Yb2O3のODF解析 (MTEX, LaboTex)

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

2021年01月10日 *HelperTex Office*

- 1. 概要
- 2. Symmetrycode
 - 2.1 MYICDDに登録
 - 2. 2 空間群が登録されていないデータの場合
 - 2.3 XRD極点図のLaboTex向けEPFデータ作成
 - 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
 - 3. 2 LaboTexの解析
 - 3.3 MTEXODF後のPFデータExportしXRD極点図として
 - 3.3.1 MTEX解析
 - 3. 3. 2 LaboTex解析
- 4. Yb2O3, Symmetry (43)のEBSDデータ作成
 - 4.1 MTEX解析
 - 4. 2 LaboTex解析

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	Cubi	ic**	Hexa	gonal	Tetra	agonal	Tri	gonal	Ortho- rhombic	Mono- clinic	Triclinic
		0	Т	D ₆	C ₆	D_4	C_4	D ₃	C ₃	D_2	C ₂	C1
Lab	oTex	7	6	11	10	5	4	9	8	3	2	1
stru	icture code											
	triclinic* (C1)	360°	360°	360°	360°	360°	360°	360°	360°	360°	360°	360°
φ ₁	monoclinic* (C2)	180°	180°	180°	180°	180°	180°	180°	180°	180°	180°	180°
	orthorhombic*(D2)	90°	90°	90°	90°	90°	90°	90°	90°	90°	90°	90°
	axial*	_***	-	-	-	-	-	-	-	-	-	-
Φ	•	90°	90°	90°	180°	90°	180°	90°	180°	90°	180°	180°
• 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:\U00e4CTR\U00e4DATA\U00e4EBSDtoLaboTex\U00e4SpaseG.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	61	
201	Pn3	23	6↓	
202	Fm 3	23	6↓	
203	Fd3	43	7↓	
204	Im 3	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。

🎽 MakeMyl	DD-add-d-value 1.27	T[21/03/31] by CTR	_		×
File Help D	isplay				
* 101 fee					
Inputfile(*.tx	t) ———				
~				di	sp
_Outputfile(*	(.txt)				
home:	C:\CTR\work\My	CDD			
filename				di	sp
		_			
	Filemake				
		4			

入力データを選択

MakeMyl Eile Help D	CDD-add-d-value 1.27T[21/03/31] by CTR	_		×
Inputfile(*.t:	xt) C:\CTR\ICDD\00-043-1036-Y2O3.txt		disp	
Outputfile(*txt) C:\CTR\work\MyICDD			
filename	YttriumOxide		disp	
	Filemake			

C:¥CTR¥work¥MYICDD に登録

🌌 MakeMyl	CDD-add-d-value 1.27T[21/03/31] by CTR	_		×
File Help D	isplay			
Inputfile(*.t	xt) C:\CTR\ICDD\No_1010332-Yb2O3.TXT		disp	
Outputfile(*.txt) C:\CTR\work\MyICDD			
filename	Ytterbiumoxide-23		disp	
	Filemake			

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

File Help						
Ytterbiumoxi	de-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		da	ata_1010332(C	COD)		Ytterbium oxide
_symmetry_s	space_group_	name_H-M	' 213'			
_symmetry_l	nt_Tables_nu	mber 1	99			
_Symmetry		23				

2. 2 空間群が登録されていないデータの場合

MaterialDat	aManual Free 1	.01 by CTF	2			_		×
File Help								
Create Materi	al data							
Ê	Material nam	ne(File n	ame) Ytterbiumo	xide.TXT			
Crystal	Cubic					~	New	
Lattuce co	nstat							
a axis	10.39	b a	xis	10.39	c axis	10.39		
α	90.0	β		90.0	Y	90.0		
Input mill	ler index(3 Axis)	& I/lo-						
B-4	Alex - 74-13	Examp	le —					
Between	ithe data (tab)	1	1	1 100.0				
		8	6	2	0.1	1.0188		^
		8	2	6 0	1.7	1.0002		
		9	4	3	0.7	1.0032		
		9	3	4	0.4	1.0092		
		9	0	5	0.1	1.0092		
								/
1.54056	\ \		Labo	Tex(a<=b<=b<:	=c α<=90 β<9	0 γ<=90		
Chemical Fo	ormula:				_			
	Yb2 O	3						
_⊂if								1
cif								
_symme	etry_space_grro	oup_name	e_H-I	N				
_symmet	ry_Int_Tables_r	number		0				
symmetry	1			0		Set		
Disp	Canc	el	R	eturn structu	ire	Modificatio	on	
								-
<u> </u>								

