Hexagonal, Symmetry 6&62

六方晶EBSDデータの解析 (MTEX, LaboTex)

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1. 概要

Hexagonalは、	D-Hexagonal,	C-Hexagonal	の解析方法があります。

	Symmetry	Cub	ic**	Hexa	gonal	Tetr	agonal	Tri	gonal	Ortho-	Mono-	Triclinic
										rhombic	clinic	
		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°
ø 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°
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

Hexagonalでは

ſ	169	DR	8	10	C21H39C	018-Hexa-C6D	ISP		
	<u>100</u>	<u>FU</u> De1	0	101	Hexagona	al			
	109		0	104	23.725	(1.0)			
	170	P65	6	101	23 725	(1.0)			
	171	P62	6	101	7 035	(0.3345)			
	172	P64	6	10↓	1.900	(0.0040)			
	173	P63	6	10↓	90.0	symmetry sr	pace group	name H-M	1 'P6'
	174	P6	6	10↓	90.0	symmetry In	t Tables ni	imber	168
	175	P6/m	6	101	120.0			e c	100
	176	P63/m	Ă	iñi		_Symmetry		0	
	177	P622	Ğ2	111					
	178	D6122	62	111					
	170	D6522	62	111					
	179	FUUZZ	02	114					
	100	POZZZ	02	114					
	181	P6422	62						
	182	P6322	62	↓					
	183	P6mm	62	11↓					
	184	P6cc	62	11↓					
	185	P63cm	62	11↓	http://www.com	T: DODIOD			
	186	P63mc	62	11↓	li itanium-	-TI-D6DISP			
	187	P6m2	62	11↓	Hexagon	al			
	188	Pfic2	62	111	2.95	(1.0)			
	189	P62m	62 62	111	2.95	(1.0)			
	100	P620	62	111	4.686	(1.5885)			
	101	DG/mmm	62	111	90.0 sv	mmetry space	e group na	me H-M	'P63/mmc'
	102		62	111	90.0 S	vmmetry Int T	ables numb	per 1	94
	192		02	111	120.0 0	vmmetrv		62	
	193	PO3/mcm	02	111	_0	ymmeny		02	
	194	P63/mmc	6Z	↓					

があり、TiやMgはSymmetry (62) である。

本資料では、TableNo168のC21H39O18 とNo194のTiを扱ってみます。

ICDDからCTRのDataBaseへの登録はYb2O3のODF解析を参照してください。

2. C21H39O18、Symmetry (6) の解析

2.1 EBSDデータ作成

▲ EBSDAngdataMaker 1.00T[21/03/31] by CTR - □ ×
File Help
Material
Materialname C21H39O18-Hexa-C6
LatticeConstants 23.725 23.725 7.935 90.0 90.0 120.0
GRID: SqrGrid#
Number 20 400
Data eulerangle(f1,F,f2) angles ウインドウの領域切り取り(W)
□ 1 0.000 45 0.000 □ 2 170 80 0.000
3 340 100 0.000 4 0.000 0.000
5 0.000 0.000 6 0.000 0.000
9 0.000 0.000 0.000 0.000 0.000 0.000
Makefileholder U:¥2021-01-10-Hexagonal¥C21H39O18-Hexa-C6¥C21H39O18-Hexa-C6.ang
makefile

TextDisplay 1.14S U:¥2021-01-10-Hexagonal¥C21H39O18-Hexa-C6¥C21H39O18-Hexa-C6.ang

File Help # # Phase 1 # MaterialName C21H39O18-Hexa-C6 # Formula # Symmetry 6 # LatticeConstants 23.725 23.725 7.935 90.0 90.0 120.0 # # GRID: SqrGrid# 0.000 0.785 0.000 0.000 0.000 1.0 1.0 1 1 2.967 1.396 0.000 1.000 0.000 1.0 1.0 1 1 5.934 1.745 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

