

C u b i c S y m m e t r y 2 3 & 4 3

Y b 2 O 3 の O D F 解析 (M T E X, L a b o T e x)

2 0 2 1 年 0 1 月 1 0 日

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1. 概要

C u b i c に関して、L a b o T e x では O - C u b i c と T - C u b i c で O D F 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 C u b i c 材料は O - C u b i c であるが、T - C u b i c と考えられる材料である Y b 2 O 3 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↓

S y m m e t r y は 6 で T - C u b i c とし て 解 析 を 行 っ て み ま す。

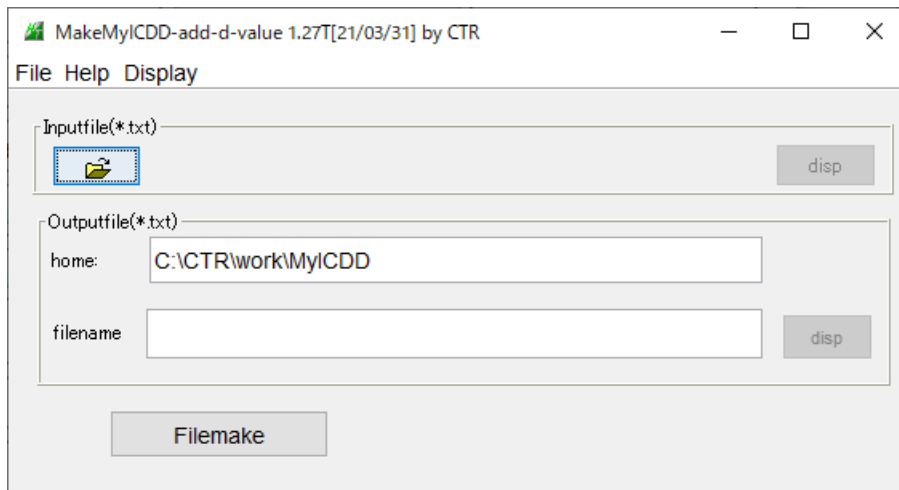
従来 の D a t a B a s e に は 空 間 群 情 報 が 登 録 さ れ て い ま せ ん。

新 規 登 録 方 法、修 正 方 法、S y m m e t r y を 利 用 し て い る ソ フ ト ウ ェ 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。



MakeMyICDD-add-d-value 1.27T[21/03/31] by CTR

File Help Display

Inputfile(*.txt)

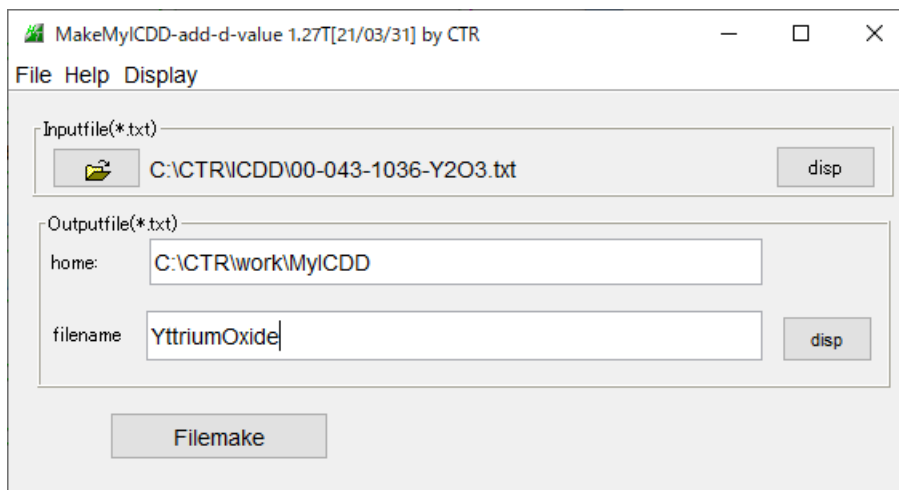
Outputfile(*.txt)

home: C:\CTR\work\MyICDD

filename

Filemake

入力データを選択



MakeMyICDD-add-d-value 1.27T[21/03/31] by CTR

File Help Display

Inputfile(*.txt)

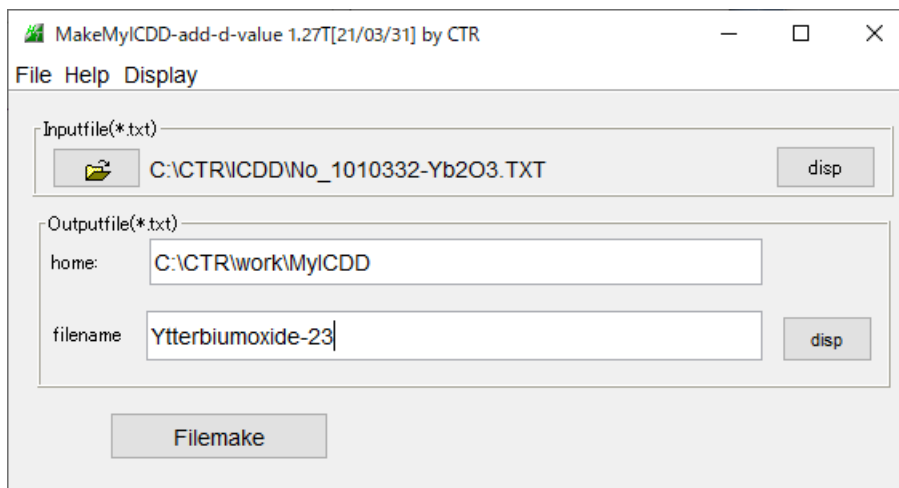
Outputfile(*.txt)

home: C:\CTR\work\MyICDD

filename YttriumOxide

Filemake

C:\CTR\work\MyICDDに登録



MakeMyICDD-add-d-value 1.27T[21/03/31] by CTR

File Help Display


Inputfile(*.txt)

Outputfile(*.txt)

home: C:\CTR\work\MyICDD

filename Ytterbiumoxide-23

Filemake

 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

MaterialDataManual Free 1.01 by CTR

File Help

Create Material data

Material name(File name) Ytterbiumoxide.TXT

Crystal Cubic New

Lattice constat

a axis 10.39 b axis 10.39 c axis 10.39

α 90.0 β 90.0 γ 90.0

Input miller index(3 Axis) & I / Io

Between the data (tab)

Example

1	1	1	100.0	
8	8	2	0.1	1.0188
8	2	6	1.7	1.0188
9	5	0	0.1	1.0092
9	4	3	0.7	1.0092
9	3	4	0.4	1.0092
9	0	5	0.1	1.0092

Wave length 1.54056

☐ LaboTex(a<=b<=c α <=90 β <90 γ <=90)

Chemical Formula: Yb2 O3

cif

cif

_symmetry_space_ggroup_name_H-M

_symmetry_Int_Tables_number 0

symmetry 0 Set

Disp Cancel Return structure Modification

c i f ファイルを選択か直接入力する。

cif

cif

_symmetry_space_ggroup_name_H-M I213

_symmetry_Int_Tables_number 199

symmetry 23 Set

Disp Cancel Return structure Modification

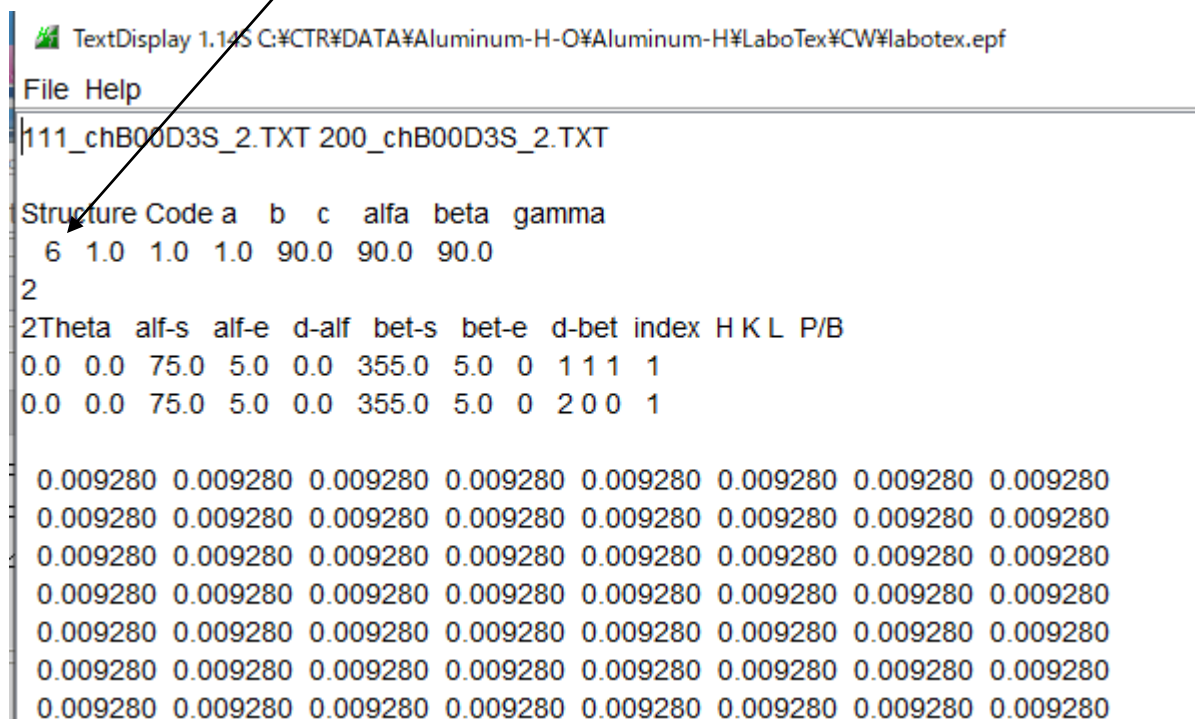
Modification

で変更する。

Disp

で確認出来ます。

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

EBSDtoLaboTex 3.05T[21/03/31] by CTR

File Help amgdatacheck

Material

Material Ytterbiumoxide-23

Lattice constant

Structure Code(symmetries after Schoenflies) 6 - T (cubic)

