

R h o m b o h e d r a l と H e x a g o n a l

2025年09月21日

H e l p e r T e x O f f i c e

概要

最近、 β -Polypropyleneを扱い、以下の資料が目に残った。

until 1994 that Meille [9] and Lotz [10] independently established that the β -crystal was a rhombohedral crystal structure, and that the unit cell parameters were $a = b = 11.01 \text{ \AA}$, $c = 6.5 \text{ \AA}$, $\alpha = \beta = 90^\circ$, $\gamma = 60^\circ$, and a density of 0.921 g/cm^3 . Due to their unique molecular

rhombohedralであるが、Hexagonalとして扱っている。

手元にrhombohedralファイルがないため、CODからdownloadし
変換比較を行ってみます。

Cell Parameters and Symmetry

	Lower Range	Upper Range	
a	5	10	☒ Range
b	5	10	☐ Tolerance
c	5	10	
alpha	40	60	
beta	40	60	
gamma	40	60	
space group			
crystal system	rhombohedral		

Logic interface:

☒ AND ☐ OR

送信

Reset

	Mineral
	Author
	Chemistry Search
a=5to10 and b=5to10 and c=5to10 and alpha=40to60 and beta=	Cell Parameters and Symmetry
	Diffraction Search
	General Search
	Search Tips
Search Reset	

Logic interface

☒ AND ☐ ORViewing (About [File Formats](#))☒ amc long form ☐ amc short form ☐ cif

Download

☒ amc ☐ cif ☐ diffraction data☐ [Alunite](#)

Pabst A



American Mineralogist 32 (1947) 16-30

Some computations on svanbergite, woodhouseite and alunite
_database_code_amcsd 0000037

7.058 7.058 7.058 59.08 59.08 59.08 R-3m

atom x y z

K 0 0 0

Al .5 0 0

S .305 .305 .305

O1 .393 .393 .393

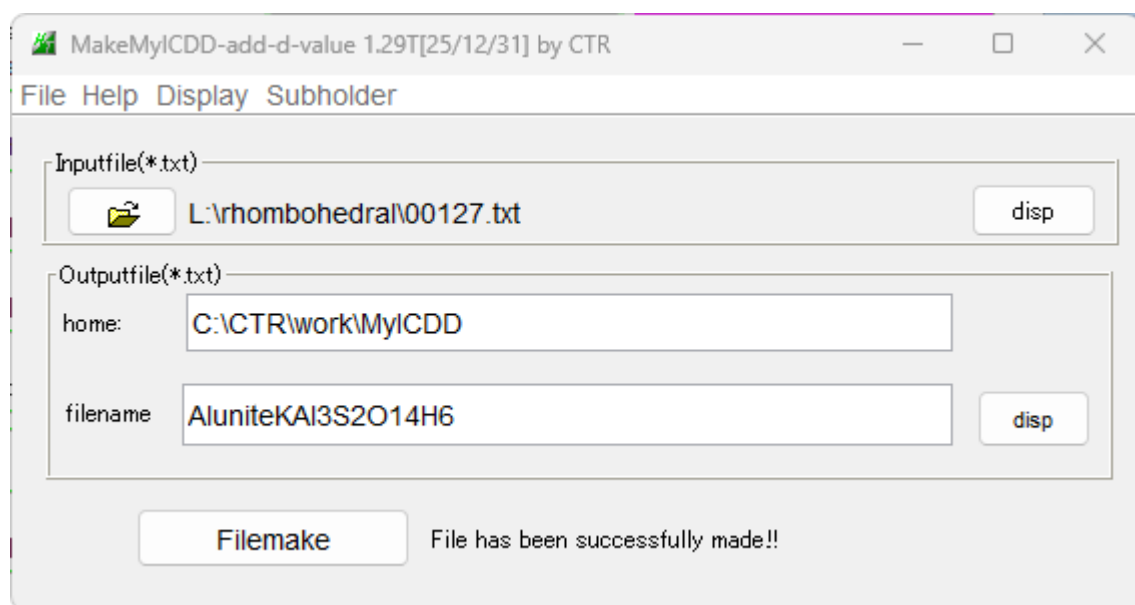
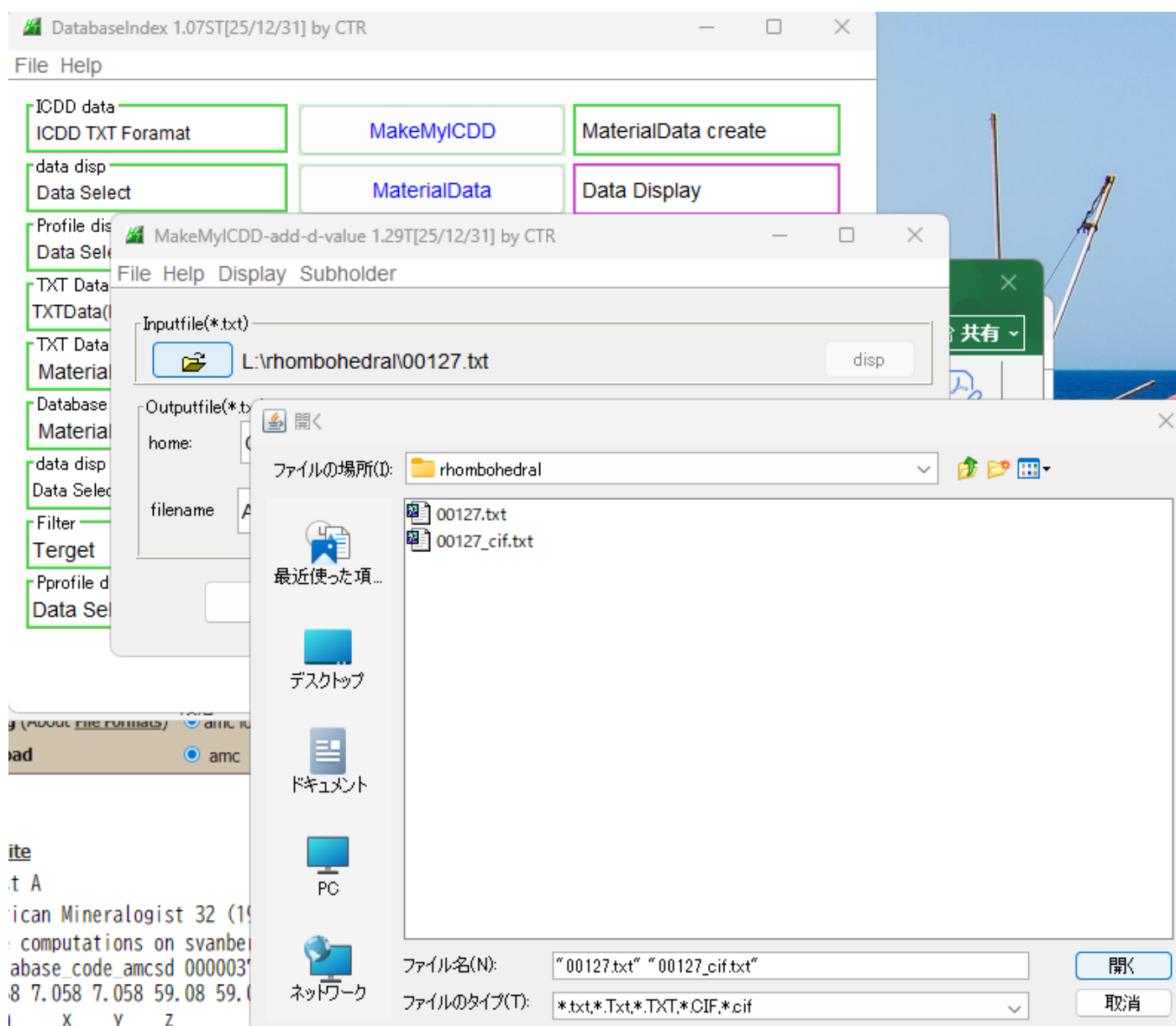
O2 .512 .157 .157

