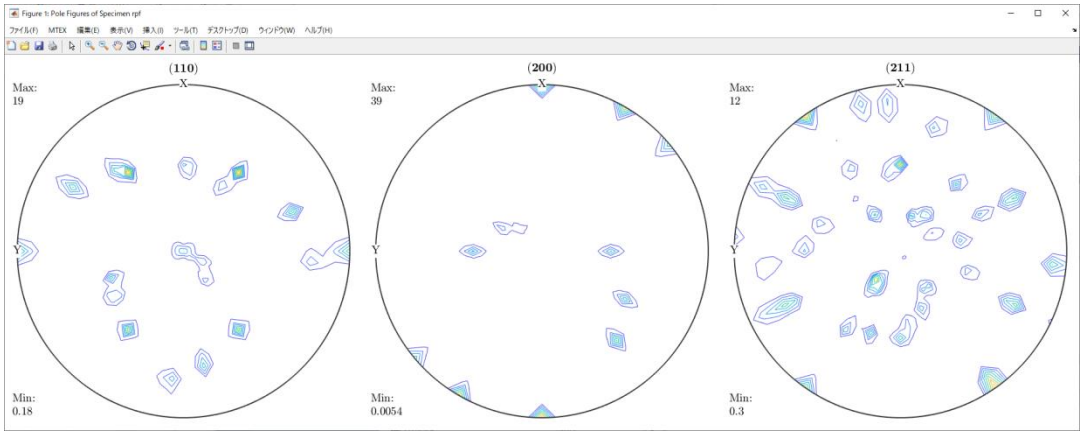
plot(pf,'contour','projection','eangle')



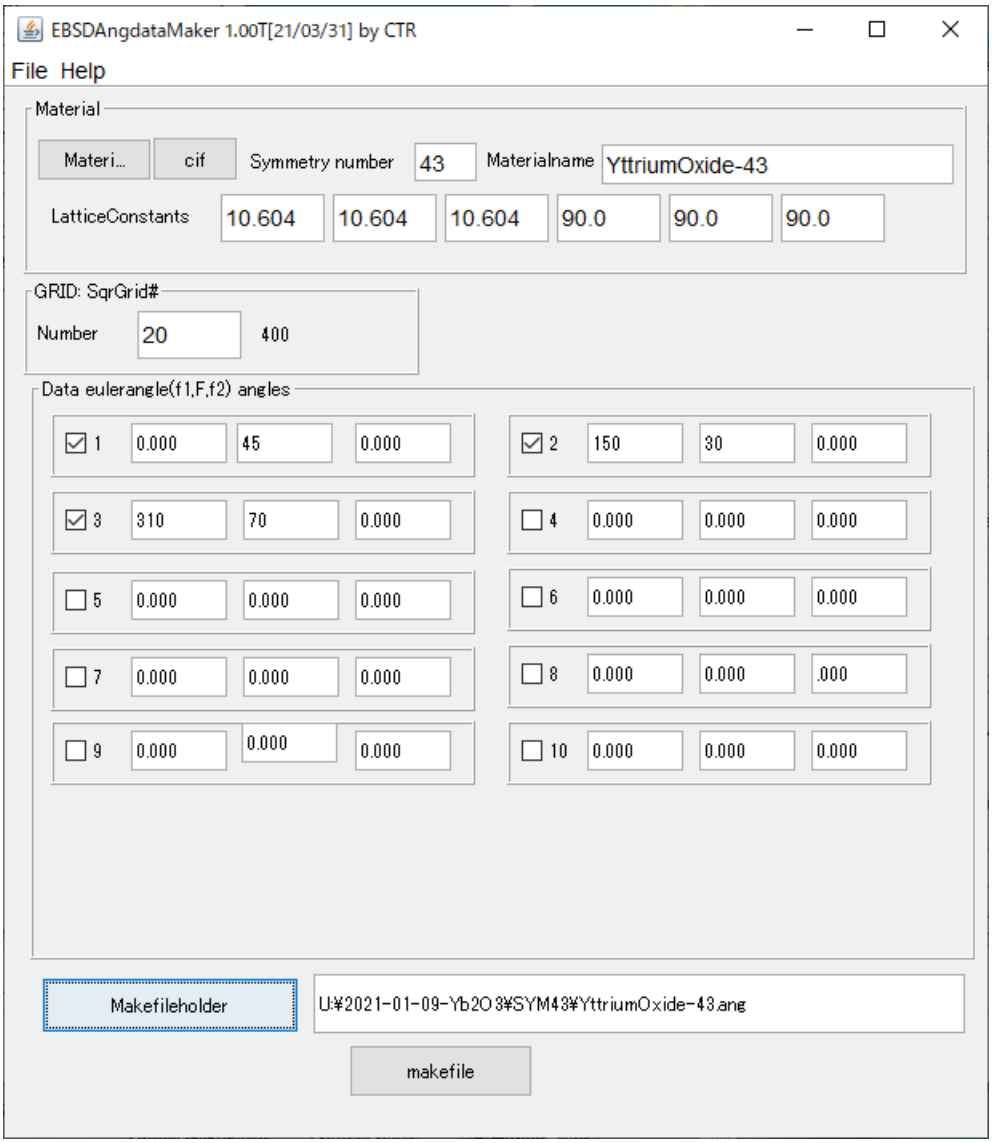
odf=calcODF(pf,'halfwidth',2*degree)