a 1.0 b 1.0 c 1.0 alfa 90.0 beta 90.0 gamma 90.0

Step for output O...

5.0

Weight for data

1-present

Angle Unit

1-rad

Angle Convention

0-Bunge

Input data format

Check data Line 200 Phase position 8 Select phasenumbe 1 IQ 6

No of data Line

Out data Line 8 P1 1 F 2 P2 3

3: # Formula

4: # Symmetry 23

5: # LatticeConstants 10.39 10.39 10.39 90.0 90.0 9

6: #

7: # GRID: SqrGrid#

8: 0.000 0.785 0.000 0.000 0.000 1.0

Comment

U:¥2021-01-09-Yb2O3¥Ytterbiumoxide-23.ang

LaboTexFile(toRadian.SOR)

TexToolsFile(OIMRad.ang)

ToAngle

Brucker(Angle-TXT)-MTEX(Radian-Ang)

DataAppend

toRadian

0: U:¥2021-01-09-Yb2O3¥Ytterbiumoxide-23.ang

1:

2: Structure Code a b c alfa b

3: 6 1.0 1.0 1.0 90.0 90.0 90.0

4: 0.0 0.785 0.0 1.0

5: 5.934 2.793 0.0 1.0

Comment

U:¥2021-01-09-Yb2O3¥Ytterbiumoxide-23.ang

LaboTexFile(toRadian.SOR)

TexToolsFile(OIMRad.ang)

ToAngle

3. Y b 2 O 3、S y m m e t r y (2 3) の E B S D データ作成

EBSDAngdataMaker 1.00T[21/03/31] by CTR

File

Help

Material

Materi...cifSymmetry number23MaterialnameYtterbiumoxide-23

LatticeConstants10.3910.3910.3990.090.090.0

GRID: SqrGrid#

Number20400

Data eulerangle(f1,F,f2) angles

☒10.000450.000

☒2150300.000

☒3310700.000

☐40.0000.0000.000

☐50.0000.0000.000

☐60.0000.0000.000

☐70.0000.0000.000

☐80.0000.000.000

☐90.0000.0000.000

☐100.0000.0000.000

Makefileholder

U:¥2021-01-09-Yb2O3¥SYM23¥Ytterbiumoxide-23.ang

makefile

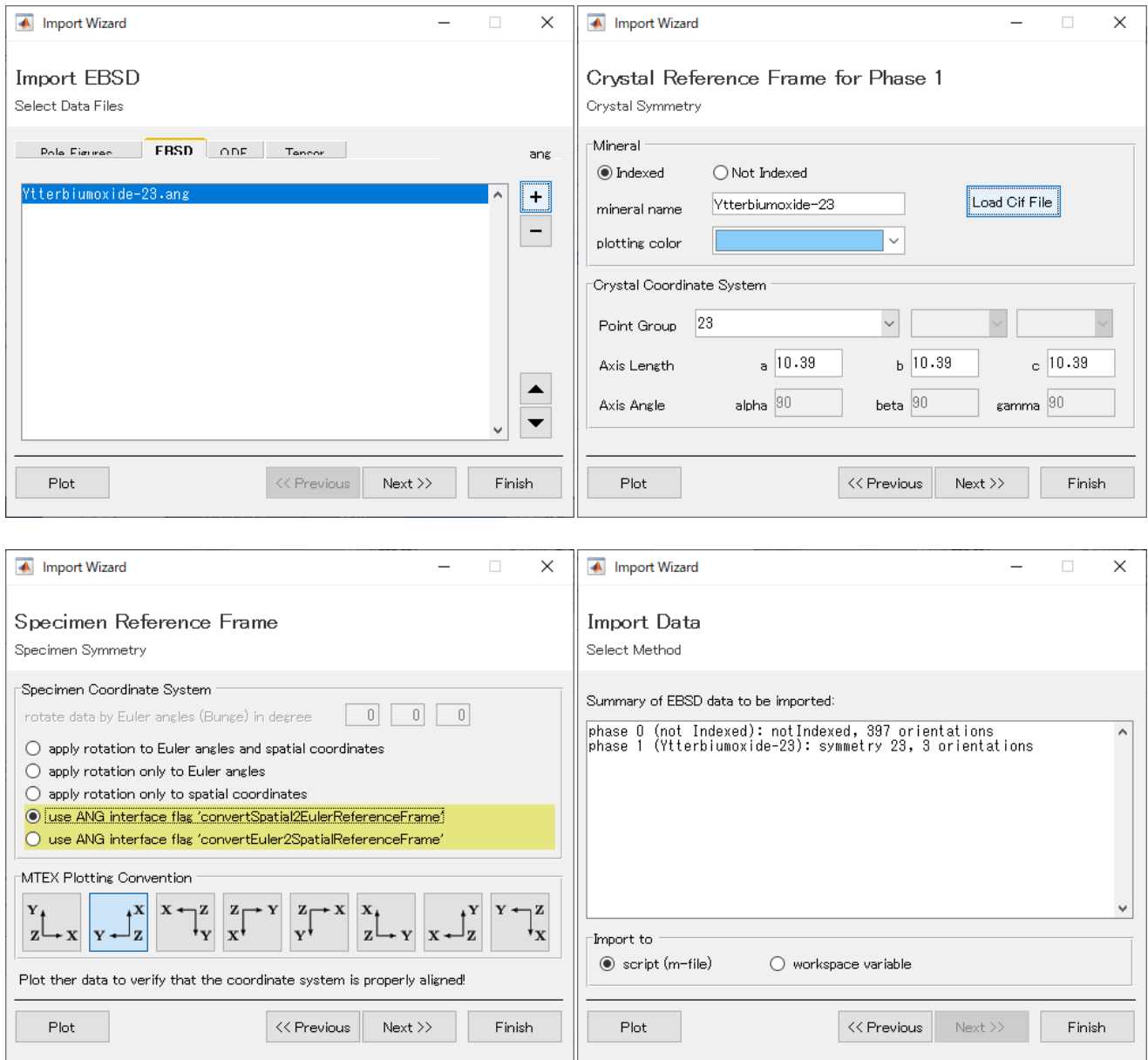
TextDisplay 1.14S U:¥2021-01-09-Yb2O3¥SYM23¥Ytterbiumoxide-23.ang