OH3 -.174 .276 .276

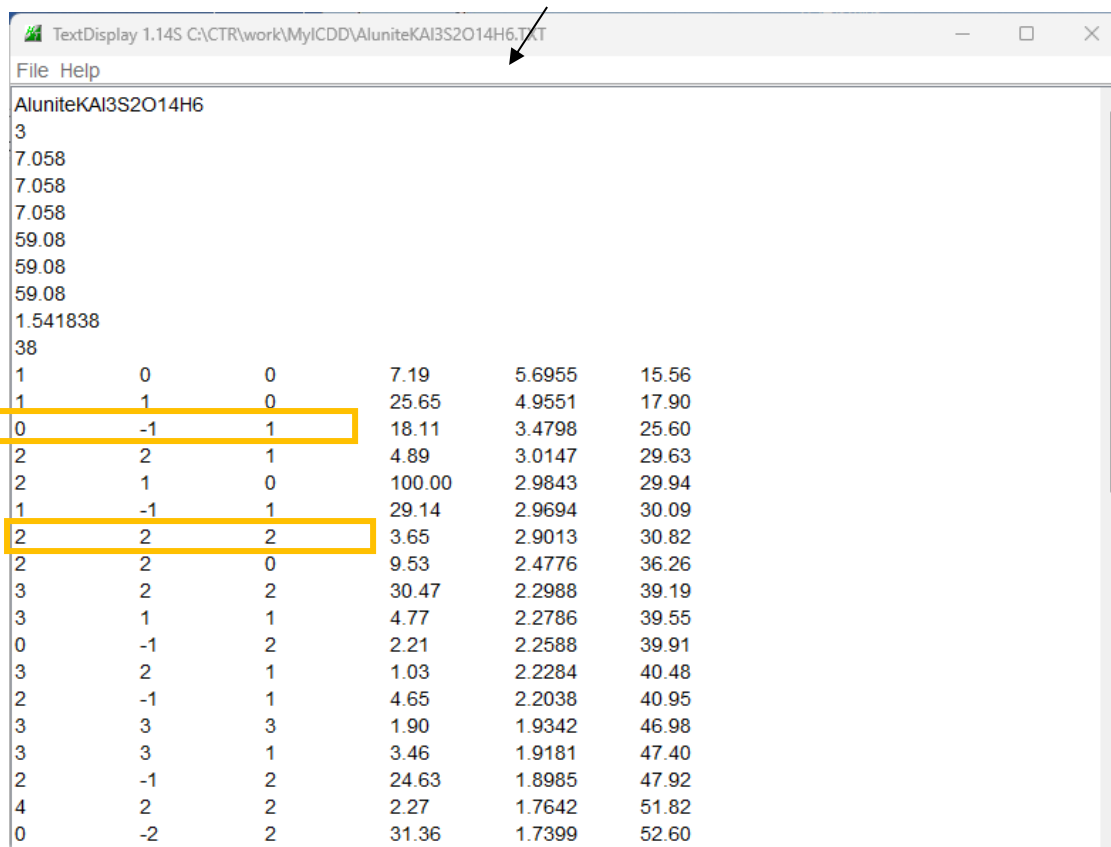
[Download AMC data \(View Text File\)](#)[Download CIF data \(View Text File\)](#)[Download diffraction data \(View Text File\)](#)[View Jmol 3-D Structure \(permalink\)](#)

CIFとdiffractionファイルをdownload

downloadしたCIFとdiffractionからMYICDDデータを作成



MYICDDにAluniteKAI3S2O14H6. TXTファイルが作成される



TextDisplay 1.14S C:\CTR\work\MyICDD\AluniteKAI3S2O14H6.TXT

File Help

AluniteKAI3S2O14H6

3

7.058

7.058

7.058

59.08

59.08

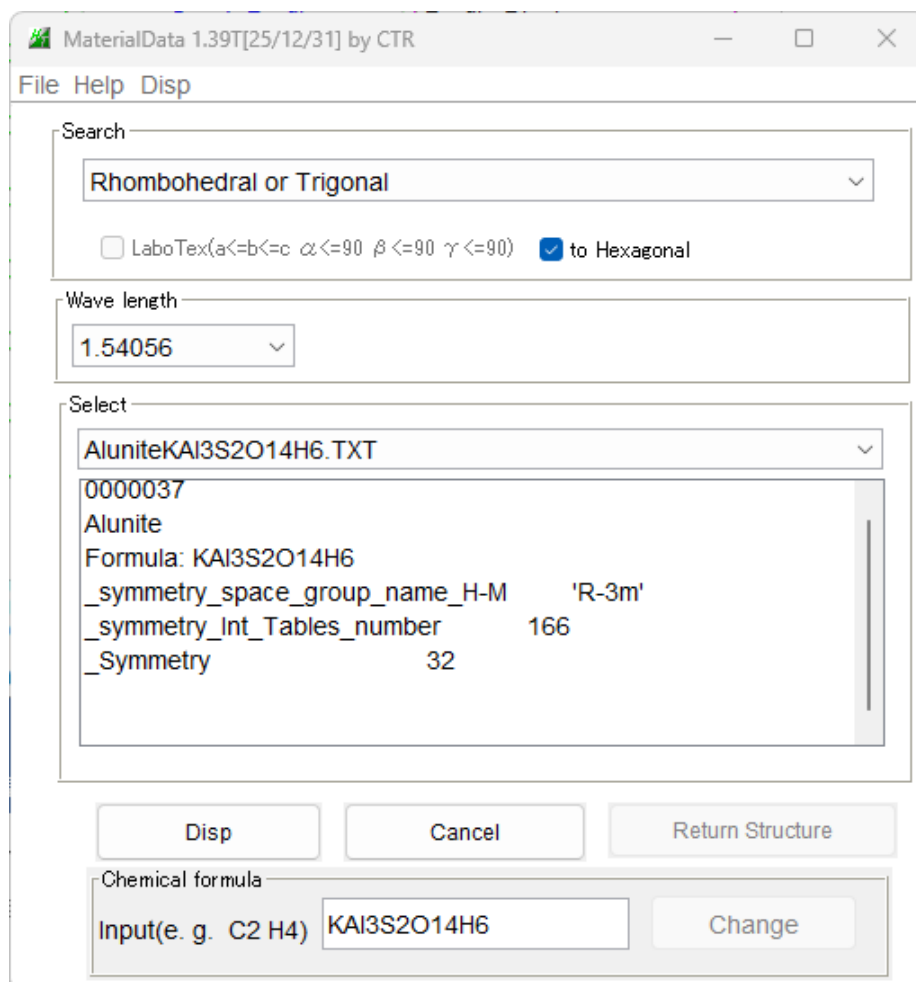
59.08

1.541838

38

1	0	0	7.19	5.6955	15.56
1	1	0	25.65	4.9551	17.90
0	-1	1	18.11	3.4798	25.60
2	2	1	4.89	3.0147	29.63
2	1	0	100.00	2.9843	29.94
1	-1	1	29.14	2.9694	30.09
2	2	2	3.65	2.9013	30.82
2	2	0	9.53	2.4776	36.26
3	2	2	30.47	2.2988	39.19
3	1	1	4.77	2.2786	39.55
0	-1	2	2.21	2.2588	39.91
3	2	1	1.03	2.2284	40.48
2	-1	1	4.65	2.2038	40.95
3	3	3	1.90	1.9342	46.98
3	3	1	3.46	1.9181	47.40
2	-1	2	24.63	1.8985	47.92
4	2	2	2.27	1.7642	51.82
0	-2	2	31.36	1.7399	52.60

MaterialDataで確認



MaterialData 1.39T[25/12/31] by CTR

File Help Disp

Search

Rhombohedral or Trigonal

☐ LaboTex($a \leq b \leq c$ $\alpha \leq 90$ $\beta \leq 90$ $\gamma \leq 90$) ☒ to Hexagonal

Wave length

1.54056

Select

AluniteKAI3S2O14H6.TXT

0000037

Alunite

Formula: KAI3S2O14H6

_symmetry_space_group_name_H-M 'R-3m'

_symmetry_Int_Tables_number 166

_Symmetry 32

Disp Cancel Return Structure

Chemical formula

Input(e. g. C2 H4) KAI3S2O14H6 Change

Hexagonal 変換表示

TextDisplay 1.14S C:\CTR\work\MYICDD\DISP\disp.txt

File Help

AluniteKAl3S2O14H6DISP

Hexagonal

6.959626484683846 (1.0)
 6.959626484683846 (1.0)
 17.407730282293024 (2.5012)
 90.0
 90.0
 120.0
 1.54056
 38

