ＲｈｏｍｂｏｈｅｄｒａｌとＨｅｘａｇｏｎａｌ

２０２５年０９月２１日

ＨｅｌｐｅｒＴｅｘ　Ｏｆｆｉｃｅ

概要

最近、β－Ｐｏｌｙｐｒｏｐｙｌｅｎｅを扱い、以下の資料が目に留まった。

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 Å, c = 6.5 Å, α = β = 90°, γ = 60°, 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。

ＣＯＤからｄｏｗｎｌｏａｄ

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**	○ **OR**	
Viewing (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

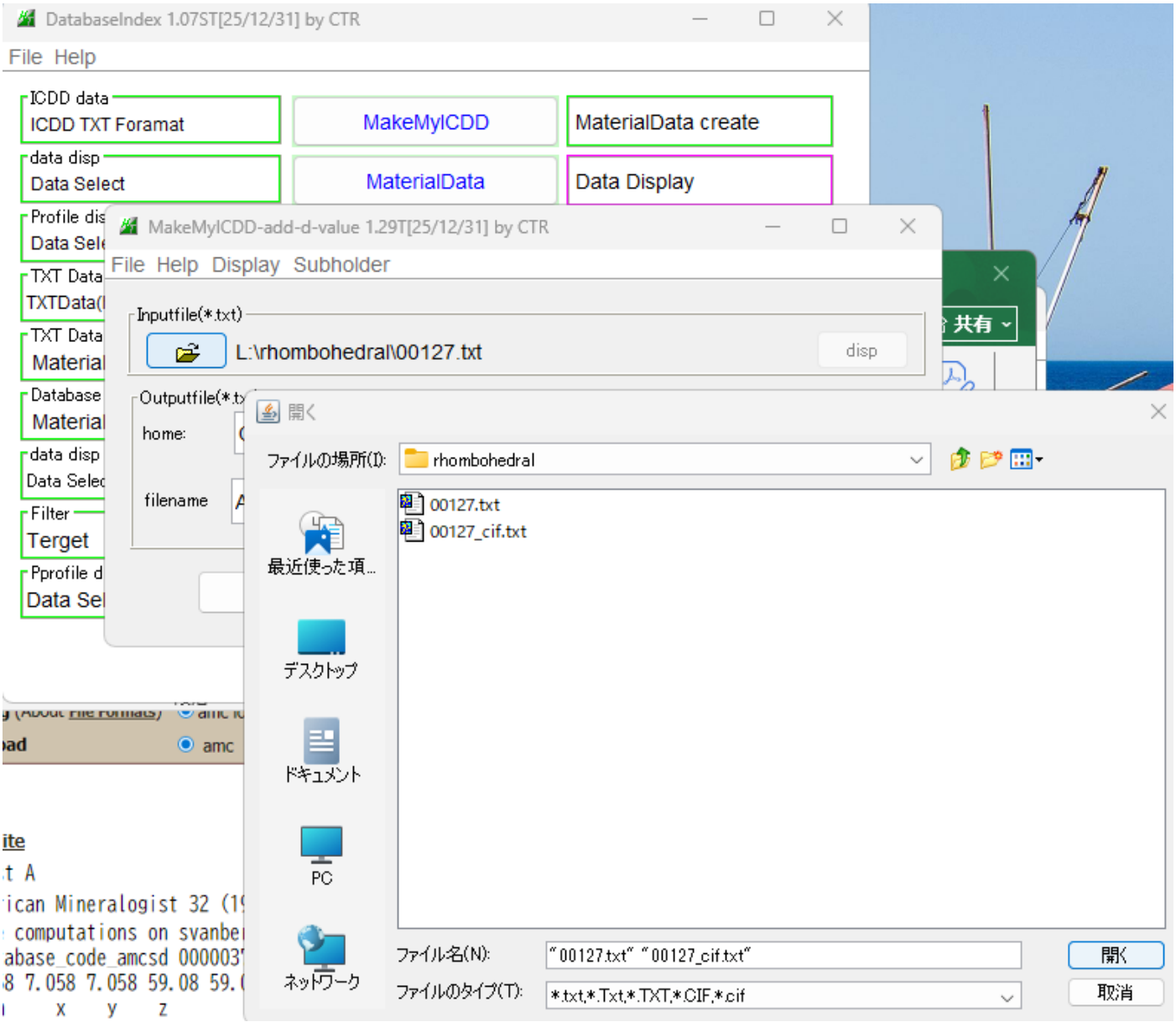
7.058 7.058 7.058 59.08 59.08 59.08 R-3m