rpf=calcPoleFigure(odf,h)



４．Ｙｂ２Ｏ３，Ｓｙｍｍｅｔｒｙ（４３）のＥＢＳＤデータ作成



TextDisplay 1.14S U:¥2021-01-09-Yb2O3¥SYM43¥YttriumOxide-43.ang

File Help

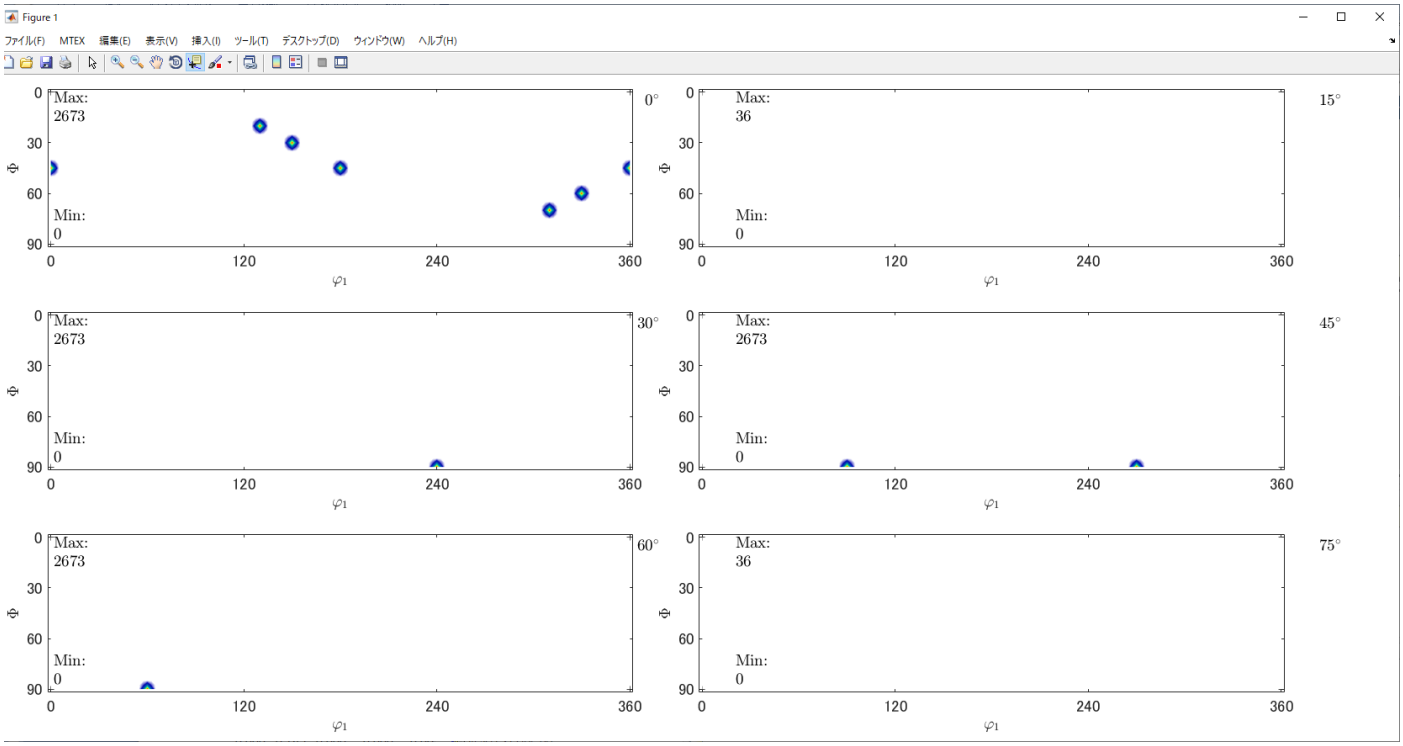
```
#
# Phase 1
# MaterialName      YttriumOxide-43
# Formula
# Symmetry          43
# LatticeConstants  10.604   10.604   10.604   90.0   90.0   90.0
#
# GRID: SqrGrid#
  0.000   0.785   0.000     0.000     0.000      1.0      1.0  1        1
  2.618   0.524   0.000     1.000     0.000      1.0      1.0  1        1
  5.411   1.222   0.000     2.000     0.000      1.0      1.0  1        1
  0.000    0000   0.000     3.000     0.000      1.0      1.0  0        1
  0.000    0000   0.000     4.000     0.000      1.0      1.0  0        1
```