File

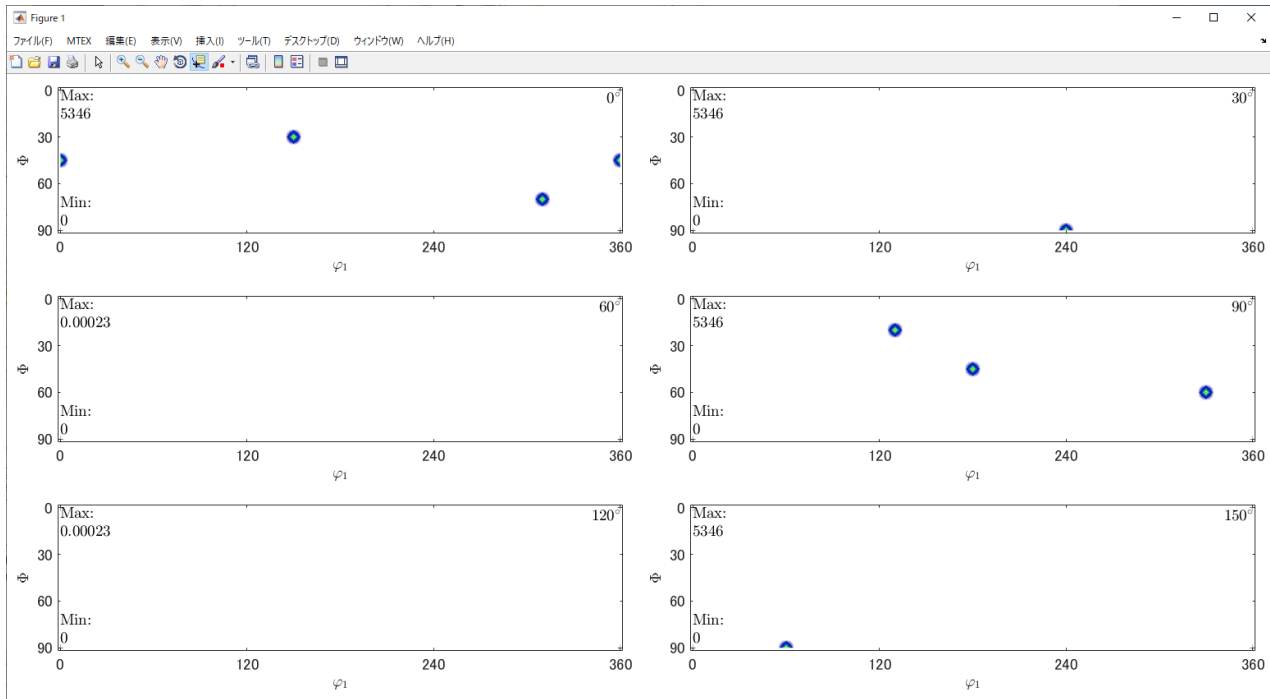
Help

```
#
# Phase 1
# MaterialName    Ytterbiumoxide-23
# Formula
# Symmetry        23
# LatticeConstants 10.39 10.39 10.39 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
```

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

EBSDtoLaboTex 3.05T[21/03/31] by CTR

File Help amgdatacheck

Material
Material Ytterbiumoxide-23

Lattice constant
Structure Code(symmetries after Schoenflies) 6 - T (cubic)

a 1.0 b 1.0 c 1.0 alfa 90.0 beta 90.0 gamm 90.0

Step for output O... 5.0 Weight for data 1-present Angle Unit 1-rad Angle Convention 0-Bunge

Input data format
Check data Line 200 Phase position 8 Select phasenum 1 IQ 6
No of data Line
Out data Line 8 P1 1 F 2 P2 3

```
5: # Lattice constants 10.00 10.00 10.00 90.0 90.0 90.0
6: #
7: # GRID: SqrGrid#
8: 0.000 0.785 0.000 0.000 0.000 1.0
9: 2.618 0.524 0.000 1.000 0.000 1.0
10: 5.411 1.222 0.000 2.000 0.000 1.0
11: 0.000 0.000 0.000 3.000 0.000 1.0
```

Comment
U¥2021-01-09-Yb2O3\$SYM23\$Ytterbiumoxide-23.ang

LaboTexFile(toRadian.SOR) TexToolsFile(OIMRad.ang) ToAngle
Bruker(Angle-TXT)-MTEX(Radian-Ang) DataAppend toRadian

Lattice constant
Structure Code(symmetries after Schoenflies) 6 - T (cubic)

a 1.0 b 1.0 c 1.0 alfa 90.0 beta 90.0 gamm 90.0

Step for output O... 5.0 Weight for data 1-present Angle Unit 1-rad Angle Convention 0-Bunge

Input data format
Check data Line 200 Phase position 8 Select phasenum 1 IQ 6
No of data Line
Out data Line 8 P1 1 F 2 P2 3

```
2: Structure Code a b c alfa b
3: 6 1.0 1.0 1.0 90.0 90.0 90.0
4: 0.0 0.785 0.0 1.0
5: 2.618 0.524 0.0 1.0
6: 5.411 1.222 0.0 1.0
```

La b o T e xに読み込み

New Sample

Choose Experimental Data (LaboTex Single Orientations Files)

☐ EPF
 ☐ PPF
 ☒ SOR
 ☐ NJC
 ☐ NJA
 ☐ RW1
 ☐ epf
 Selected : 1

Ytterbiumoxide-23toRadian.SOR

Path: U:\2021-01-09-Yb2O3\SYM23\ Ytterbiumoxide-

Info: U:\2021-01-09-Yb2O3\SYM23\Ytterbiumoxide-23.ang

Crystal Symmetry: T (Cubic)

Project Name: Demo

Choose Defocussing Correction

☒ Correction (On/Off)

☒ Correction Data from File
 ☐ Correction Data from Formula

(COR,POW,DFB,ASC,PPG,NJA,DAT,POL,NJC,COA,RWA,UXD,EXP)

Cor(1x1).cor
Cor(5x5).cor

Path: C:\LaboTex2\USER\1EBSD.LAB\COR\

Info:

Sample Name: SiO2toRadian-T
T_Cubic

Sample Name: Yb203-23

Cancel Create of ODF from Single Orientations Data

Project

Demo

Crystal Symmetry

T-Cubic

Angle Convention for Data

Bunge

Grid Cells for Output ODF

5.0*5.0

Angle Unit

Radians

Weight

Yes

Phase

0

Descriptions

U:\2021-01-09-Yb2O3\SYM23\Ytterbiumoxide-23.ang

Single Orientations Files

Ytterbiumoxide-23toRadian.SO

Calculations Progress

Merge (files)



No of single orien.

'SOR' Output File Options

Add (HKL)<UVW>

Max. Value of Miller Indices = 15

Hexagonal Axis Convention of Data (important only in Hexagonal C.S.)

☒ 
☐ 

Warning: If your file contains non-indexed data, then you should use "EBSD Format - Defined by User" (Menu "Edit", "LaboTex Options", "Data Formats")

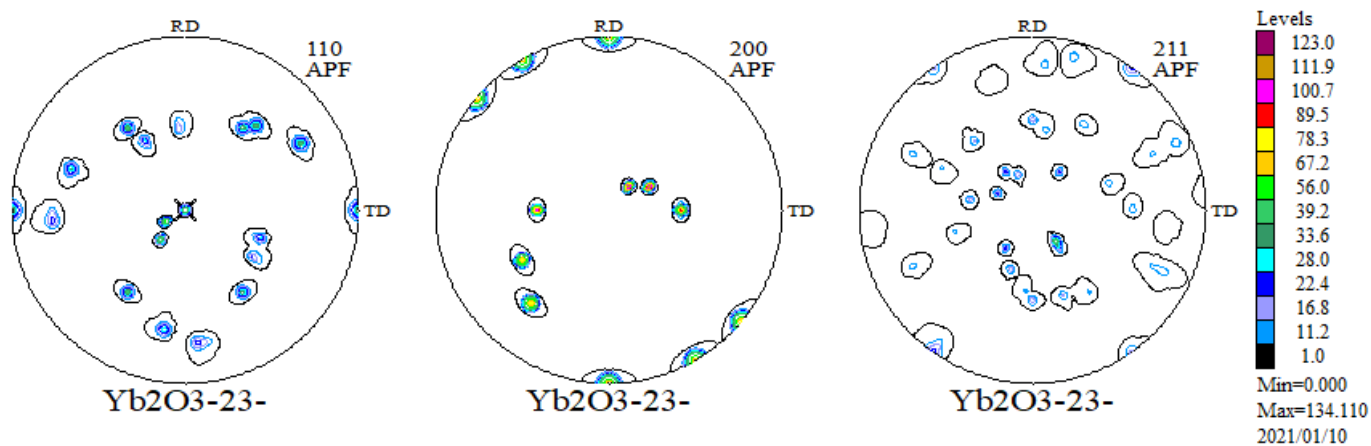
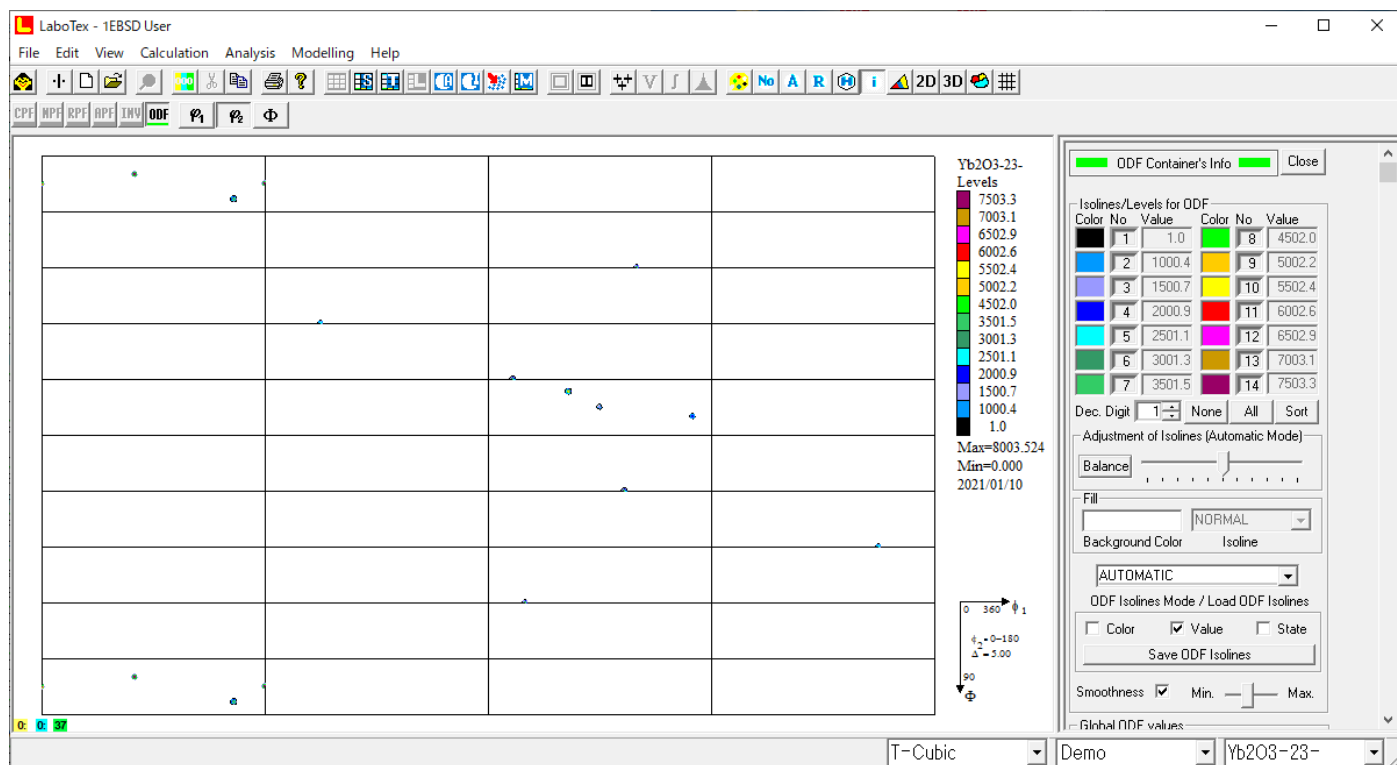
In this format you can exclude non-indexed data from ODF calculation.