1	0	1	7.19	5.6955	15.545
0	1	2	25.65	4.9551	17.886
1	-2	0	18.11	3.4798	25.577
0	1	5	4.89	3.0147	29.607
1	1	3	100.0	2.9843	29.916
2	-2	1	29.14	2.9694	30.069
0	0	6	3.65	2.9013	30.793
0	2	4	9.53	2.4776	36.227
1	0	7	30.47	2.2988	39.154
2	0	5	4.77	2.2786	39.517
1	-3	1	2.21	2.2588	39.877
1	1	6	1.03	2.2284	40.445
3	-2	2	4.65	2.2038	40.916
0	0	9	1.9	1.9342	46.937
0	2	7	3.46	1.9181	47.355
3	-3	3	24.63	1.8985	47.874
2	0	8	2.27	1.7642	51.778
2	-4	0	31.36	1.7399	52.554

Rhombohedral

7.058 7.058 7.058 59.08 59.08 59.08 R-3m

からHexagonal

6.9596 x 6.9596 x 17.4077 x 90 x 90 x 120 に
 変換されています。

LaTeXでHexagonal $c/a = 2.5$ のTD-Splitを作成

HexaConvert 1.145T[25/12/31] by CTR

File Step Help random Dispfile

A ☐ X-Axis[100] ([2-1-10])

B ☒ X-Axis[210] ([10-10])

Miller Notation (3 Axis Notation)

☐ 0

☐ 1

☐ 3

1

0

0

hkl

uvw

Miller Bravais Notation (4 Axis Notation)

☒ 0

☐ 1

☐ -1

☐ 3

2

-1

-1

0

hkil

uvwx

Euler(p1Pp2)

☐

0.0

43.909

30.0

Material select

HEXA.txt

c/a

2.501

Input ψ 2 Angles

0

Calc

DISP

Position

10

Disp size

200

DISP

BG Corr

Black

Line size

1.0

MINUS

Polefigure

FWHM

5

degree

Step

1

Polefigure

1,1,1

☒ Orthorhombic

Disp

Gratio

1.0

☒ Lorentzcut(max/20)

Holder

C:\CTR\work\HexaConvert

OK

Return Structure

Model ODF

Crystal Symmetry

D_{6h} (Hexagonal)

Sample Symmetry

Orthorhombic

Grid Cells for Output ODF

5.0*5.0

Step

0.50

Diagram Range +/-

45.0

Component No. 1.

100.0%

0.50

FWHM $\phi_1 = 10.0$

45.0

Component No. 1.

100.0%

0.50

FWHM $\phi_1 = 10.0$

45.0

Component No. 1.

100.0%

0.50

FWHM $\phi_1 = 10.0$

45.0

No

Texture Component

On

Distribution

FWHM ϕ_1

FWHM ϕ_2

FWHM ϕ_3

Volume Fraction

Sample Name

013-100

Project Name

Demo

Cell Parameters (Relative)

a

1.0

b

1.0

c

2.501

α

90.0

β

90.0

γ

120.1

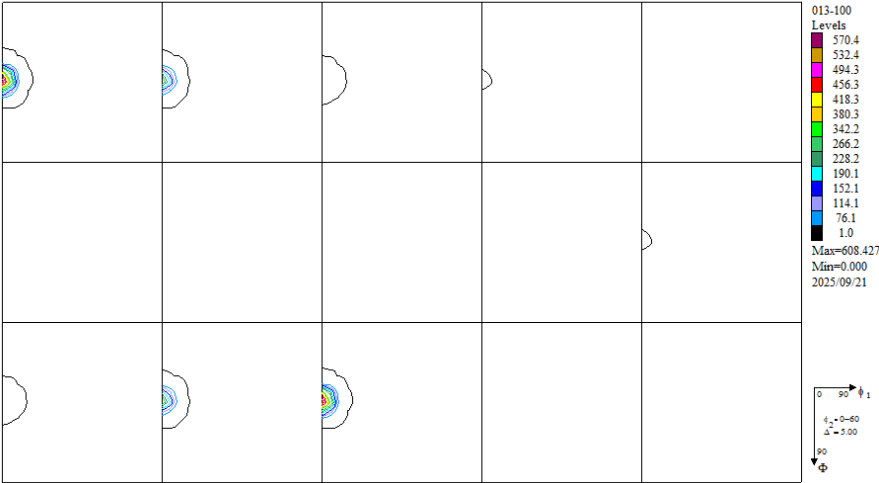
☒ Max Linearity

Background

0

Creation of Model ODF

Exit



Additional Pole Figures (APF) Calculation

Choose APF hkl for Calculation

h: 0 1 2 3 4 5 6 7 8 9
k: 0 1 2 3 4 5 6 7 8 9
l: 0 1 2 3 4 5 6 7 8 9

APF hkl: 1 1 3

Calculation Progress (100.0 %)

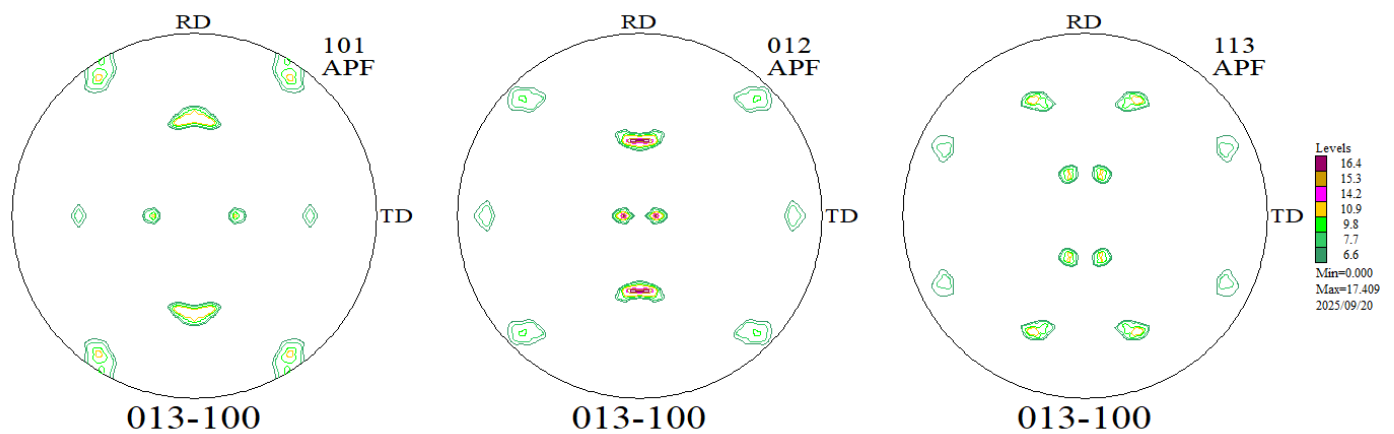
START APF CALCULATION

END

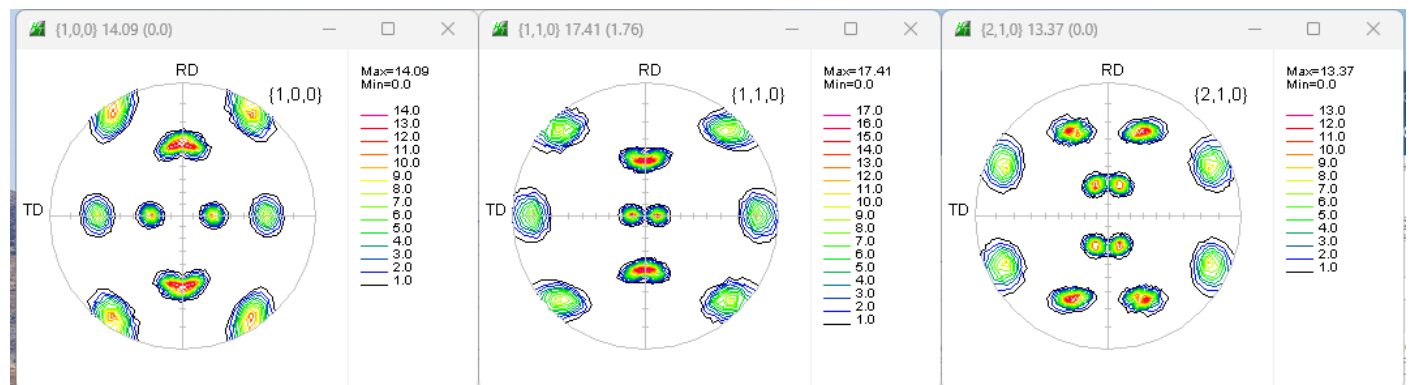
Calculated APF hkl

1 0 1
0 1 2
1 1 3

Hexagonal



Rhombohedral に指数変換



Rhombohedralによる解析

PFtoODF3 9.00T[25/12/31] by CTR

File Option Symmetric Software Data Help

Lattice constant

Material AluniteKAI3S2O14H6.txt

Structure Code(Symmetries after Schoenfiles) cif 9 - D3 (trigonal)

a 1.0 <=b 1.0 <=c 1.0 alpha 59.08 beta 59.08 gamm 59.08

Initialize

Start

getHKL<-Filena...