c i f ファイルを選択か直接入力する。

cif		
_symmetry_space_grroup_name_H-M	I213]
_symmetry_Int_Tables_number	199	
symmetry	23	Set
eif cif _symmetry_space_grroup_name_H-M [213 _symmetry_Int_Tables_number 199 symmetry 23 Set Disp Cancel Return structure Modification Modification		
Modification	Disp	

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。

						_	
PFtoODF3 8.501[21/03/31] by CTR					_		×
File Option Symmetric Software Data Help				-1			
				Initializ	e		
Material Ytterbiumoxide-23.txt					S	tart	
Structure Code(Symmetries after Schoenfiles) Cif	6 - T (cubic))	~	• ce	etHKL<-F	Filename	
a 1.0 <=b 1.0 <=c 1.0 alpha 90.0	beta 90.0	0 gan	nm 90.0		≱ AllFileS	Select	
PF Holder							
C:#CTR#DATA#Aluminum-H-O#Aluminum-H							
PF Data SelectFile(TXT(b,intens),TXT2(a,b,intens.))	h,k,l	2Theta	Alpha scope	AlphaS	AlphaE	Select	
111_chB00D3S_2.TXT	1,1,1	0.0	0.0->75.0	0.0	75.0		の領域
200_chB00D3S_2.TXT	2,0,0	0.0	0.0->75.0	0.0	75.0	\checkmark	
	2.0.0	0.0		0.0	0.0		
File Help				pi			
Structure Code a b c alfa beta gamma							
2Theta alf-s alf-e d-alf bet-s bet-e d-bet	index H K	L P/B					
0.0 0.0 75.0 5.0 0.0 355.0 5.0 0 111	1						
0.0 0.0 75.0 5.0 0.0 355.0 5.0 0 200) 1						
0.009280 0.009280 0.009280 0.009280 0.0	09280 0.0	09280	0.009280	0.0092	280		
0.009280 0.009280 0.009280 0.009280 0.0	09280 0.0	09280	0.009280	0.0092	280		
0.009280 0.009280 0.009280 0.009280 0.0	0.0 09280	09280	0.009280	0.0092	280		
0.009280 0.009280 0.009280 0.009280 0.0	09280 0.0	09280	0.009280	0.0092	280		
0.009280 0.009280 0.009280 0.009280 0.0	09280 0.0	09280	0.009280	0.0092	280		
0.009280 0.009280 0.009280 0.009280 0.0	09280 0.0	09280	0.009280	0.0092	280		
0.009280 0.009280 0.009280 0.009280 0.0	09280 0.0	09280	0.009280	0.0092	280		

2. 4 EBSDデータからLaboTex入力のSORファイル作成

нер	amgdatacheck
Materi	al
	Material Ytterbiumoxide-23
.attice	constant
Stru	Icture Code(symmetries after Schoenfiles) 6 - T (cubic) ~
a	1.0 b 1.0 c 1.0 alfa 90.0 beta 90.0 gamm 90.0
Step f 5.0	or output 0 Weight for data 1-present Angle Unit Angle Convention 0-Bunge
Input o	Jata format
Cł F ^{No}	peck data Line 200 Phase position 8 Select phasenumber 1 IQ 6
0	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#
C	>
Comme	ent
U:¥20	21-01-09-Yb2O 3¥Ytterbiumoxide-23 ang
Lat	boTexFile(toRadian.SOR) TexToolsFile(OIMRad.ang) To Angle
Bru	iker(Angle TXT)-MTEX(Radian Ang) DataAppend toRadian
	0: U:¥2021-01-09-Yb203¥Ytterbiumoxide-23.ang
	1: 2: Structure Code a h a alfa
	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
	at
mmer	
mmer :¥202	1-01-09-Yb2O3¥Ytterbiumoxide-23lang
mmer :¥202	1-01-09-Yb2O3¥Ytterbiumoxide-23.ang