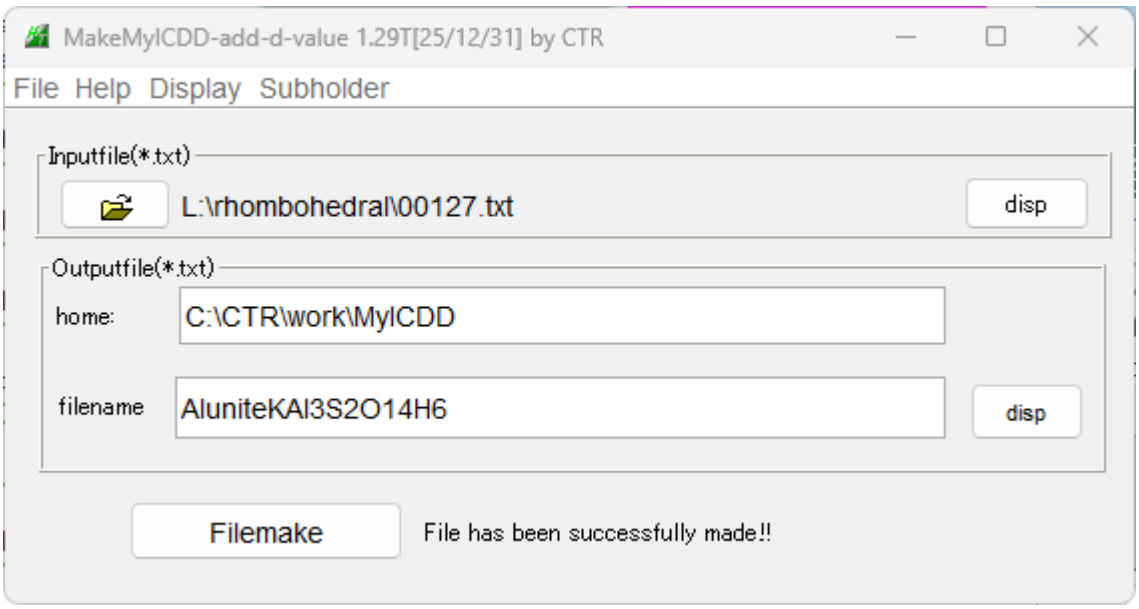
atom	x	y	z
K	0	0	0
Al	.5	0	0
S	.305	.305	.305
O1	.393	.393	.393
O2	.512	.157	.157
OH3	-.174	.276	.276

Download AMC data (View Text File)
Download CIF data (View Text File)
Download diffraction data (View Text File)
View JMOL 3-D Structure (permalink)