Non-indexed data can create false maximum on the ODF!

In case of problems, please contact the office@labosoft.com.pl

RUN

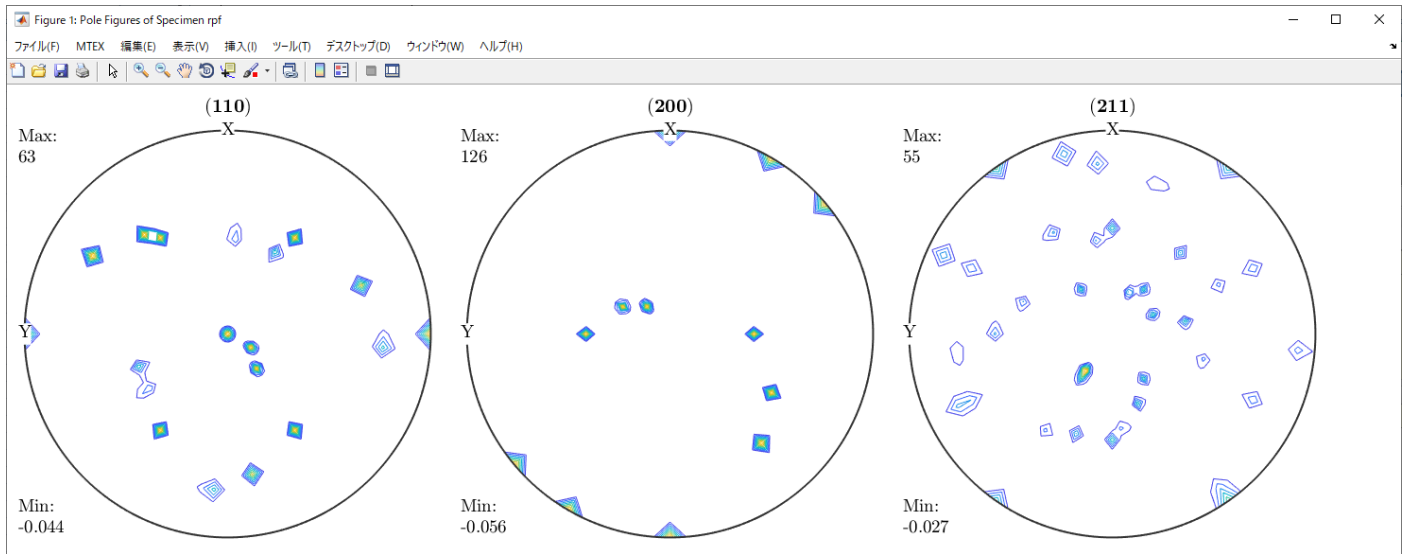
END



MTEXとODF図は一致

3. 3 MTEXODF後のPFデータE x p o r t 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')
```

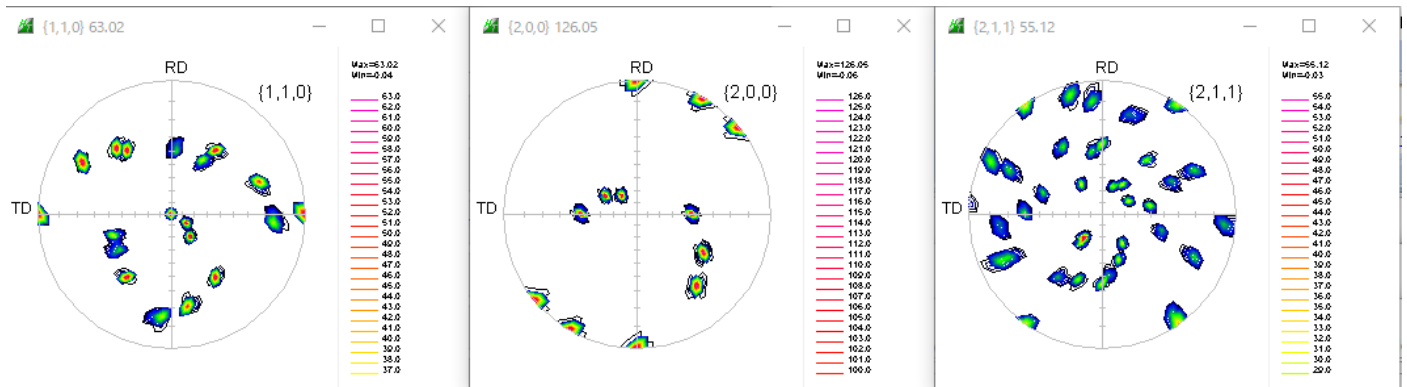


極点図のTD方向はL a b o T e xに対し180度回転している。

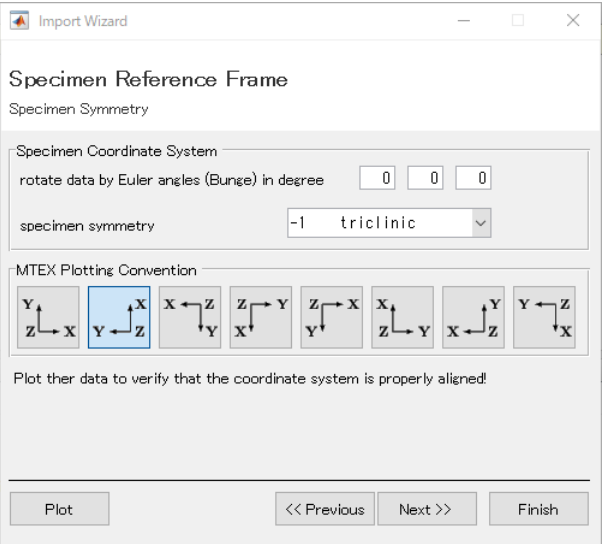