3. Yb2O3、Symmetry (23)のEBSDデータ作成

 EBSDAngdataMaker 1. File Help 	00T[21/03/3	31] by CTR					-		×
Material									
Materi cif	Symmetry	number 🚦	23 Ma	terialnai	me Yttert	iumoxide-2	23		
LatticeConstants 1	0.39	10.39	10.39	9	0.0	90.0	90.0		
GRID: SqrGrid#									
Number 20	400								
Data eulerangle(f1,F,f2)	angles ——								
1 0.000	45	0.000		2	150	30	0.000)	
3 310	70	0.000		4	0.000	0.000	0.000)	
5 0.000	0.000	0.000		6	0.000	0.000	0.000)	
7 0.000	0.000	0.000		8	0.000	0.000	.000		
9 0.000	0.000	0.000		10	0.000	0.000	0.000)	
Makefileholder	U:	¥2021-01-	09-Yb2O3¥	SYM23¥	fYtterbiumo	oxide-23.ang			
		m	akefile						

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

File Help

#									
# Phase	e 1								
# MaterialName Ytterbiumoxide-23									
# Formu	ıla								
# Symm	etry	23							
# Lattice	eConsta	nts 10.3	39 10.39	9 10.39	90.0	90.0 90.0			
#									
# GRID:	SqrGrid	d#							
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

Import Wizard – 🗆 X	Import Wizard – 🗆 🗙
Import EBSD Select Data Files	Crystal Reference Frame for Phase 1 Crystal Symmetry
Pole Figure FBSD ODE Tencor and	Mineral Mineral Indexed Not Indexed mineral name Ytterbiumoxide-23 Load Cif File plotting color Crystal Coordinate System Point Group 23 Axis Length a 10.39 b 10.39 c 10.39 Axis Angle alpha 90 beta 90 gamma 90
Plot Kext >> Finish	Plot Kext >> Finish
Million Import Wizard – 🗆 X	Mittard – X
Specimen Reference Frame Specimen Symmetry	Import Data Select Method
Specimen Coordinate System rotate data by Euler angles (Bunge) in degree 0 0 o apply rotation to Euler angles and spatial coordinates o apply rotation only to Euler angles o apply rotation only to Euler angles o apply rotation only to spatial coordinates • juse ANG interface flag 'convertSpatial2EulerReferenceFrame! • use ANG interface flag 'convertEuler2SpatialReferenceFrame'	Summary of EBSD data to be imported: phase 0 (not Indexed): notIndexed, 397 orientations phase 1 (Ytterbiumoxide-23): symmetry 23, 3 orientations
MTEX Plotting Convention $\begin{array}{c} Y \\ z \rightarrow x \end{array} \xrightarrow{Y} z \end{array} \xrightarrow{X} \begin{array}{c} x \rightarrow z \\ y \rightarrow z \end{array} \xrightarrow{Y} y \end{array} \xrightarrow{Z} \begin{array}{c} z \rightarrow y \\ x \rightarrow y \end{array} \xrightarrow{Y} y \xrightarrow{Y} y$	Import to script (m-file) O workspace variable
Plot Kernick Kernick Finish	Plot K Previous Next >> Finish

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 –	×
ile Help amgdatacheck	
_ Material	
Material Ytterbiumoxide-23	
Lattice constant	
Structure Code(symmetries after Schoenfiles) 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 Weight for data Angle Unit Angle Convention	
5.0 V 1-present V 1-rad V 0-Bunge V	
Input data format	
Check data Line 200 Phase position 8 Select phasenumber 1 IQ 6	
Out data Line 8 P1 1 F 2 P2 3	
0. # LatticeConstants 10.00 10.00 10.00 00.0	^
0. # 7. # GRID: SarGrid#	
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 0000 0.000 3.000 0.000 1.0	~
< 2	*
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(symmetric	es after So	hoenfile	s) 6 - ⁻	F (cubic)		~	
a 1.0 b 1.0 c	1.0	alfa 🤉	30,0 E	eta 90.0	gamm	90.0	
Step for output O 5.0 v	for data— :ent	~/	Angle Unit – 1-rad	~ Ar	ngle Conven 0-Bunge	tion ~	
_Input data format	/	/					
Check data Line 200	Phase p osi	tion <mark>8</mark>	Select pł	nasenumber	1 IQ	6	
No of data Line	_/						
Out data Line 8	P	1 1	F	2	P2 3	}	
2: Structure Co	Ide	a	b	с	alfa	. 1	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				
							¥
<						>	