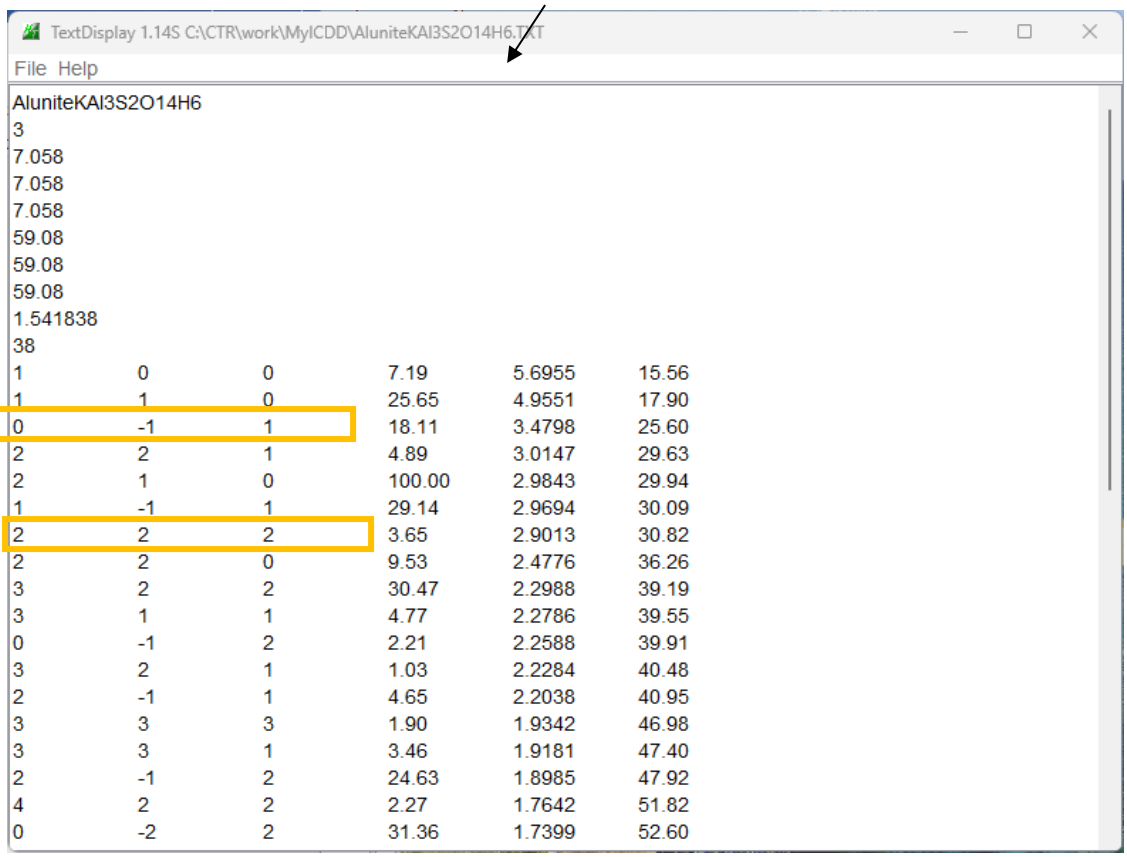
ＣＩＦとｄｉｆｆｒａｃｔｉｏｎファイルをｄｏｗｎｌｏａｄ

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