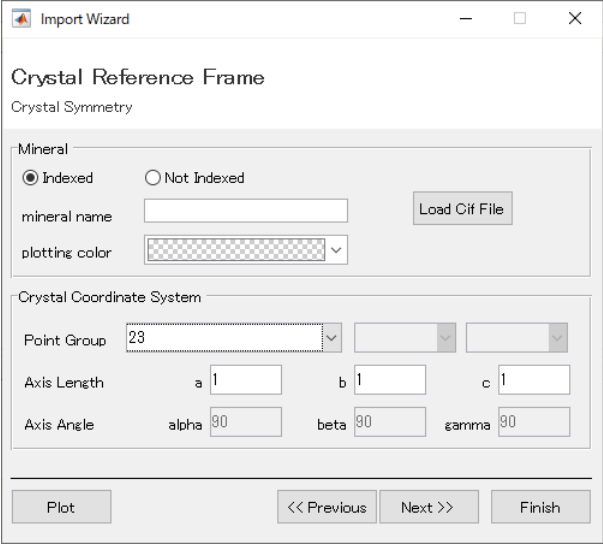
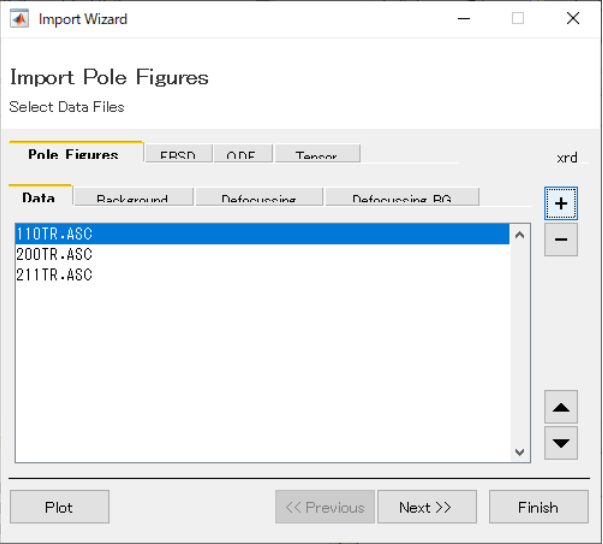
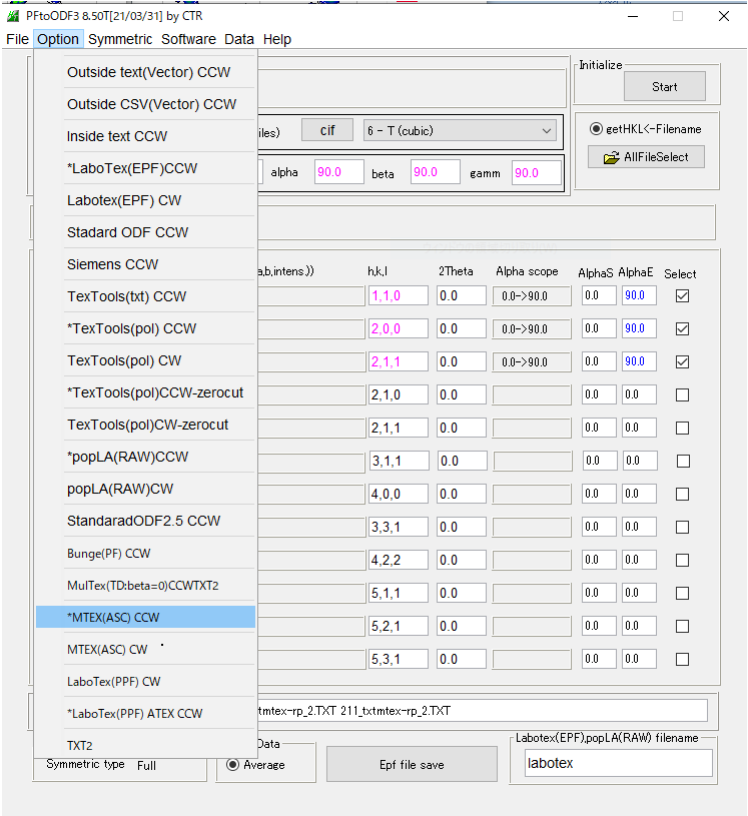
M T E X - C C W 一般的

L a b o T e x - C W

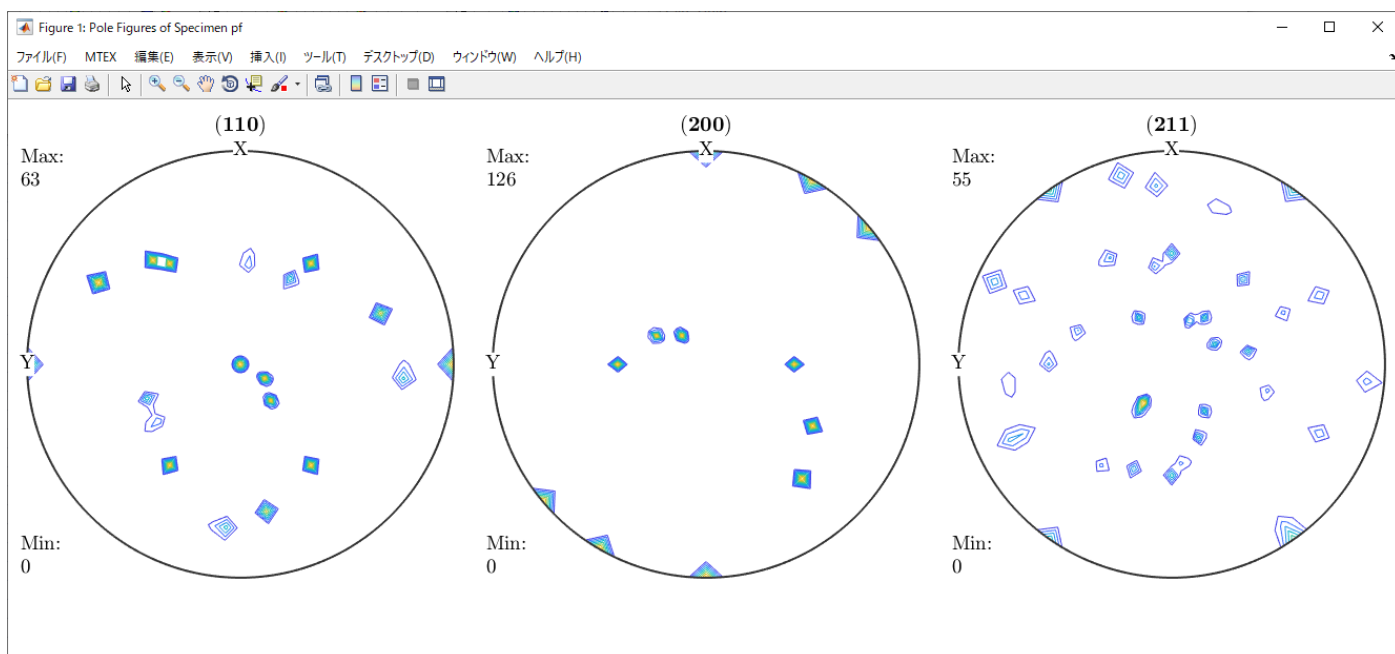
再計算極点図をE x p o r t



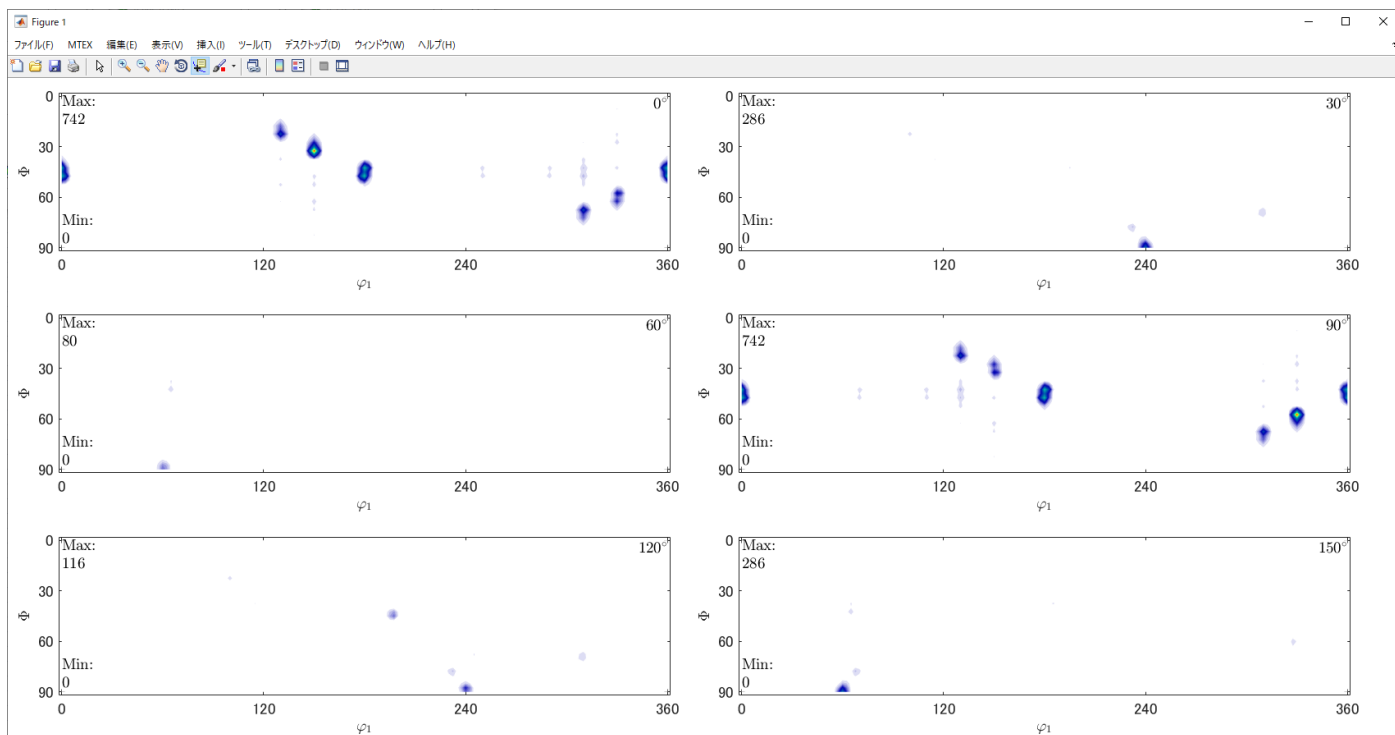
3. 3. 1 MTEX解析



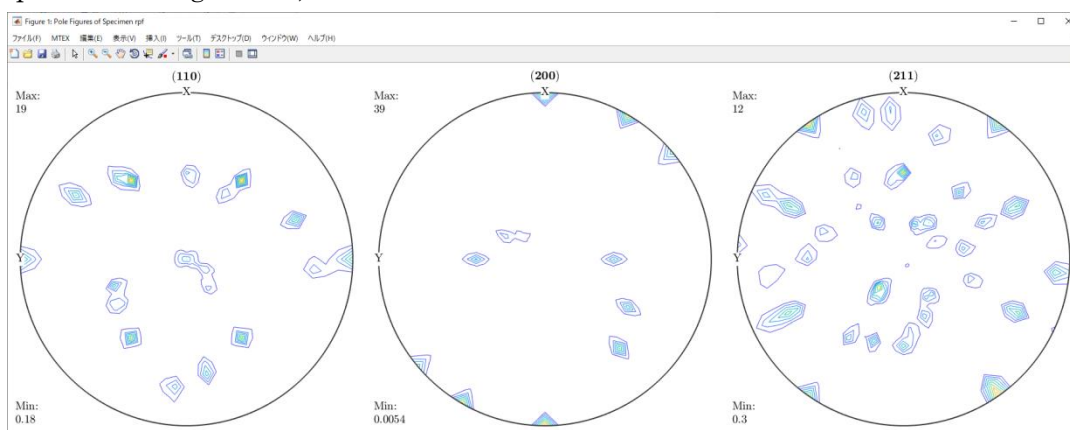
```
plot(pf,'contour','projection','eangle')
```



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