2. 2 MTEXの解析

✓ Import Wizard – □ ×	Import Wizard – 🗆 X
Crystal Reference Frame for Phase 1 Crystal Symmetry	Specimen Reference Frame Specimen Symmetry
Mineral Mineral Not Indexed mineral name C21H39O18-Hexa-C6 plotting color Crystal Coordinate System Point Group 6 Axis Length a 23.725 b 23.725 c 7.935 Axis Angle alpha 90 beta 90 gamma 120	Specimen Coordinate System rotate data by Euler angles (Bunge) in degree 0 0 0 apply rotation to Euler angles and spatial coordinates apply rotation only to Euler angles apply rotation only to spatial coordinates Use ANG interface flag 'convertSpatial2EulerReferenceFrame' Use ANG interface flag 'convertEuler2SpatialReferenceFrame' MTEX Plotting Convention $Y \rightarrow z$ $Y \rightarrow z$ $X \rightarrow Y$ $X \rightarrow Y$ $X \rightarrow Y$ $X \rightarrow Y$ $Y \rightarrow Z$ Plot ther data to verify that the coordinate system is properly aligned!
Plot << Previous Next >> Finish	Plot << Previous Next >> Finish

odf = calcDensity(ebsd('C21H39O18-Hexa-C6').orientations,'halfwidth',2*degree)



ODFデータをEXportし、GPODFDisplayで表示



2. 3 LaboTexの解析

AngデータからSORデータ変換

🖀 EBSDtoLaboTex 3.05T[21/03/31] by CTR — 🗆 🗙	Lattice constant
File Help amgdatacheck	
Material C21H39O18-Hexa-C6	Structure Code(symmetries after Schoenfiles)
Lattice constant	
Structure Code(symmetries after Schoenfiles) 10 - C6 (hexagonal) V	a 2.9899 b 2.9899 c 1.0 alfa 90.0 beta 90.0 gamm 120.0
a 2.9899 b 2.9899 c 1.0 alfa 90.0 beta 90.0 gamm 120.0	Step for output O Weight for data Angle Unit Angle Convention
Step for output 0 Weight for data Angle Unit Angle Unit Angle Convention Bunge ~	5.0 1-present 0-Bunge
Check data Line 200 Phase nosition Q Salact phase number 1 10 6	_ Input data format
No of data Line	Check data Line 200 pt
Out data Line 8 P1 1 F 2 P2 3	Check data Line 200 Phase position 8 Select phasenumber 1 IQ 6
4: # Synnetry 6	No of data Line
5:#LatticeConstants 23.725 23.725 7.935 90.0 90.0 8:#	Out data Line 8 P1 1 F 2 P2 3
7: # GRID: SqrGrid# 8: 0.000 0.785 0.000 0.000 0.000 1.0	
9: 2.967 1.396 0.000 1.000 0.000 1.0	1.
٢	
Comment	2:Styructure Code a b c alfa b
	3: (10) 2.9899 2.9899 1.0 90.0 90.0 120.0
	4: 0.9 0.785 0.0 1.0
LaboTexFile(toRadian,SOR) TexToolsFile(OIMRad.ang) ToAngle	5: 2.967 1.396 0.0 1.0
Bruker(Angle=TXT)=MTEX(Radian=Ang) DataAppend toRadian	6: 5.934 1.745 0.0 1.0 🗸
	< >>

L a b o T e x の O D F 解析結果



C21H39O18 Levels 2188.5

2188.5 2042.6 1896.7 1750.8 1604.9 1459.0

1439.0 1333.1 1021.3 875.4 729.5 583.6 437.7 291.8 1.0 Max=2334.361 Min=0.000 2021/01/11 0 90 ∳1 ¢-0-60 5.00 180

Symmetrization to orthorhombic

2. 4 MTEX, LaboTex再極点図比較

cs=ebsd('C21H39O18-Hexa-C6').CS h={Miller(1,0,0,cs),Miller(1,1,0,cs),Miller(1,0,1,cs)} rpf=calcPoleFigure(odf,h) plot(rpf,'contour','projection','eangle')