Center $\alpha=0$

AllFileSel...

PF Holder

L#rhombohedral#Rhomobo

PF Data

SelectFile(TXT(b,intens),TXT2(a,b,intens))	h,k,l	2Theta	Alpha scope	AlphaS	AlphaE	Select
100-rp_2.TXT	1,0,0	0.0	0.0->90.0	0.0	90.0	☒
110-rp_2.TXT	1,1,0	0.0	0.0->90.0	0.0	90.0	☒
210-rp_2.TXT	2,1,0	0.0	0.0->90.0	0.0	90.0	☒
	2,1,1	0.0		0.0	0.0	☐
	2,1,1	0.0		0.0	0.0	☐
	3,1,1	0.0		0.0	0.0	☐
	4,0,0	0.0		0.0	0.0	☐
	3,3,1	0.0		0.0	0.0	☐
	4,2,2	0.0		0.0	0.0	☐

Comment

Symmetric type Full

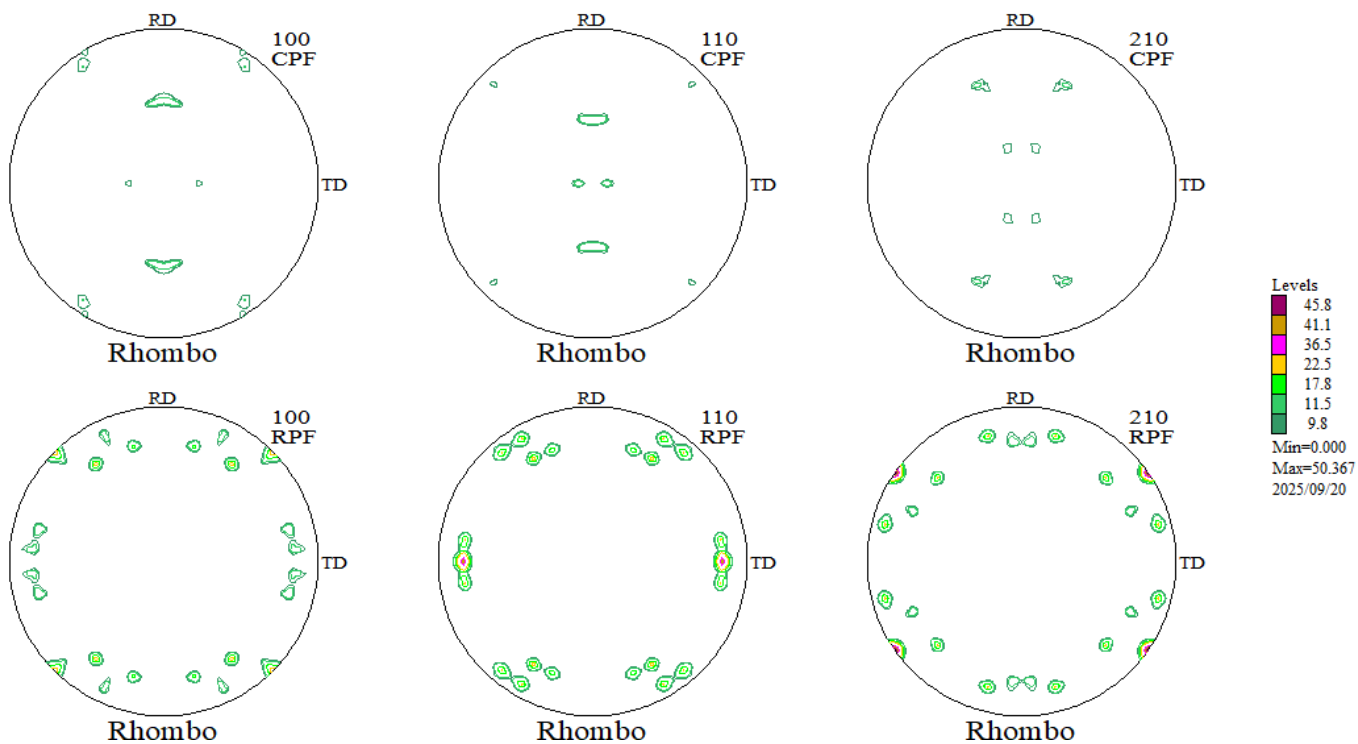
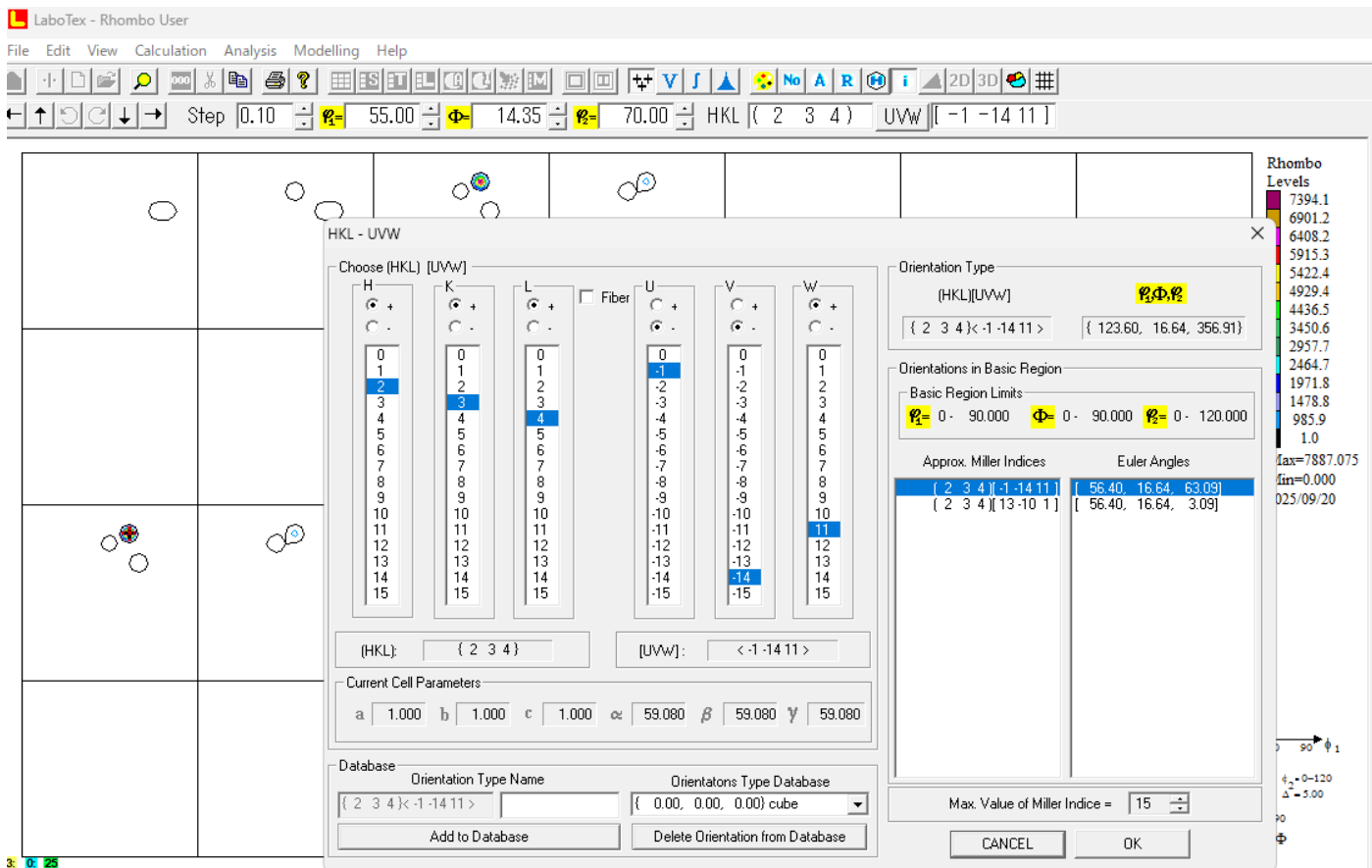
CenterData

Average

Epf file save

Labotex(EPF),popLA(RAW) filename

labotex



計算で来ていない

TexTools

ODF Calculation Setup

Crystal info.