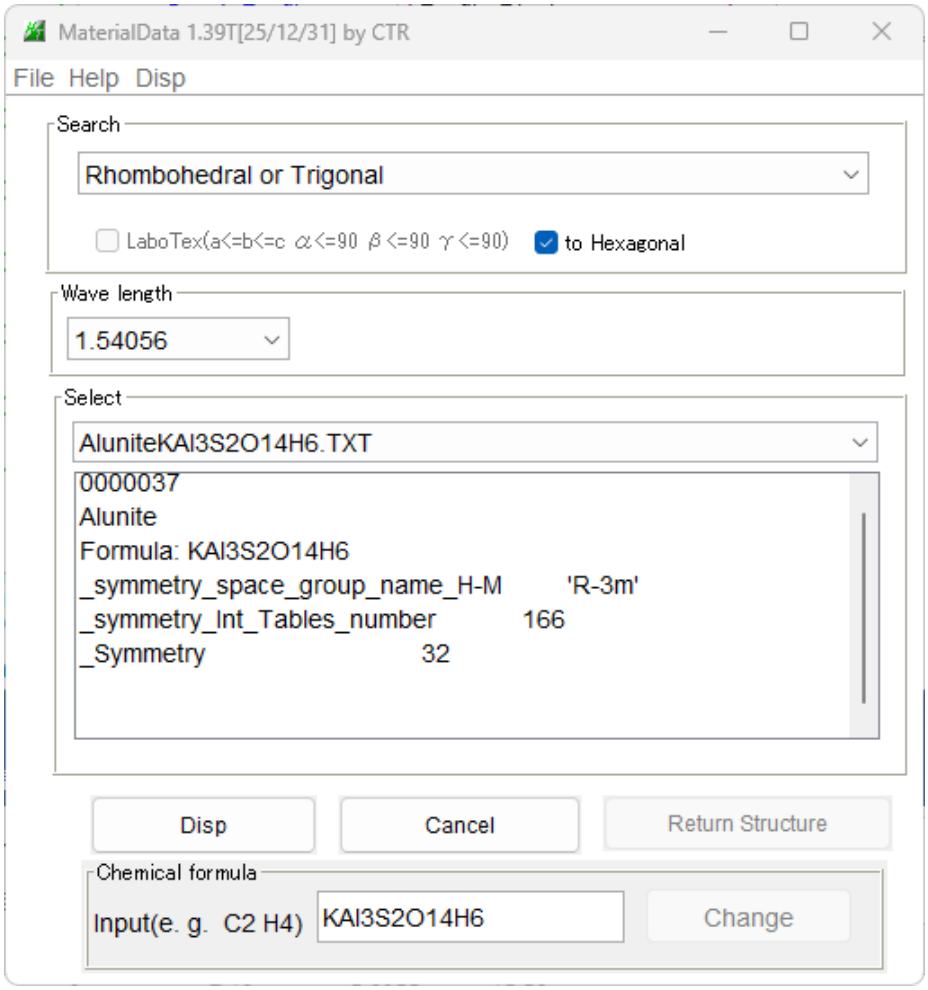




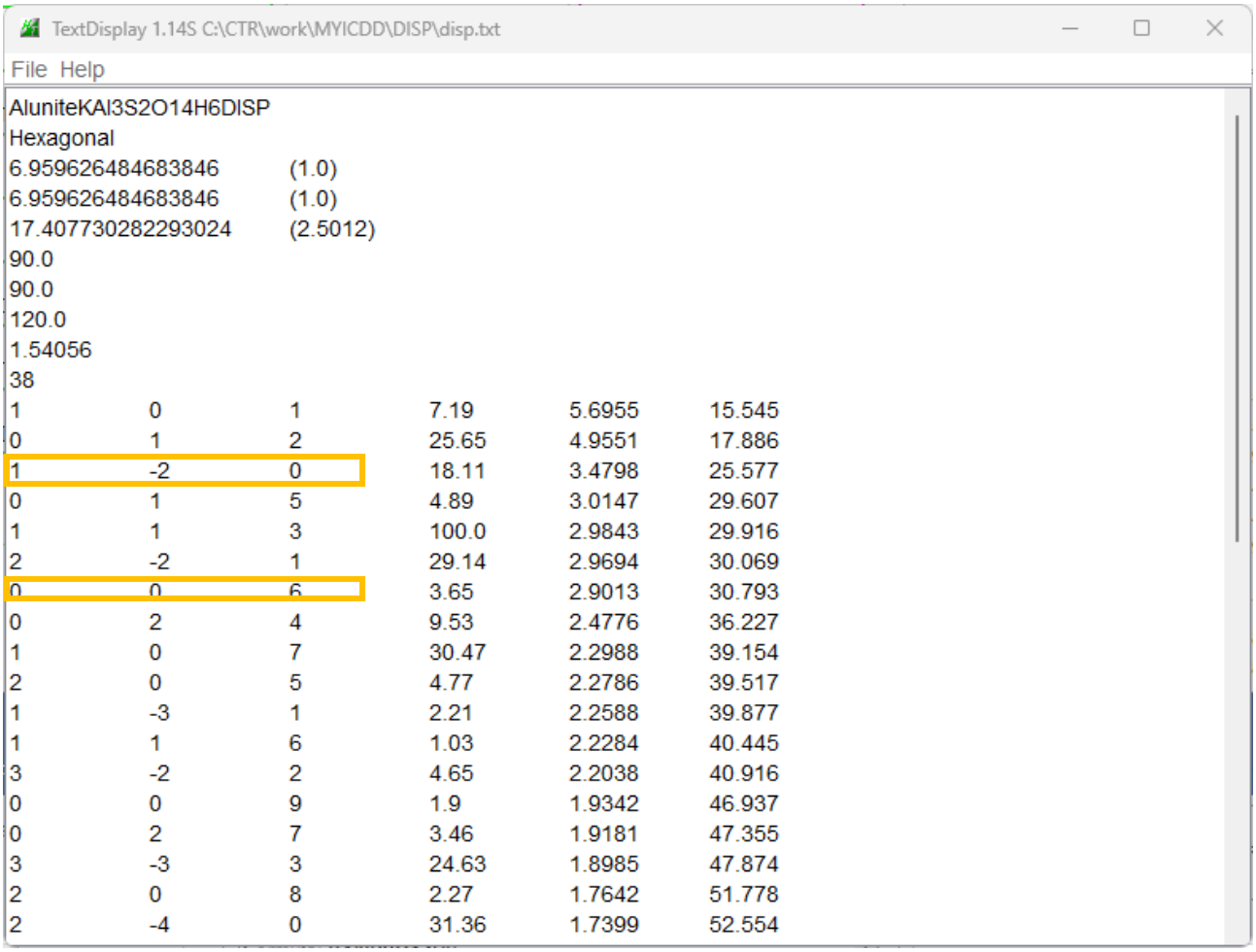
ＭＹＩＣＤＤにＡｌｕｎｉｔｅＫＡｌ３Ｓ２Ｏ１４Ｈ６．ＴＸＴファイルが作成される



ＭｔｅｒｉａｌＤａｔａで確認