４．１　ＭＴＥＸ解析

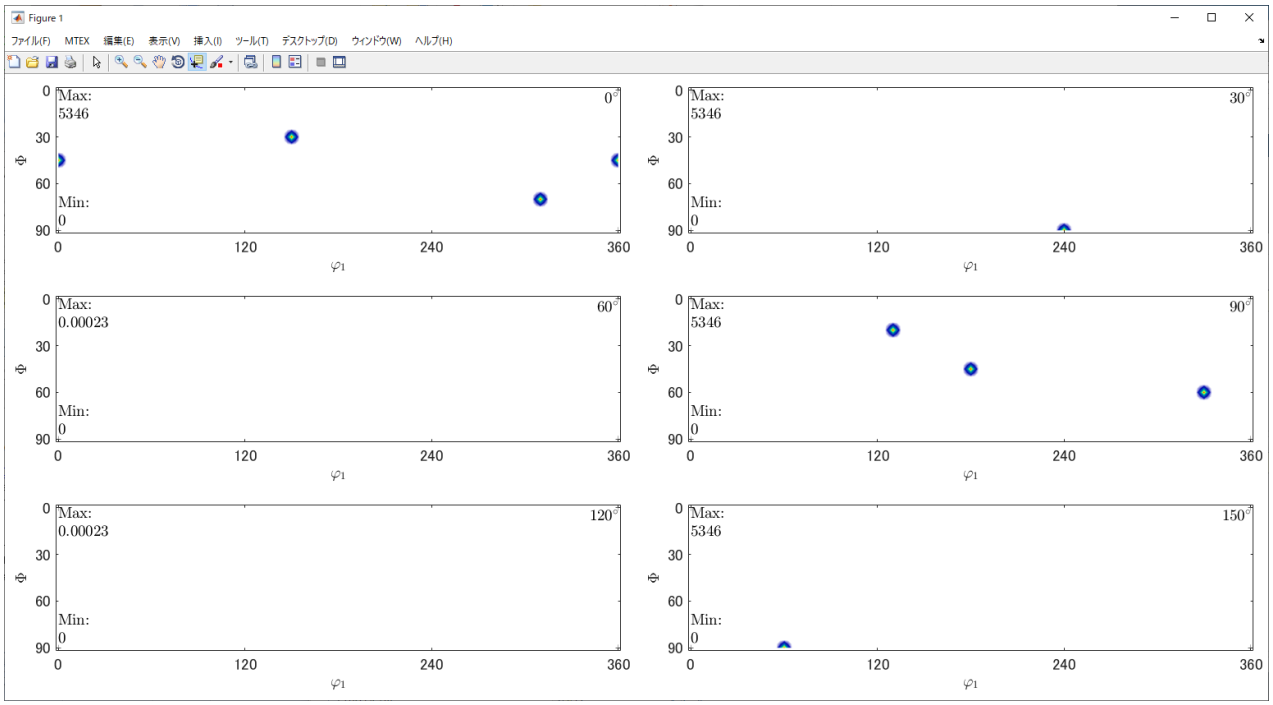
処理はＳｙｍｍｅｔｒｙ（２３）と同様に

odf = calcDensity(ebsd('YttriumOxide-43').orientations,'halfwidth',2*degree)