Crystal system: **Rhombohedral/Trigonal**

a: α :

b: β :

c: γ :

Pole figure info.

Number of pole figures:

1st PF | 2nd PF | 3rd PF

h: k: l:

Browse PF file location:

☒ Normalizing pole figures before ODF calculation

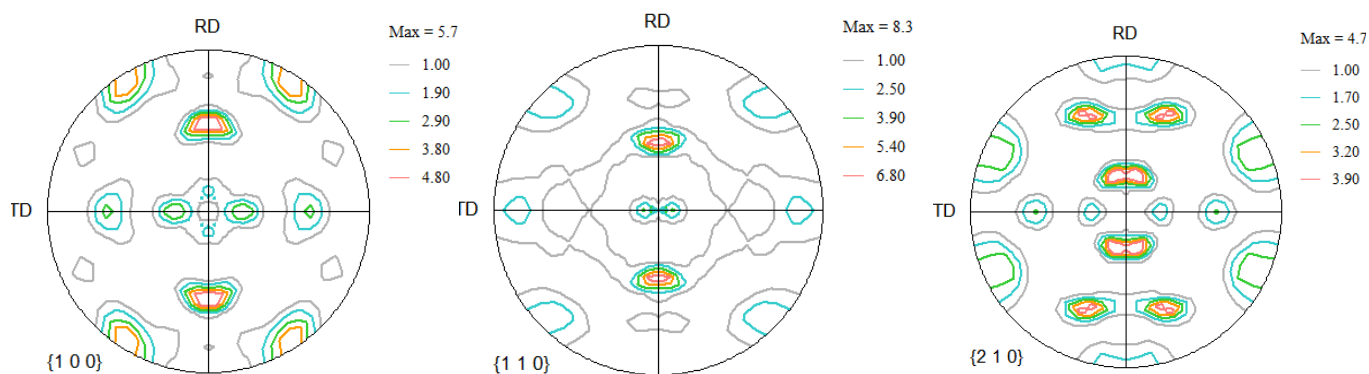
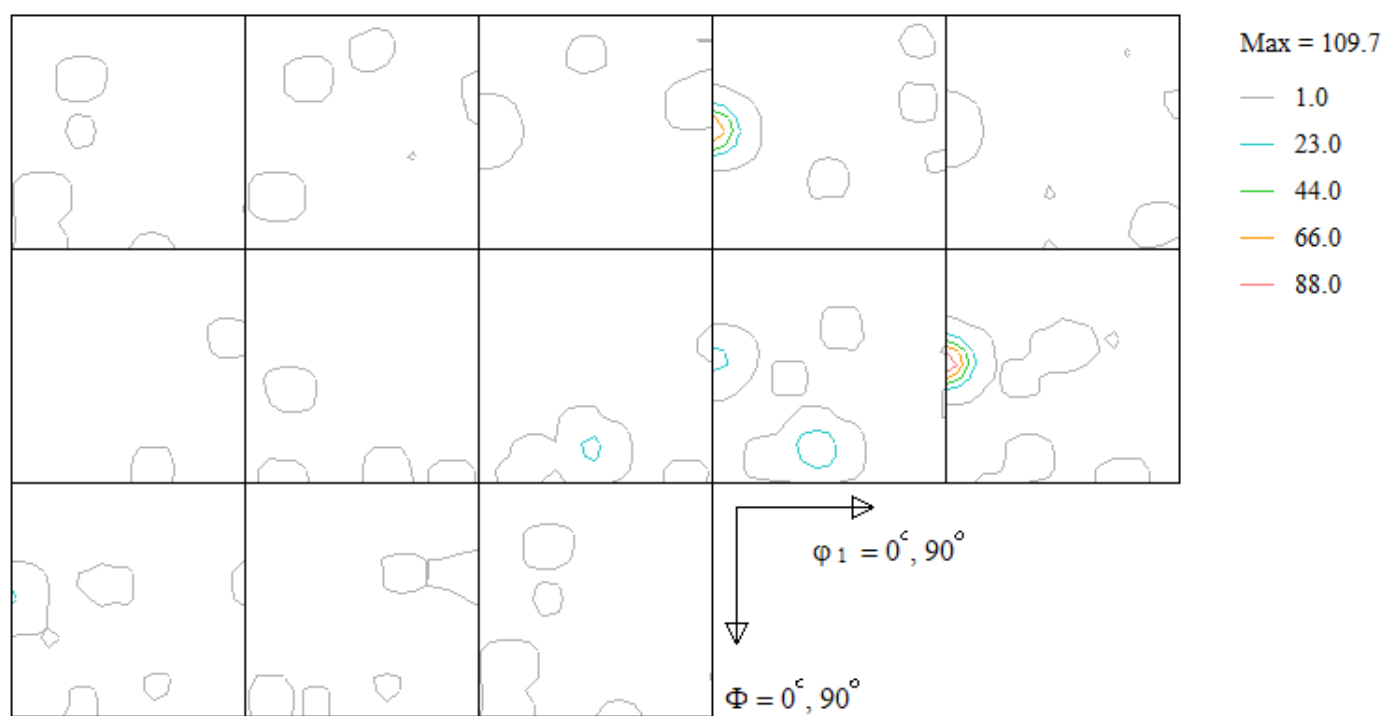
☒ With Orthogonal sample symmetry

Resolution:

☐ Assuming fiber texture

Save as:

OK Advance Help Cancel



ゴーストが発生

M T E X

Import Wizard

Crystal Reference Frame
Crystal Symmetry

Mineral
☒ Indexed ☐ Not Indexed
 mineral name: Alunite Load Cif File
 plotting color: checkbox pattern

Crystal Coordinate System
 Point Group: $-3m1$ $X||a^*$ $Z||c$
 Axis Length: a 7.058 b 7.058 c 7.058
 Axis Angle: alpha 59.08 beta 59.08 gamma 59.08

Plot << Previous Next >> Finish

Import Wizard

Miller Indices
Correct Miller Indices

Imported Pole Figure Data Sets
 (10-10) 100TR.ASC
 (11-20) 110TR.ASC
 (21-30) 210TR.ASC

Miller Indices
 h 1
 k 0
 i
 l 0

Structure Coefficients
 c 1

For superposed pole figures separate multiple Miller indece and structure coefficients by space!

Plot << Previous **Next >>** Finish

Import Wizard

Import Data
Select Method

Summary of PoleFigure data to be imported:

```
crystal symmetry: "-3m1"
specimen symmetry: "1"
h = (10-10), r = 78 x 19 points
h = (11-20), r = 78 x 19 points
h = (21-30), r = 78 x 19 points
```

Import to
☒ script (m-file) ☐ workspace variable

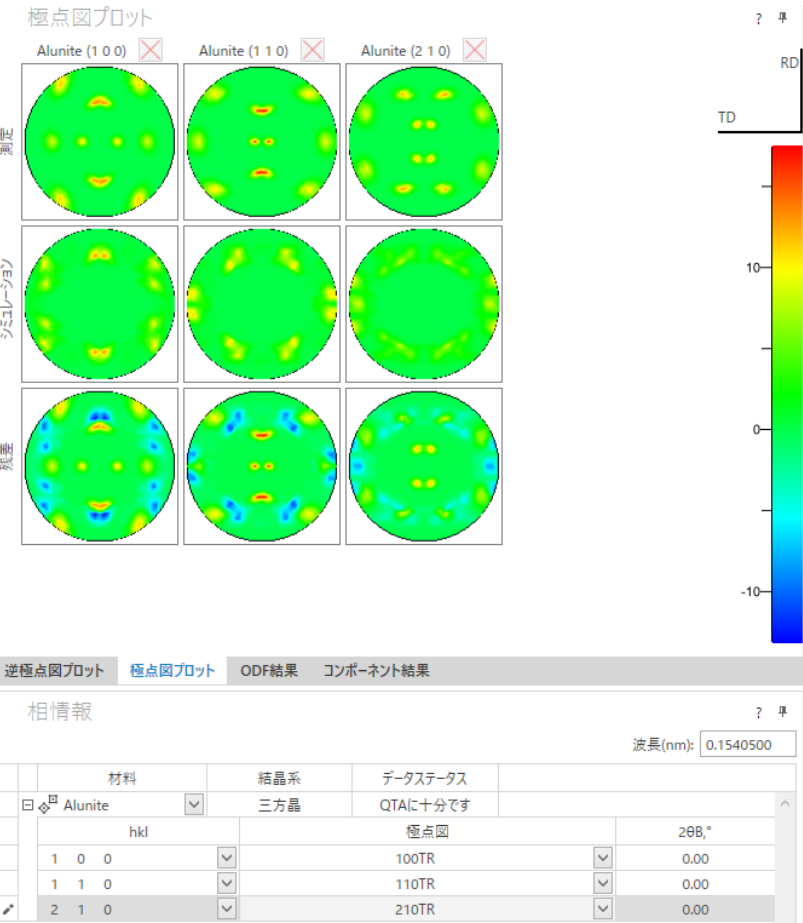
Plot << Previous Next >> Finish

```
% crystal symmetry
CS = crystalSymmetry('-3m1', [7.1 7.1 7.1], 'X||a*', 'Z||c', 'mineral', 'Alunite');
```