```
rpf=calcPoleFigure(odf,h)
```



4. Y b 2 O 3 , S y m m e t r y (4 3) の E B S D データ作成

EBSDAngdataMaker 1.00T[21/03/31] by CTR

File

Help

Material

Materi...cifSymmetry number43MaterialnameYttriumOxide-43

LatticeConstants10.60410.60410.60490.090.090.0

GRID: SqrGrid#

Number20400

Data eulerangle(f1,F,f2) angles

☒10.000450.000

☒2150300.000

☒3310700.000

☐40.0000.0000.000

☐50.0000.0000.000

☐60.0000.0000.000

☐70.0000.0000.000

☐80.0000.000.000

☐90.0000.0000.000

☐100.0000.0000.000

Makefileholder

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

makefile

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

File Help

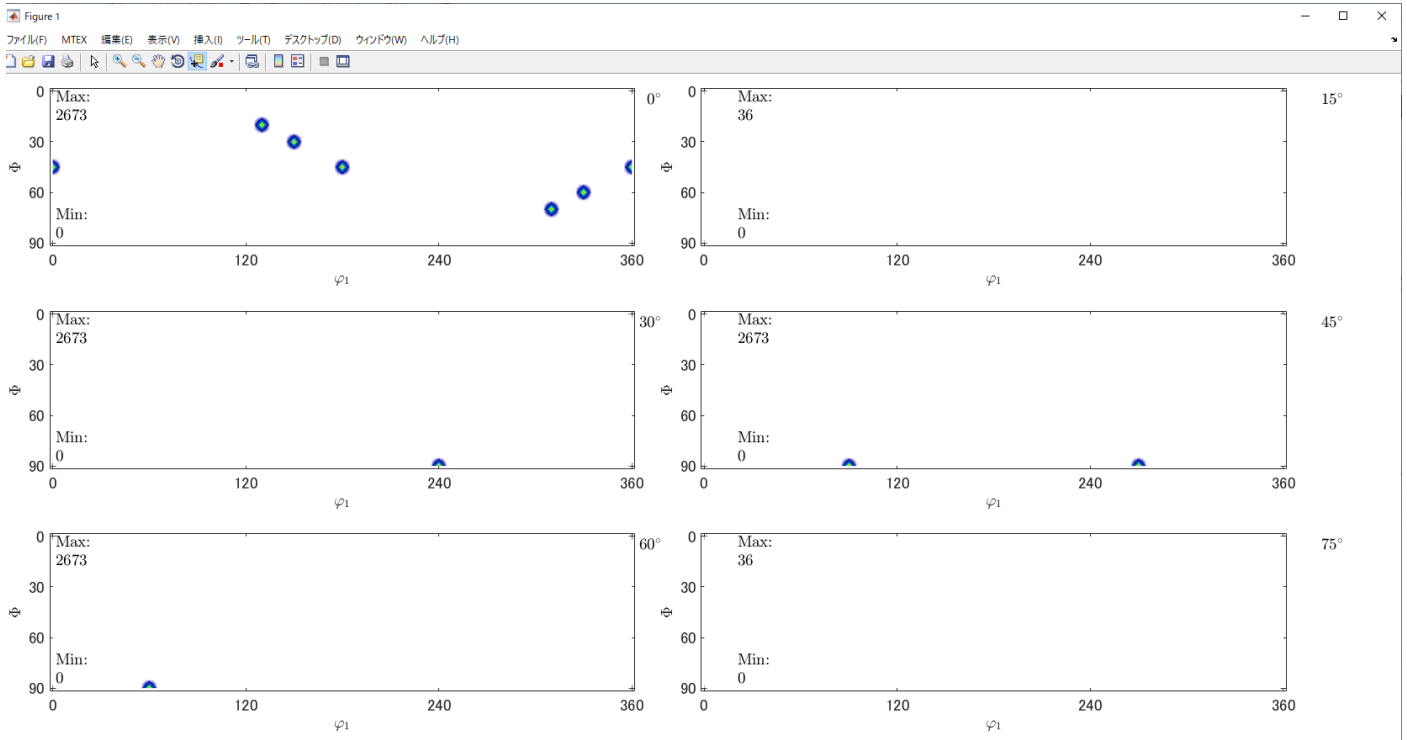
```
#
# Phase 1
# MaterialName YttriumOxide-43
# Formula
# Symmetry 43
# LatticeConstants 10.604 10.604 10.604 90.0 90.0 90.0
#
# GRID: SqrGrid#
0.000 0.785 0.000 0.000 0.000 1.0 1.0 1 1
2.618 0.524 0.000 1.000 0.000 1.0 1.0 1 1
5.411 1.222 0.000 2.000 0.000 1.0 1.0 1 1
0.000 0000 0.000 3.000 0.000 1.0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