Symmetry(43)　ϕ 2Max＝90

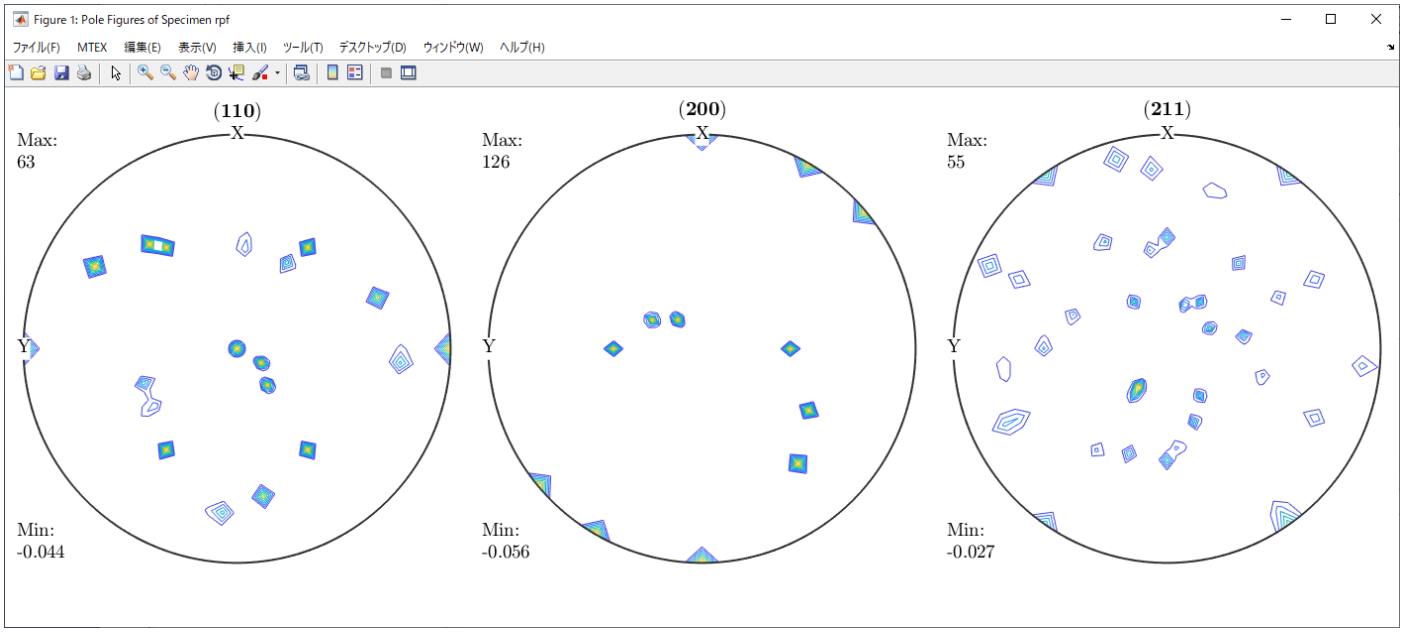


Symmetry(23)　ϕ 2Max=180