読み込んだ c i f

```
data_global↓
_chemical_name_mineral 'Alunite'↓
loop↓
_publ_author_name↓
'Pabst A'↓
_journal_name_full 'American Mineralogist'↓
_journal_volume 32↓
_journal_year 1947↓
_journal_page_first 16↓
_journal_page_last 30↓
_publ_section_title↓
;↓
Some computations on svanbergite, woodhouseite and alunite↓
;↓
_database_code_amcsd 0000037↓
_chemical_formula_sum 'K Al3 S2 O14 H6'↓
_cell_length_a 7.058↓
_cell_length_b 7.058↓
_cell_length_c 7.058↓
_cell_angle_alpha 59.08↓
_cell_angle_beta 59.08↓
_cell_angle_gamma 59.08↓
_cell_volume 243.402↓
_exptl_crystal_density_diffrn 2.826↓
_symmetry_space_group_name_H-M 'R -3 m'↓
loop↓
space group symop operation xyz↓
```

しかし、Hexagonalとして4指数変換されてします。



ODF計算

ODFを計算 ODF図をエクスポート

ODF計算

計算方式: WIMVモデル

試料の対称性: 1/4対称

α解析開始角度(°): 0.00

α解析終了角度(°): 90.00

ODFグリッド

φ₁ステップ(°): 5.00

φステップ(°): 5.00

φ₂ステップ(°): 5.00

パラメーター

結晶相: Alunite

最大繰り返し数: 10

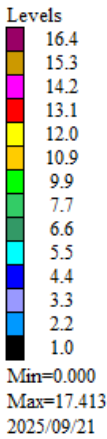
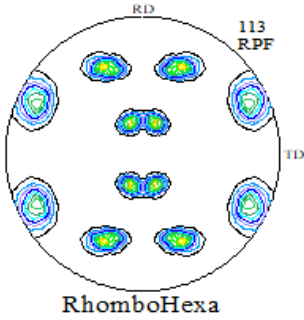
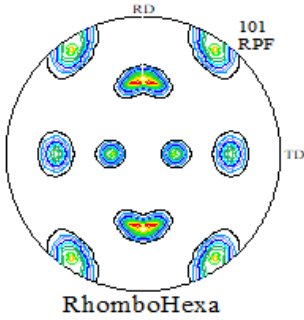
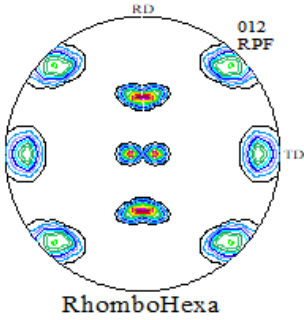
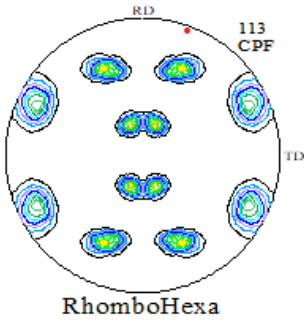
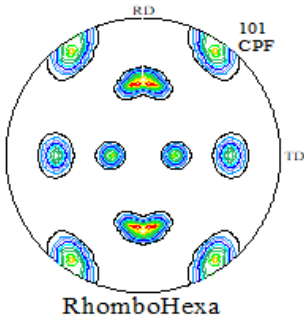
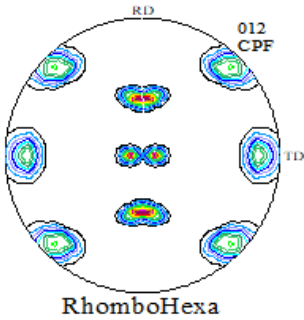
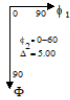
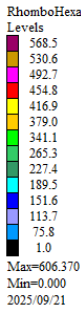
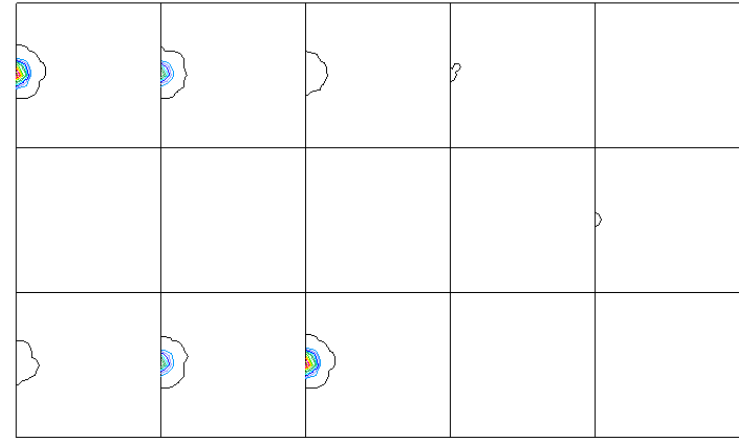
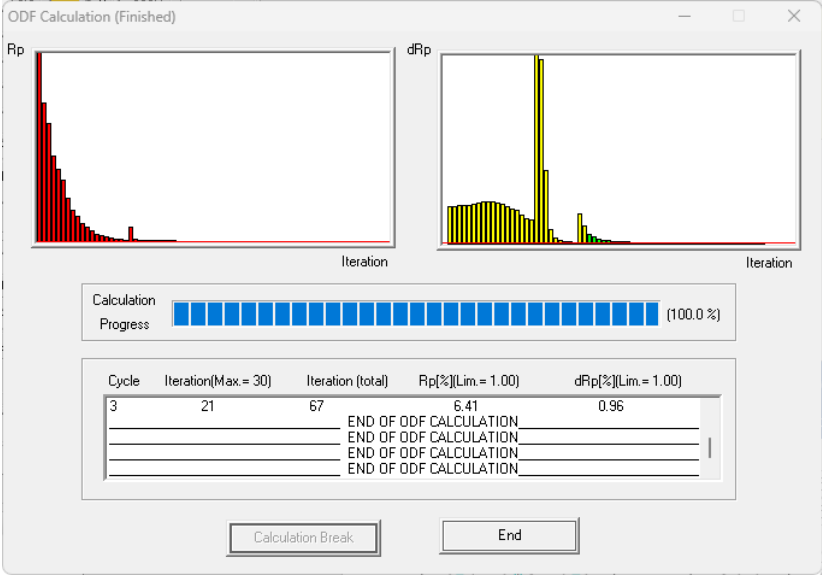
ε = 0.0100

バックグラウンドをフィッティング: ☐

RP因子=106.40 ステータス: 十分な数の測定極点図から計算

解析できない

Hexagonalで解析



正常

TeXTools

ODF Calculation Setup

Crystal info.

Crystal system: Hexagonal

a: 1, α : 90

b: 1, β : 90

c/a: 2.5, γ : 120

Pole figure info.