LaboTex



極点図の TD 方向

MTEXは左、データはCCW方向に並ぶ

LaboTexは右、データはCW方向に並ぶ

2.5 逆極点図比較

MTEX (1度間隔データ)

MTEXExport GPInverseDisplay で表示 ND

[11-20]

[10-10]

[11-20]







ND

[0001]

TD





L a b o T e x (5度間隔データ)





[100]

3. Titanium、Symmetry (62)の解析

3.1 EBSDデータ作成

BSDAngdataMaker 1.00T[21/03/31] by CTR	_		×
File Help			
∫ Material			
Materi cif Symmetry number 62 Materialname Titanium-Ti-D6			
LatticeConstants 2.95 2.95 4.686 90.0 90.0	120.0		
Number 20 400			
Data eulerangle(f1,F,f2) angles			
☑ 1 0.000 45 0.000 ☑ 2 170 80	0.00	0	
☑ 3 340 100 0.000 □ 4 0.000 0.000	0.00	0	
5 0.000 0.000 0.000 0.000	0.00	0	
7 0.000 0.000 0.000 0.000 0.000	0.00	0	
9 0.000 0.000 0.000 0.000 0.000	0.00	0	
Makefileholder U¥2021-01-10-Hexagonal¥Ti¥Titanium-Ti-D6.ang			
makefile			

TextDisplay 1.14S U:¥2021-01-10-Hexagonal¥Ti¥Titanium-Ti-D6.ang

File Help					
#					
# Phase 1					
# MaterialName Tita	inium-Ti-D)6			
# Formula					
# Symmetry 62					
# LatticeConstants 2.9	5 2.95	4.686 90).0 90.0	0 120.0	
#					
# GRID: SqrGrid#					
0.000 0.785 0.000	0.000	0.000	1.0	1.0 1	1
2.967 1.396 0.000	1.000	0.000	1.0	1.0 1	1
0.000 0000 0.000	2.000	0.000	1.0	1.0 0	1
0.000 0000 0.000	3.000	0.000	1.0	1.0 0	1

3. 2 MTEXの解析

Import Wizard – 🗆 X	Import Wizard – 🗆 🗙
Crystal Reference Frame for Phase 1 Crystal Symmetry	Specimen Reference Frame Specimen Symmetry
Mineral Indexed Not Indexed mineral name Titanium-Ti-D6 Load Cif File plotting color Crystal Coordinate System Point Group 622 X a Y b* Axis Length a 2.95 b 2.95 c 4.686 Axis Angle alpha 80 beta 90 gamma 120	Specimen Coordinate System rotate data by Euler angles (Bunge) in degree 0 0 0 apply rotation to Euler angles and spatial coordinates apply rotation only to Euler angles apply rotation only to Euler angles apply rotation only to spatial coordinates iuse ANG interface flag 'convertSpatial/EulerReferenceFrame! use ANG interface flag 'convertEuler2SpatialReferenceFrame! MTEX Plotting Convention $Y \downarrow \downarrow \chi$ $\chi \downarrow \chi$ Plot ther data to verify that the coordinate system is properly aligned!
Plot Kext >> Finish	Plot << Previous

odf = calcDensity(ebsd('Titanium-Ti-D6').orientations, 'halfwidth', 2*degree)





3.3 LaboTexの解析



Symmetrization to orthorhombic

			-
			1
×			1
			1
	b		
	Ĩ		



3. 4 MTEX, LaboTex再極点図比較

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



MTEX





plotIPDF(odf,yvector,'projection','eangle')





plotIPDF(odf,xvector,'projection','eangle')









U:\2021-01-10-Hexagonal\Ti\Ti-D6-Inverse.TPF ND





U:12021-01-10-Hexagonal/Ti/Ti-D6-Inverse.TPF RD