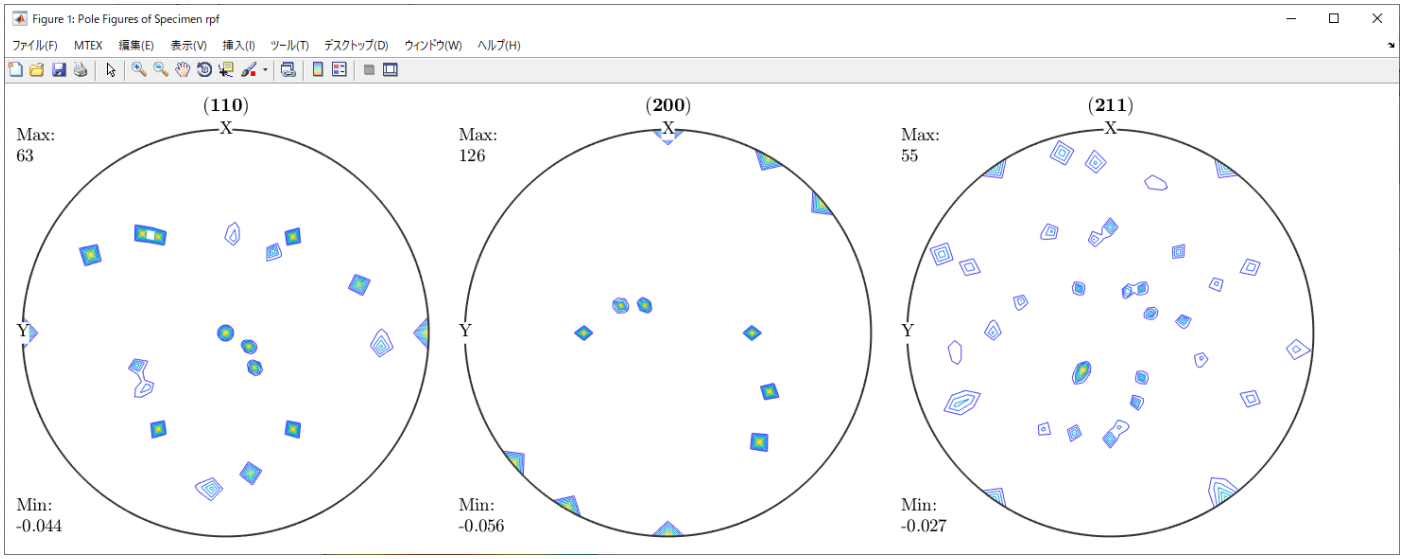


再計算極点図

Symmetry(43)



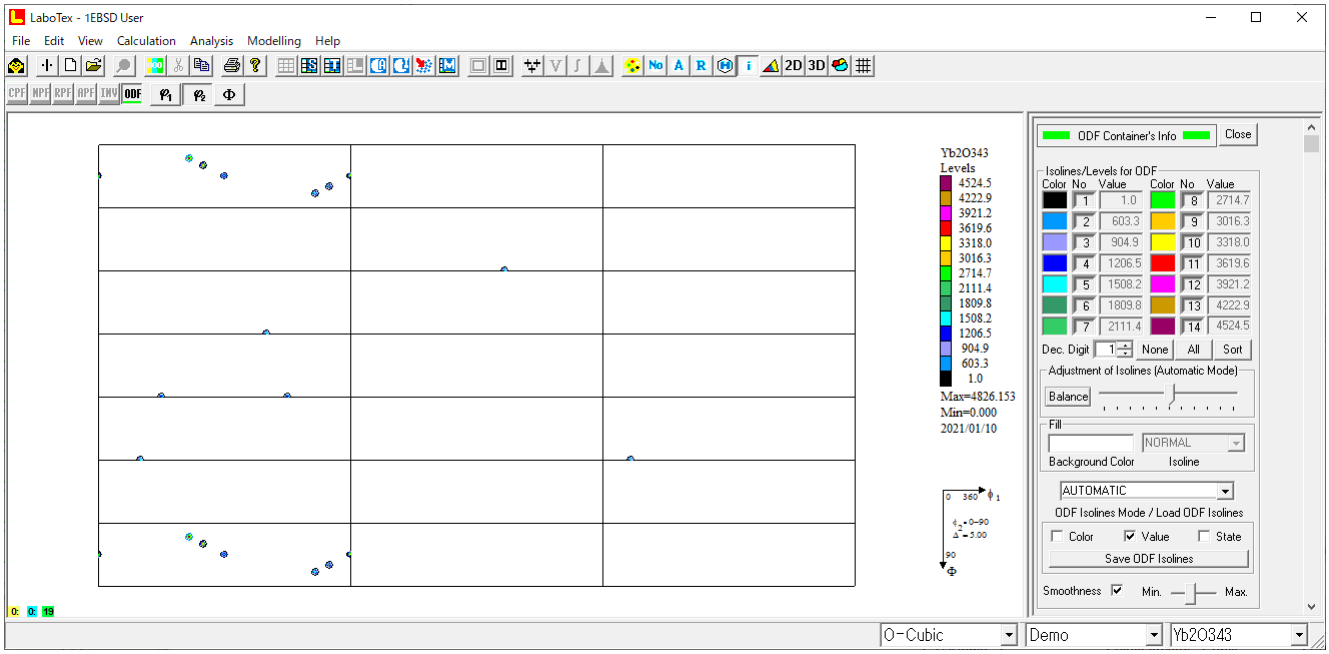
Symmetry(23)