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

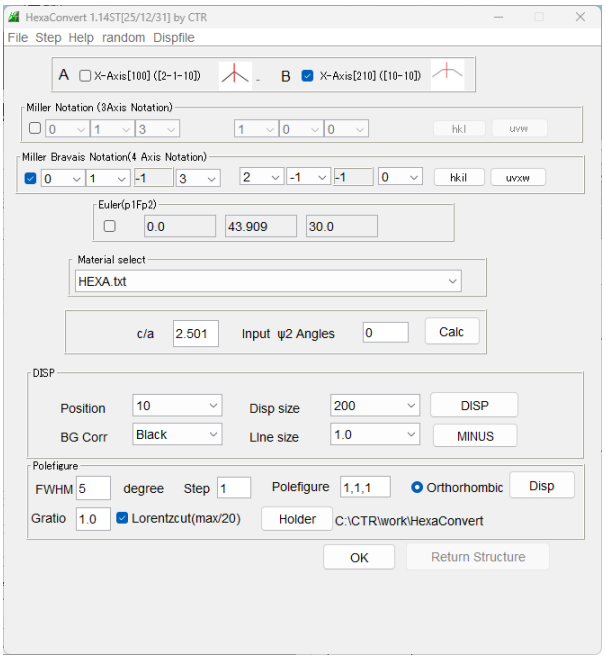
7.058 7.058 7.058 59.08 59.08 59.08 R-3m