LaboTexに読み込み

New Sample	×
Choose Experimental Data (LaboTex Single Orientations Files) CEPF CPPF SOR NJC NJA RW1 epf Selected : 1	Crystal Symmetry T (Cubic)
Ytterbiumoxide-23toRadian.SOR	Project Name Demo
Path U:\2021-01-09-Yb203\SYM23\ Ytterbiumoxide-	
Info U:\2021-01-09-Yb203\SYM23\Ytterbiumoxide-23.ang	Project Name : Demo
Choose Defocussing Correction Correction (On/Off) Correction Data from File Correction Data from Fi	Sample Name
Info	Sample Name : Yb203-23
Create of ODF from Si	ngle Orientations Data

Project	Sample-
Demo	XF503.53
Demo	1020323
Crystal Symmetry	Cell Parameters (Relative)
T-Cubic 💌	a 1.0 b 1.0 c 1.0
Angle Convention for Data	
Bunge 💌	α 90.0 β 90.0 γ 90.0
Grid Cells for Output ODF	ngle Unit Weight Phase
5.0*5.0	Radians 💌 Yes 💌 🛛 💌
Descriptions	
Single Orientations Files	Calculations Progress
Ytterbiumoxide-23toRadian.S	0 Merge (files)
	No of single orien
SUR' Uutput File Uptions	
	ax. Value of Miller Indice = 15 📑
Have a small Anda Chammer Kanniek, F) ata (important only in Hexagonal C.S.) ———
Hexagonal Axis Convention of L	· (
•	° 🔥
arning: If your file contains non-in	c deved data, then you should use "EBSD For
arning: If your file contains non-in - Defined by User'' (Menu	dexed data, then you should use "EBSD Forr "Edit", "LaboTex Options", "Data Formats")
arning: If your file contains non-in • Defined by User'' (Menu In this format you can exc	dexed data, then you should use "EBSD Forr "Edit", "LaboTex Options", "Data Formats") slude non-indexed data from ODF calculation.
arning: If your file contains non-in • Defined by User'' (Menu In this format you can exc Non-indexed data can cre	dexed data, then you should use "EBSD Forr "Edit", "LaboTex Options", "Data Formats") slude non-indexed data from ODF calculation. eate false maximum on the ODF!
arning: If your file contains non-in - Defined by User'' (Menu In this format you can exc Non-indexed data can or In case of problems, plea	dexed data, then you should use "EBSD Form "Edit", "LaboTex Options", "Data Formats") slude non-indexed data from ODF calculation. eate false maximum on the ODF! se contact the office@labosoft.com.pl
arning: If your file contains non-in - Defined by User'' (Menu In this format you can exc Non-indexed data can cr In case of problems, plea	dexed data, then you should use "EBSD Forr "Edit", "LaboTex Options", "Data Formats") clude non-indexed data from ODF calculation. eate false maximum on the ODF! se contact the office@labosoft.com.pl