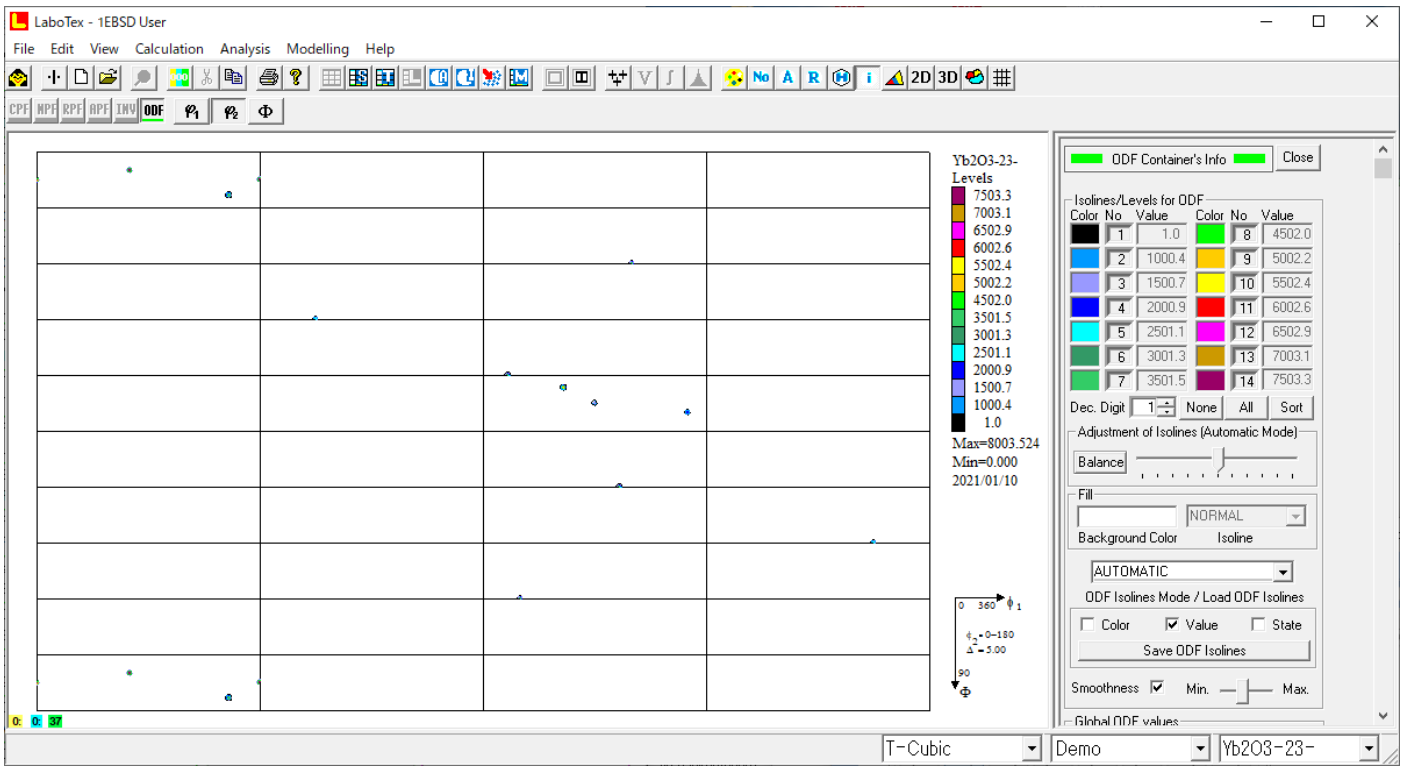
ＭＴＥＸの比較では、ＯＤＦ図は異なるが極点図は一致する

４．２　ＬａｂｏＴｅｘ解析

Symmetry(43)