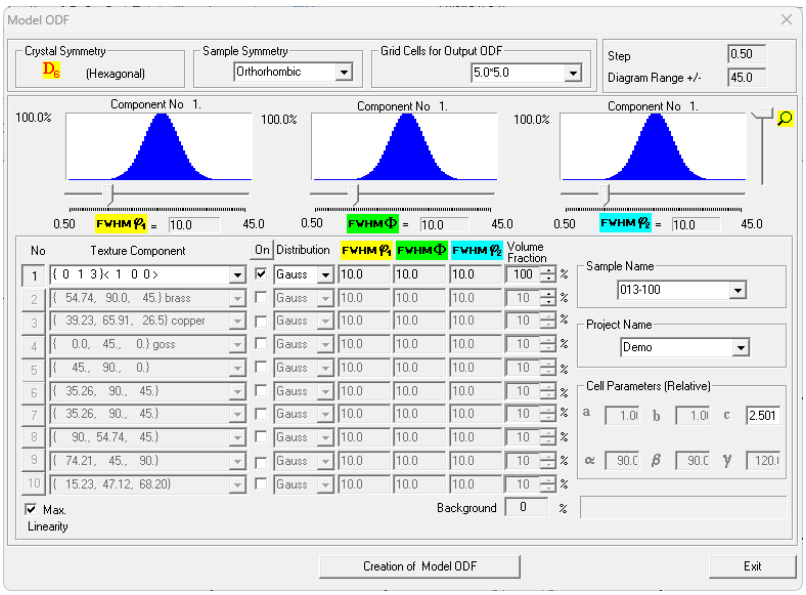
からＨｅｘａｇｏｎａｌ

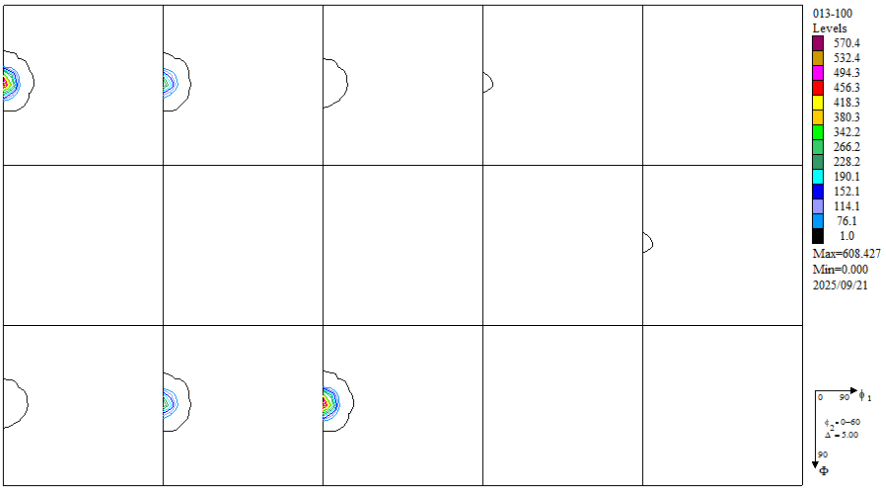
６．９５９６ｘ６．９５９６ｘ１７．４０７７ｘ９０ｘ９０ｘ１２０に