4. 1 MTEX解析

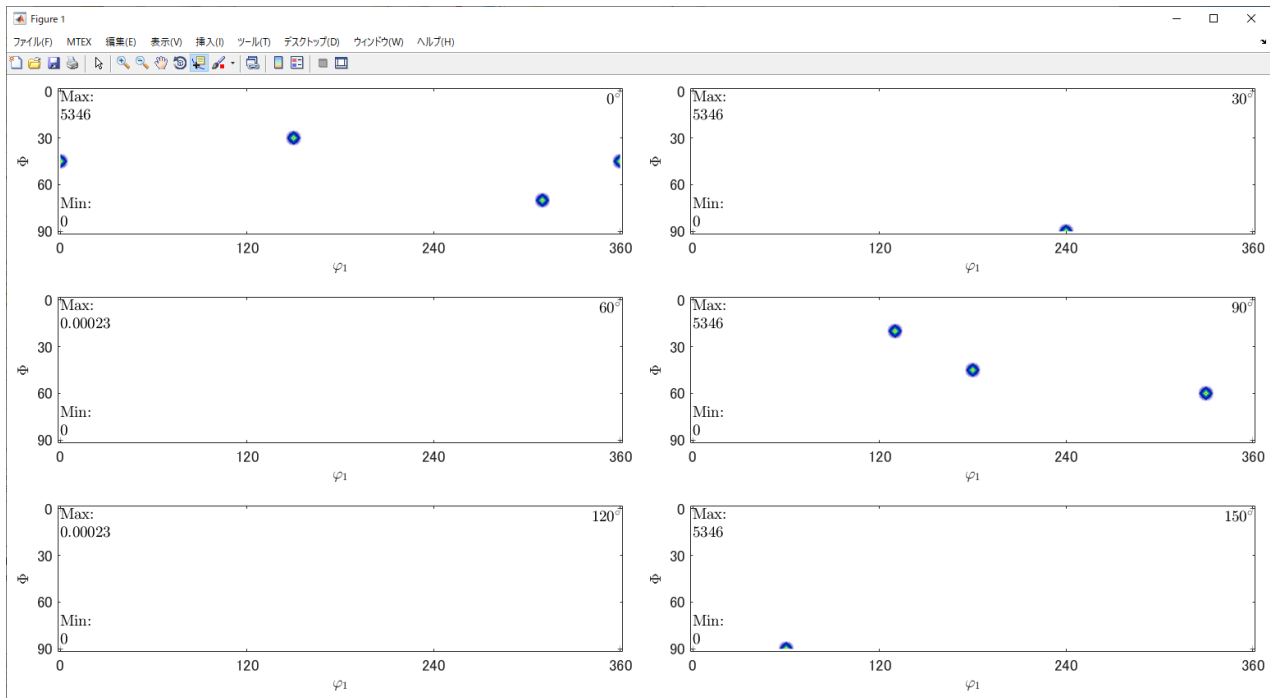
処理はSymmetry (23) と同様に

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

Symmetry(43) ϕ 2Max=90

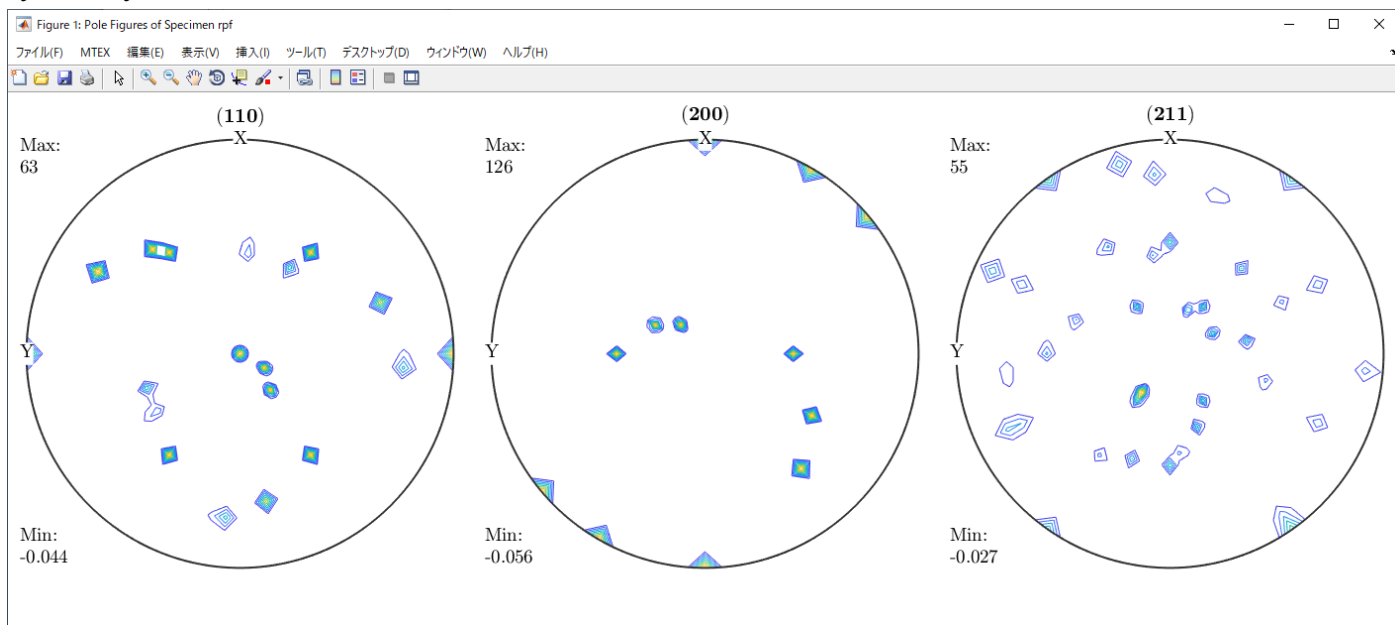


Symmetry(23) ϕ 2Max=180

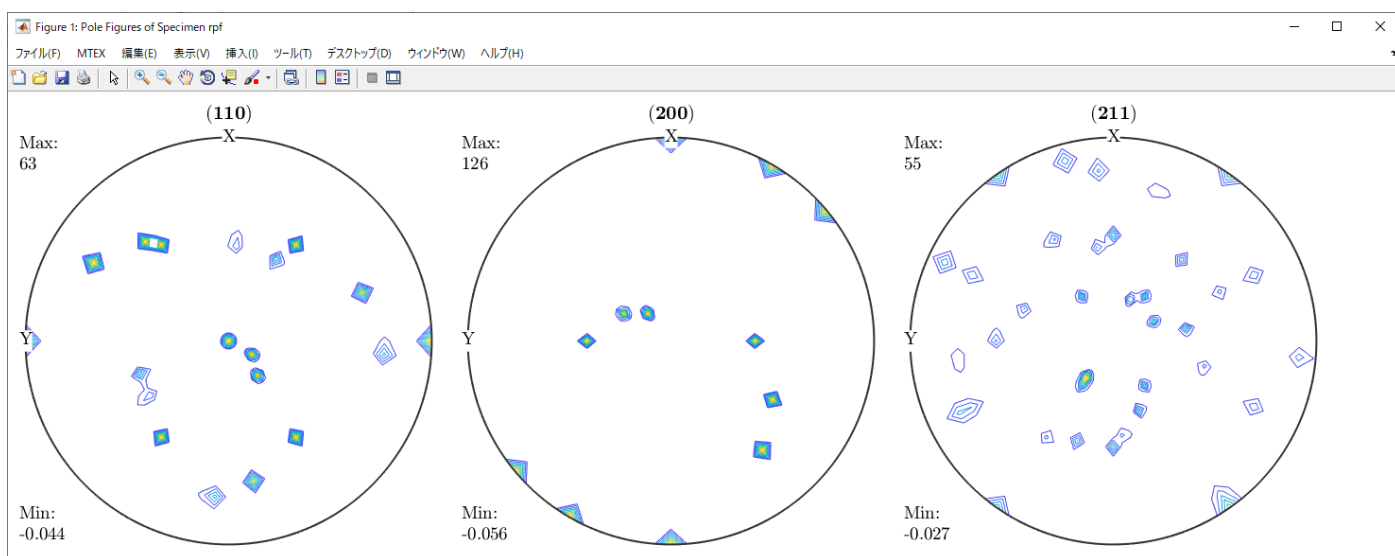


再計算極点図

Symmetry(43)



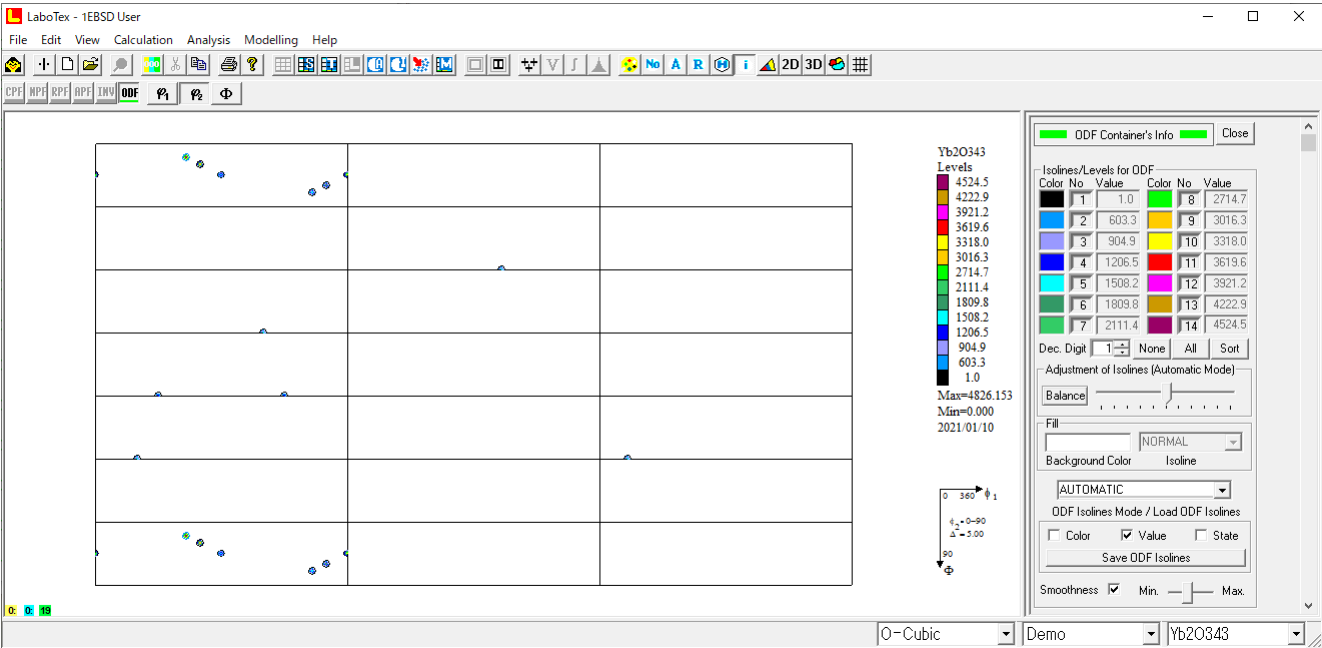
Symmetry(23)