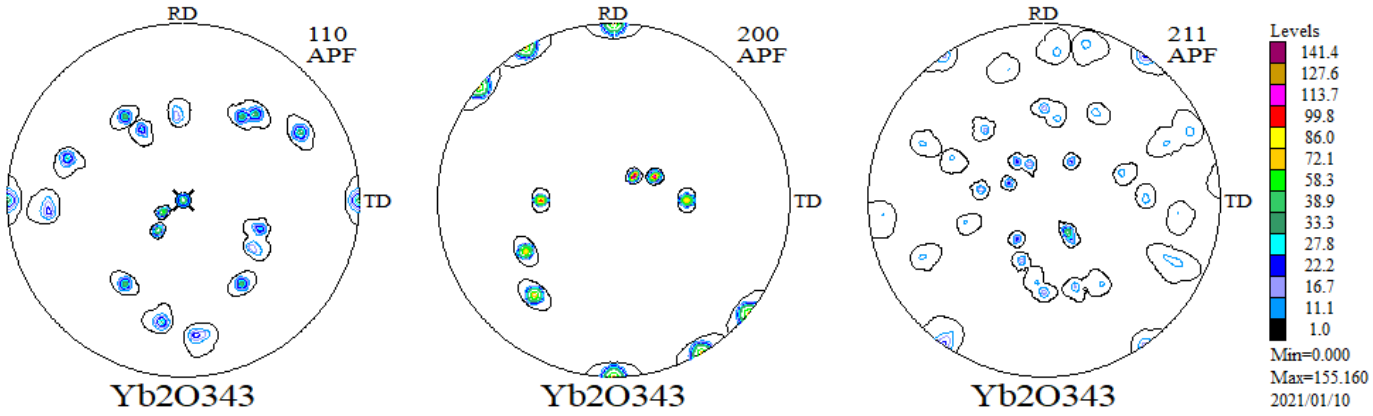


Symmetry(23)

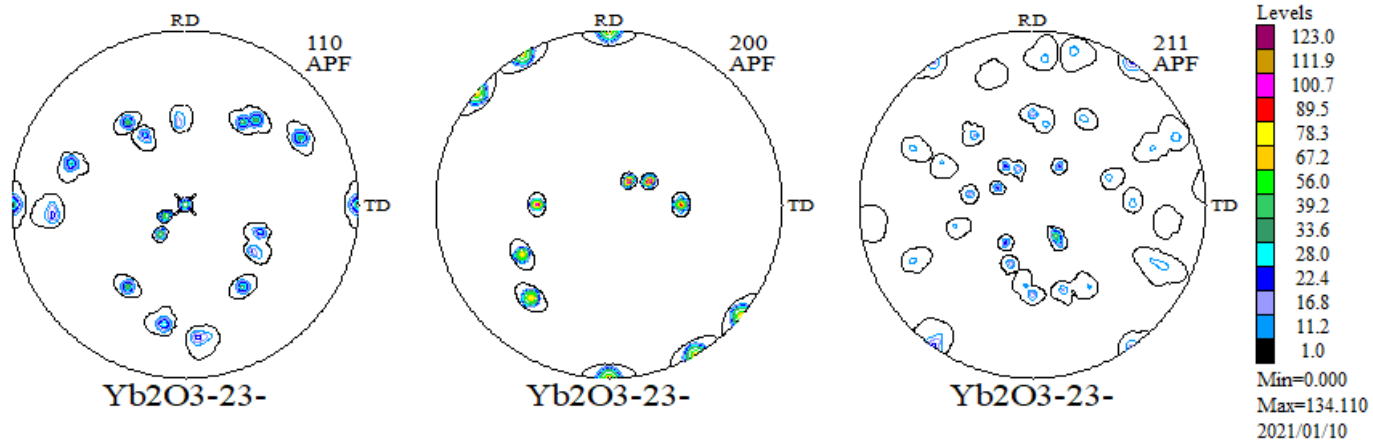


再計算極点図比較

Syymetry(43)



Symmetry(23)



使用したソフトウエア

ＥＢＳＤＡｎｇｄａｔａＭａｋｅｒ	１．００	ＥＢＳＤＡｎｇデータ作成
ＥＢＳＤｔｏＬａｂｏＴｅｘ	３．０５	ＡｎｇデータからＳＯＲデータ変換
ＭＡＴＬＡＢ	Ｒ２０１７ｂ	ＭＴＥＸ環境
ＭＴＥＸ	５．４．０	ＯＤＦ解析
ＬａｂｏＴｅｘ	５．０．５０	ＯＤＦ解析
ＰＦｔｏＯＤＦ３	８．５０	ＸＲＤＰＦ－＞ＯＤＦ
ＭａｋｅＰｏｌｅＦｉｌｅ	１．８９	ＭＴＥＸＰＦ－＞ＴＸＴ２
ＧＰＰｏｌｅＤｉｓｐｌａｙ	１．４０	ＴＸＴ２ＰＦＤｉｓｐｌａｙ