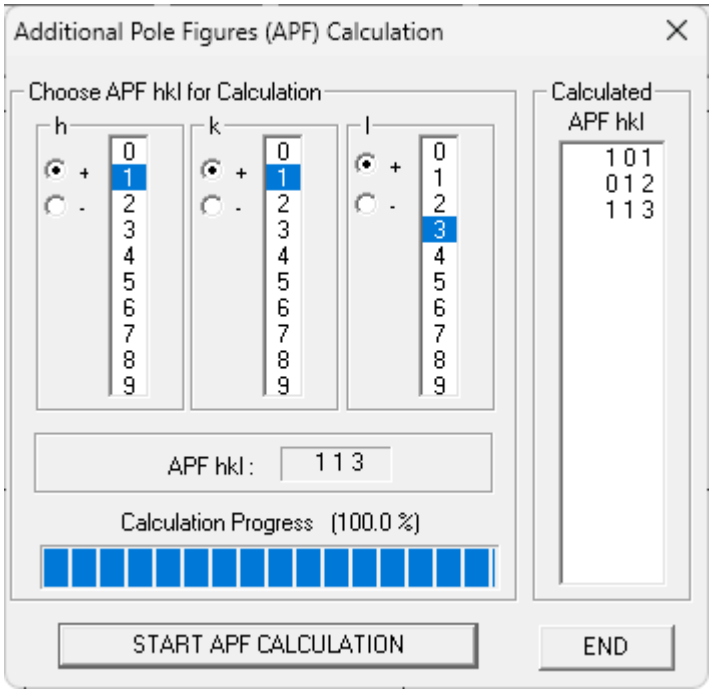
変換されています。

ＬａｂｏＴｅｘでHexagonalｃ／ａ＝２．５のＴＤ－Ｓｐｌｉｔを作成

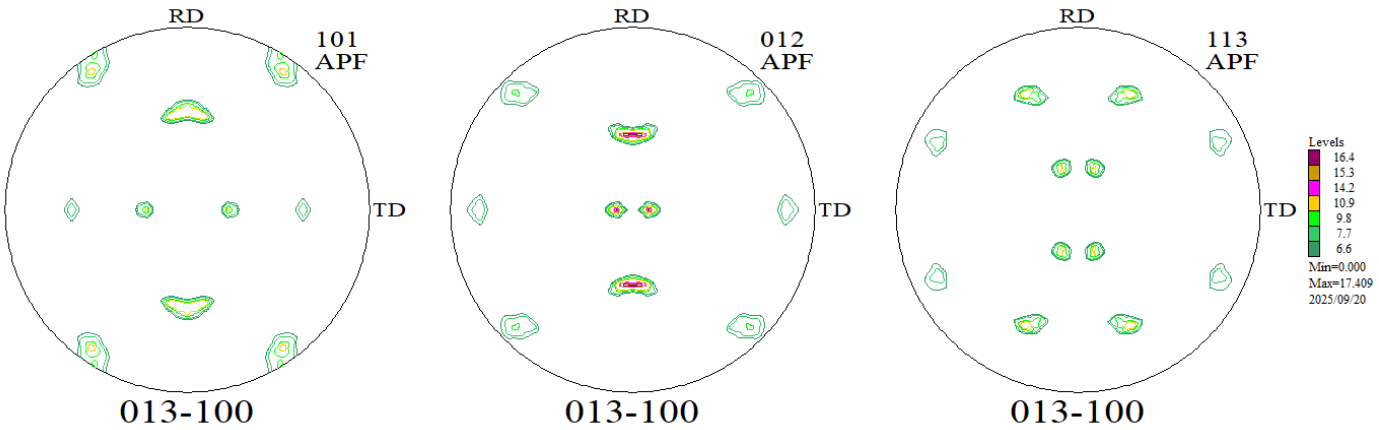