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

IVIX
 PFtoODF3 8.50T[21/03/31] by CTR
 File Option Symmetric Software Data Help

Outside text(Vester) CCW						_ Initialize		
	-					Start		
Outside CSV(Vector) CCW	_							
Inside text CCW	iles)	CIT	6 - T (cut	nic)	~	getHKL<-Filename		
*LaboTex(EPF)CCW	alpha	90.0	beta 🤇	0.0 ga	mm 90.0	AllFileSelect		
Labotex(EPF) CW]1		
Stadard ODF CCW								
Siemens CCW	a,b, intens	;))	h,k,l	2Theta	Alpha scope	AlphaS AlphaE Select		
TexTools(txt) CCW			1,1,0	0.0	0.0->90.0	0.0 90.0		
*TexTools(pol) CCW			2,0,0	0.0	0.0->90.0	0.0 90.0		
TexTools(pol) CW			2,1,1	0.0	0.0->90.0	0.0 90.0		
*TexTools(pol)CCW-zerocut			2,1,0	0.0		0.0 0.0		
TexTools(pol)CW-zerocut			2,1,1	0.0		0.0 0.0		
*popLA(RAW)CCW			3,1,1	0.0		0.0 0.0		
popLA(RAW)CW			4,0,0	0.0		0.0 0.0		
StandaradODF2.5 CCW			3,3,1	0.0]	0.0 0.0		
Bunge(PF) CCW	_		4,2,2	0.0]	0.0 0.0		
MulTex(TD:beta=0)CCWTXT2			5,1,1	0.0		0.0 0.0		
*MTEX(ASC) CCW			5,2,1	0.0		0.0 0.0		
MTEX(ASC) CW			5,3,1	0.0]	0.0 0.0		
LaboTex(PPF) CW						,, _		
*LaboTex(PPF) ATEX CCW	tmtex-rp	_2.TXT 21	l_txtmtex-rp	_2.TXT				
TXT2	Data	_			Labotex(E	PF),popLA(RAW) filename		

– 🗆 🗙

Minimport Wizard —	×	Minport Wizard - X
Import Pole Figures Select Data Files		Crystal Reference Frame Crystal Symmetry
Pole Figures EBSD ODE Tensor Data Background Defocussing Defocussing BG 110TR-ASC 200TR-ASC	xrd +	Mineral Indexed Not Indexed Load Cif File plotting color
211TR-ASC		Orystal Coordinate System Point Group 23 Axis Length a b 1 c 1 b c 1 b c 1 a b a
Plot << Previous Next >>	Finish	Plot Company Plot Finish

M Import Wizard	—		\times
Specimen Reference Frame			
Specimen Coordinate System rotate data by Euler angles (Bunge) in degree 0 0	0		
MTEX Plotting Convention	~		
$\begin{array}{c c} \mathbf{Y}_{\bullet} \\ \mathbf{z}_{\bullet} \mathbf{x} \end{array} \begin{array}{c} \mathbf{x}_{\bullet} \mathbf{x}_{\bullet} \mathbf{z}_{\bullet} \mathbf{x} \end{array} \begin{array}{c} \mathbf{x}_{\bullet} \mathbf{x}_{\bullet} \mathbf{z}_{\bullet} \mathbf{x}_{\bullet} \mathbf{x}$	x↓z	Y -	z
Plot ther data to verify that the coordinate system is properly a	ligned!		
Plot	>	Finish	

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



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







4. Yb2O3, Symmetry (43)のEBSDデータ作成

Materi	cif	Symmetr	y number	43	Material	name	Yttriu	mOxide-43			
LatticeCo	onstants	10.604	10.604	10.0	504	90.0)	90.0	90.0		
iRID: SqrG	irid#			-							
lumber	20	400									
Data euler	angle(f1,F,f2	?) angles —									
1	0.000	45	0.000			2 1	50	30	0.0	000	
3	310	70	0.000			4 0	.000	0.000	0.0	000	
5	0.000	0.000	0.000			6 0	.000	0.000	0.0	000	
7	0.000	0.000	0.000			8 0	.000	0.000	.00	DO	
9	0.000	0.000	0.000			10 0	.000	0.000	0.0	000	

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 1.0 0.000 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) $\phi 2Max = 90$







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)



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
LаbоТех	5.0.50	ODF解析
PFtoODF3	8.50	X R D P F -> O D F
MakePoleFile	1.89	$\mathbf{M}\mathbf{T}\mathbf{E}\mathbf{X}\mathbf{P}\mathbf{F}-\!\!\!>\!\mathbf{T}\mathbf{X}\mathbf{T}2$
GPPoleDisplay	1. 40	T X T 2 P F D i s p l a y