Number of pole figures: 3

1st PF: h, 2nd PF: k, 3rd PF: l

Browse PF file location: L:\rhombohedral\TexTools\textools113_2.pol

Resolution: 5.00

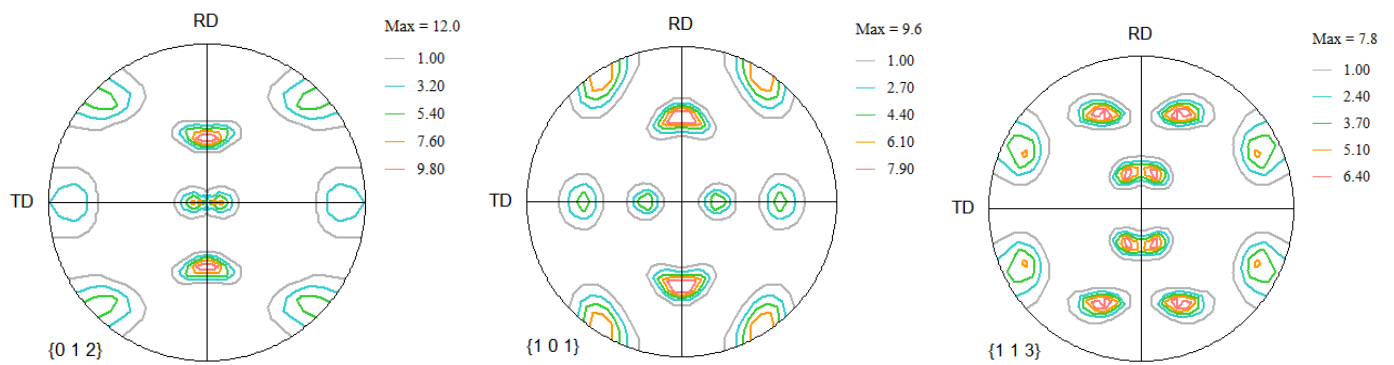
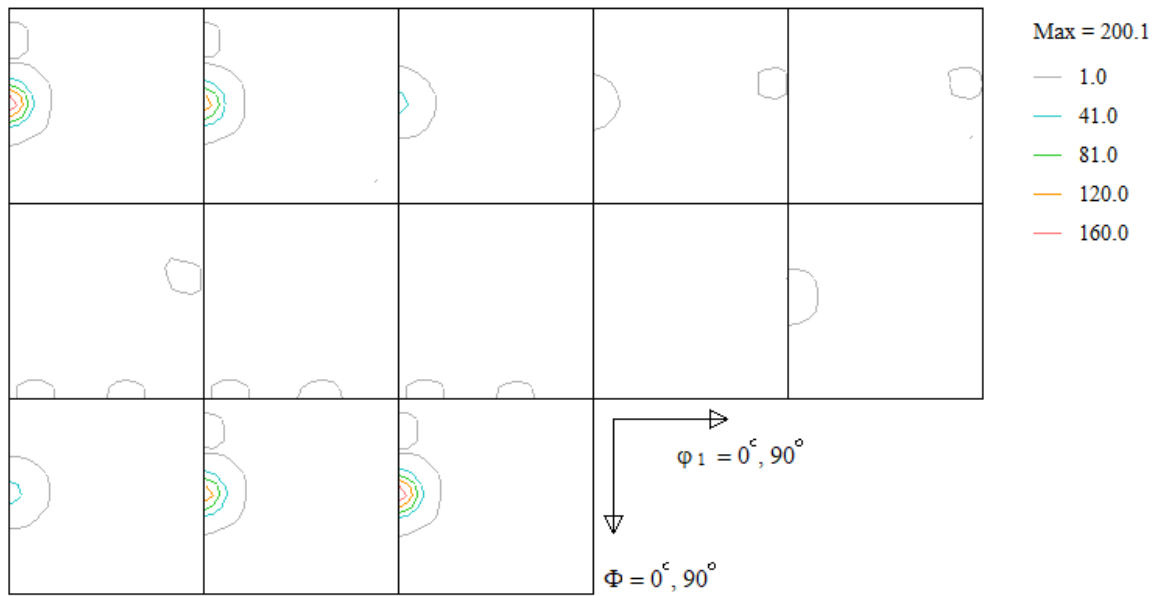
Assuming fiber texture: ☐

Normalizing pole figures before ODF calculation: ☒

With Orthogonal sample symmetry: ☒

Save as: L\rhombohedral\TexTools\Hexa.HODF

OK Advance Help Cancel



正常

MTEX (cifにRhombohedralを指定)

Import Wizard

Crystal Reference Frame

Crystal Symmetry

Mineral

☒ Indexed ☐ Not Indexed

mineral name: Alunite Load Cif File

plotting color:

Crystal Coordinate System

Point Group: $\bar{3}m1$ $X||a^*$ $Z||c$

Axis Length: a: 7.058 b: 7.058 c: 7.058

Axis Angle: alpha: 59.08 beta: 59.08 gamma: 59.08

Plot << Previous Next >> Finish

Import Wizard

Miller Indices

Correct Miller Indices

Imported Pole Figure Data Sets

(01-12)	012TR.ASC
(10-11)	101TR.ASC
(11-23)	113TR.ASC

Miller Indices

h: 0

k: 1

i:

l: 2

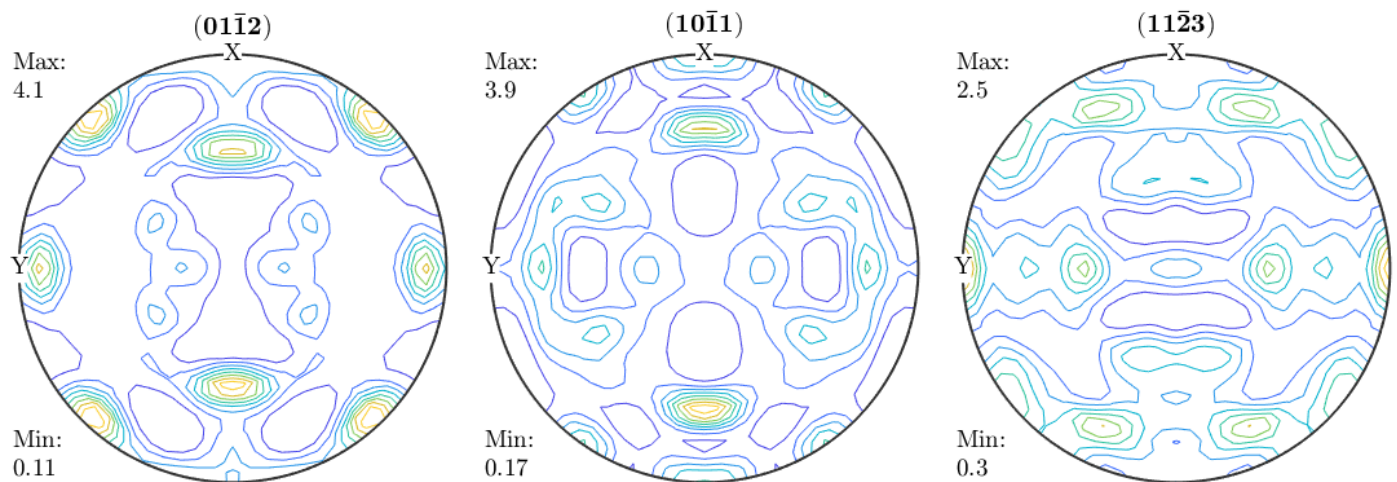
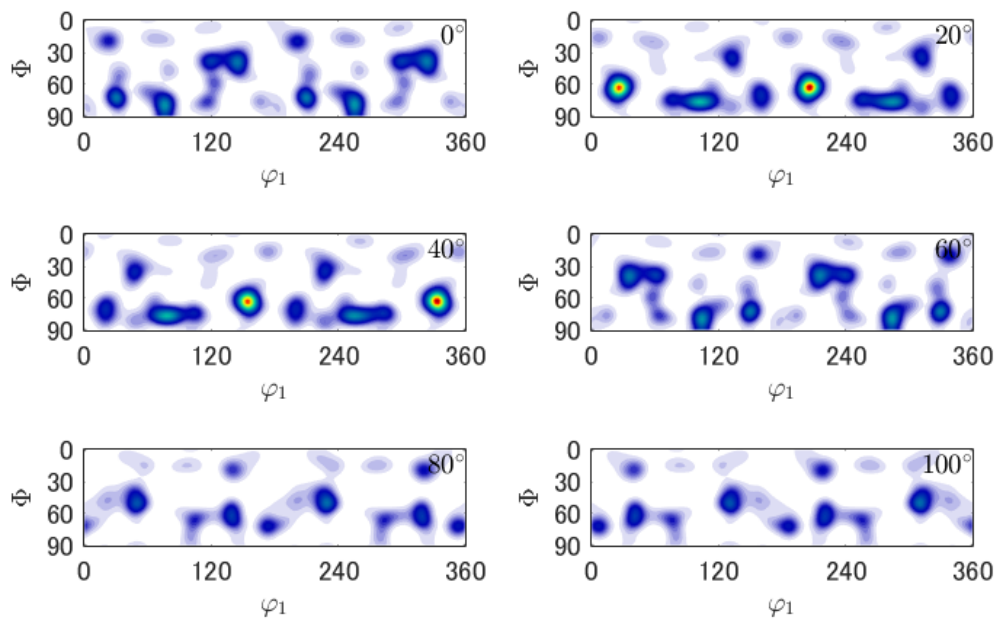
Structure Coefficients

c: 1

For superposed pole figures separate multiple Miller indice and structure coefficients by space!