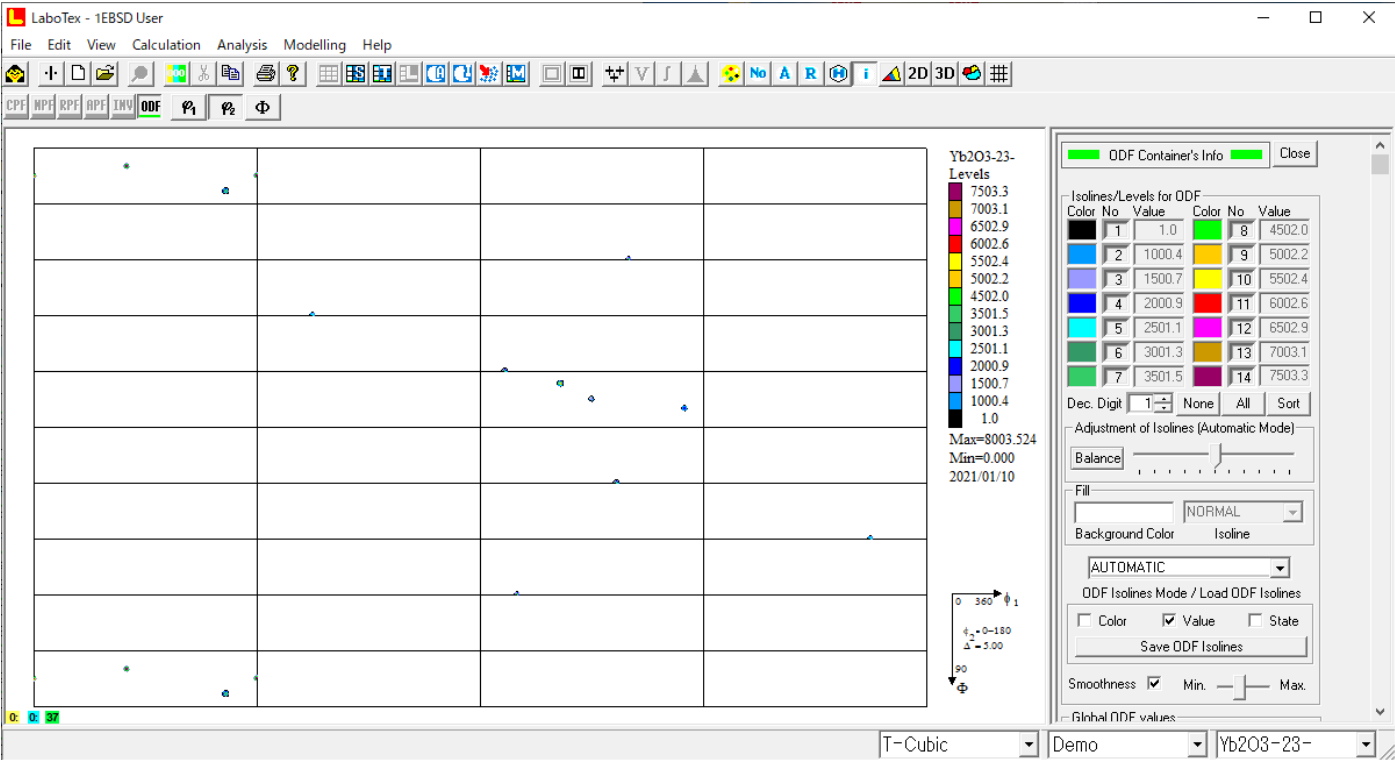
MTEXの比較では、ODF図は異なるが極点図は一致する

4. 2 L a b o T e x 解析

Symmetry(43)

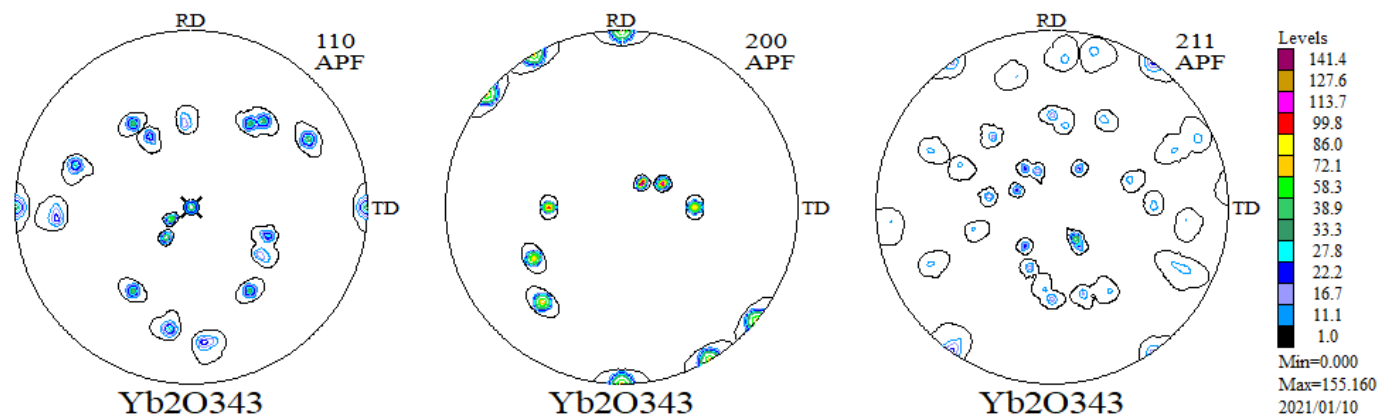


Symmetry(23)

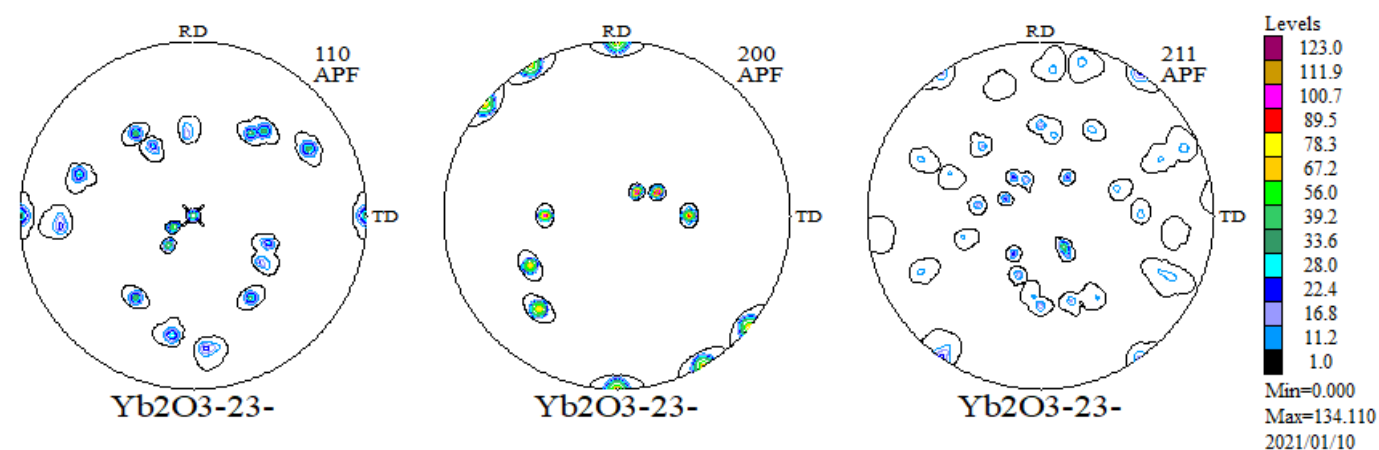


再計算極点図比較

Syymetry(43)



Symmetry(23)



使用したソフトウェア

EBSDAngdataMaker	1. 0 0	EBSDAngデータ作成
EBSDtoLaboTex	3. 0 5	AngデータからSORデータ変換
MATLAB	R 2 0 1 7 b	MTEX環境
MTEX	5. 4. 0	ODF解析
LaboTex	5. 0. 5 0	ODF解析
PFtoODF3	8. 5 0	XRD PF→ODF
MakePoleFile	1. 8 9	MTEX PF→TXT2
GPPoleDisplay	1. 4 0	TXT2 PF Display