Plot << Previous Next >> Finish

解析結果

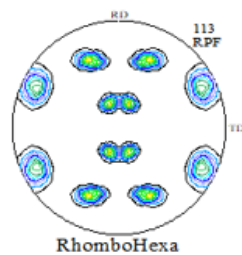
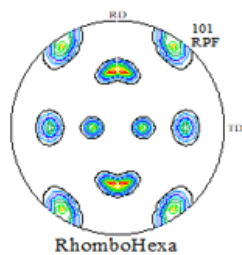
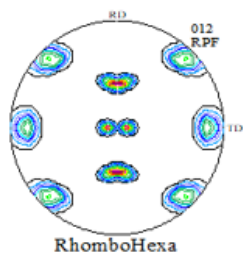
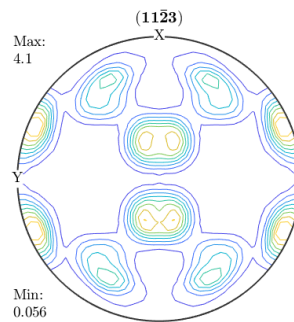
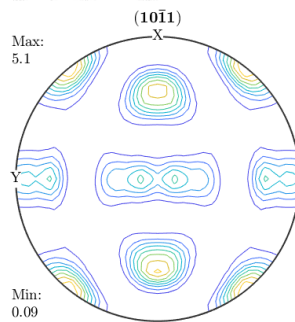
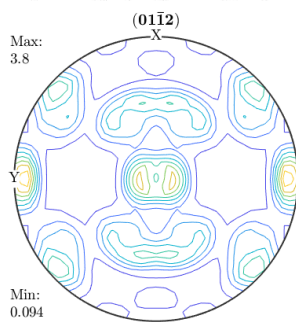
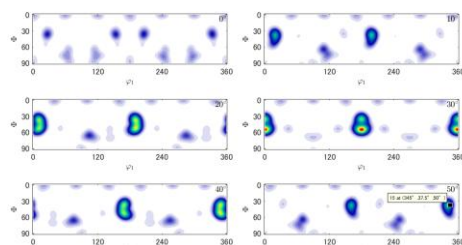


解析できない

MTEX (cifにMgを指定し、変数の変更)

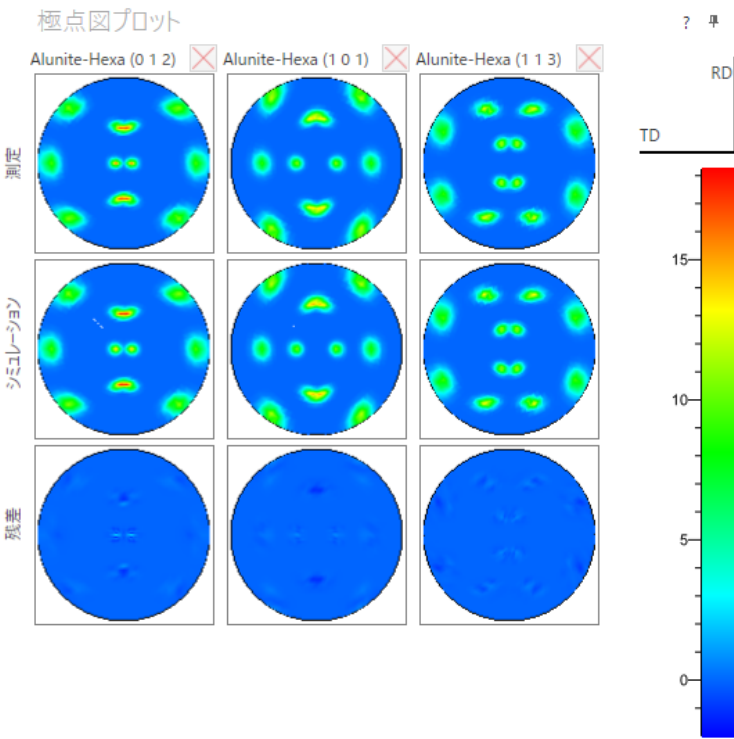
```
CS = crystalSymmetry('6/mmm', [3.2 3.2 5.2], 'X||a*', 'Y||b', 'Z||c*', 'mineral', 'Mg');
```

```
CS = crystalSymmetry('6/mmm', [6.9 6.9 17.4], 'X||a*', 'Y||b', 'Z||c*', 'mineral', 'Mg');
```



解析結果はずれている。

newODF



ODF計算

ODFを計算 ODF図をエクスポート

ODF計算

計算方式: WIMVモデル

試料の対称性: 1/4対称

α解析開始角度(°): 0.00

α解析終了角度(°): 90.00

ODFグリッド

φ₁ステップ(°): 5.00

φステップ(°): 5.00

φ₂ステップ(°): 5.00

パラメータ

結晶相: Alunite-Hexa

最大繰り返し数: 10

ε = 0.0100

バックグラウンドをフィッティング: ☐

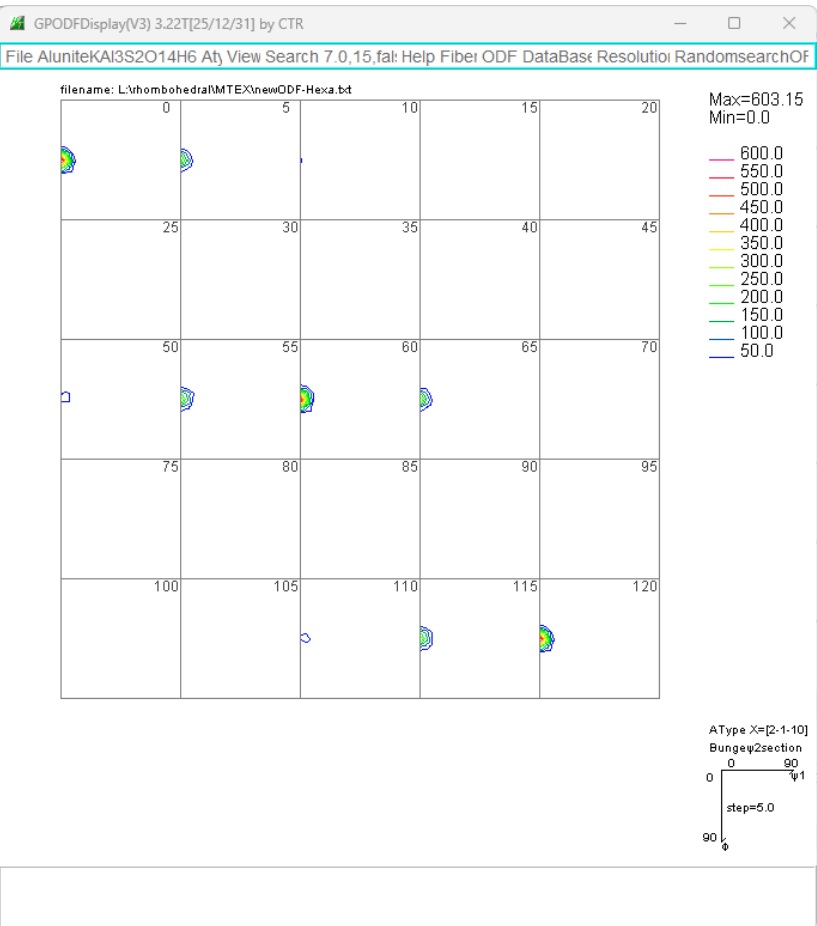
RP因子=6.86 ステータス: 十分な数の測定極点図から計算

逆極点図プロット 極点図プロット ODF結果 コンポーネント結果

相情報

波長(nm): 0.1540500

材料	結晶系	データステータス
Alunite-Hexa	三方晶	QTAに十分です
hkl	極点図	2θB,°
0 1 2	012TR	0.00
1 0 1	101TR	0.00
1 1 3	113TR	0.00



まとめ

R h o m b o h e d r a l の指定方法が悪いのか？解析できない。

R h o m b o h e d r a l 材料のODF解析はH E x a g o n a l 変換で行うこと