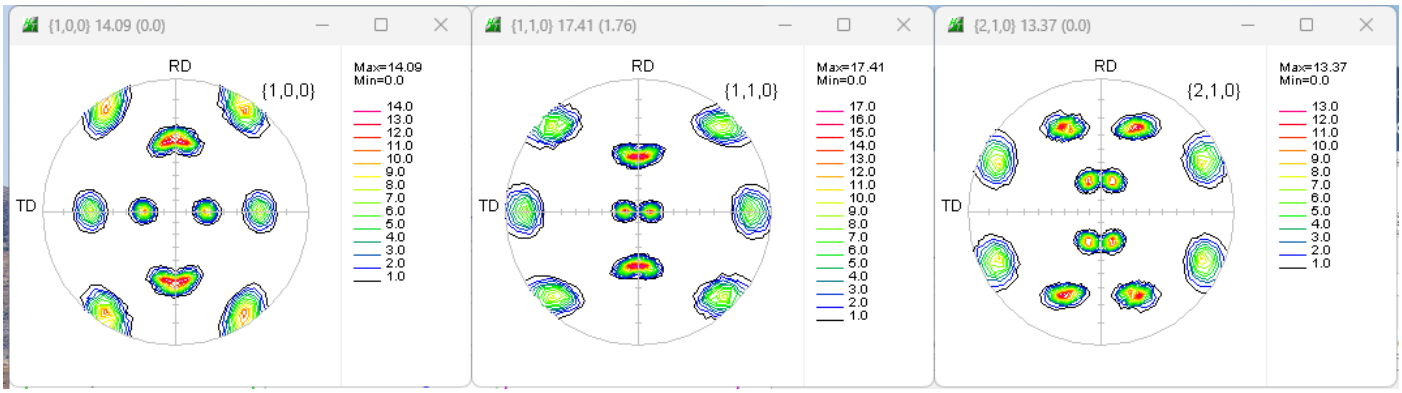




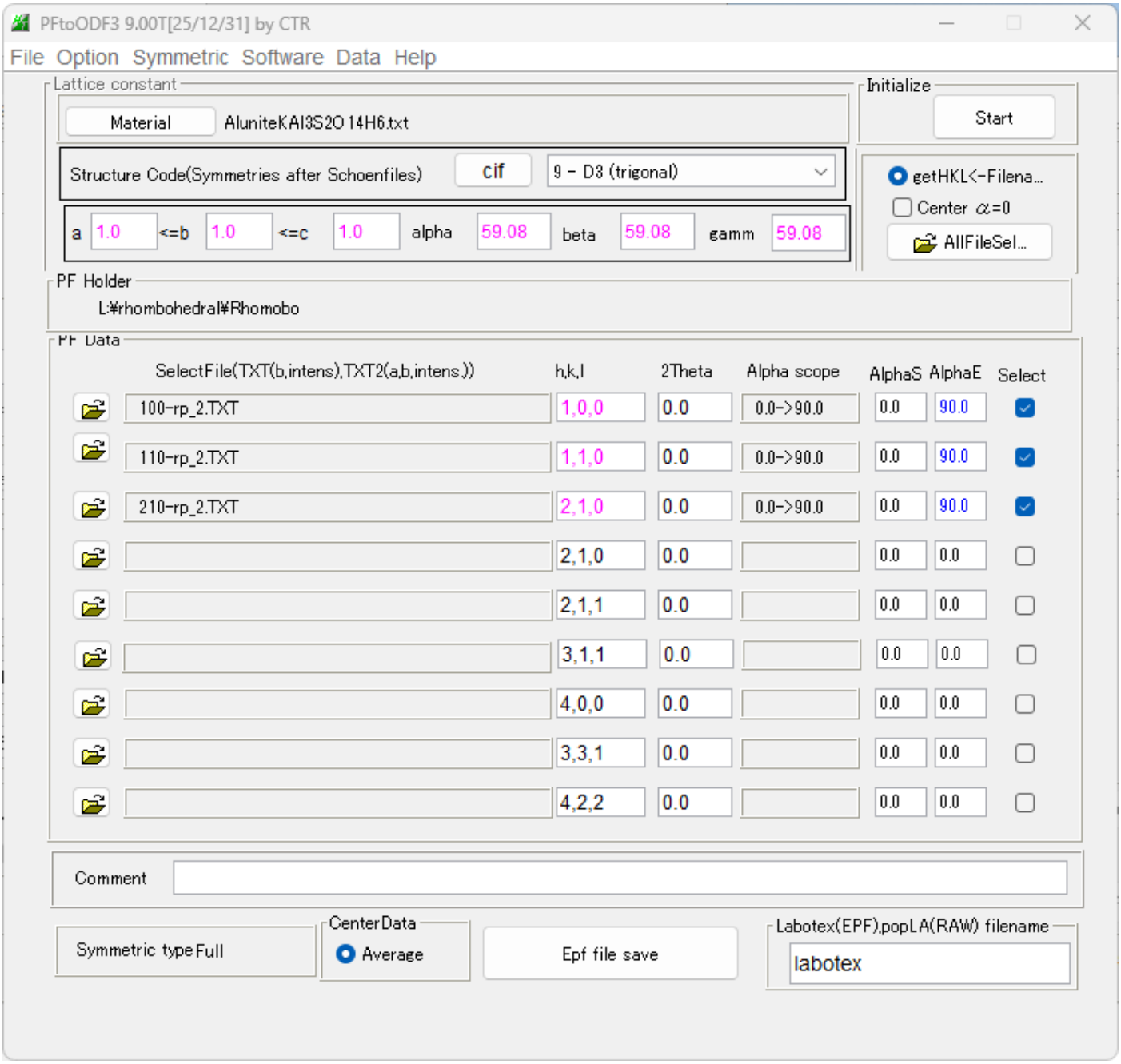
Ｈｅｘａｇｏｎａｌ



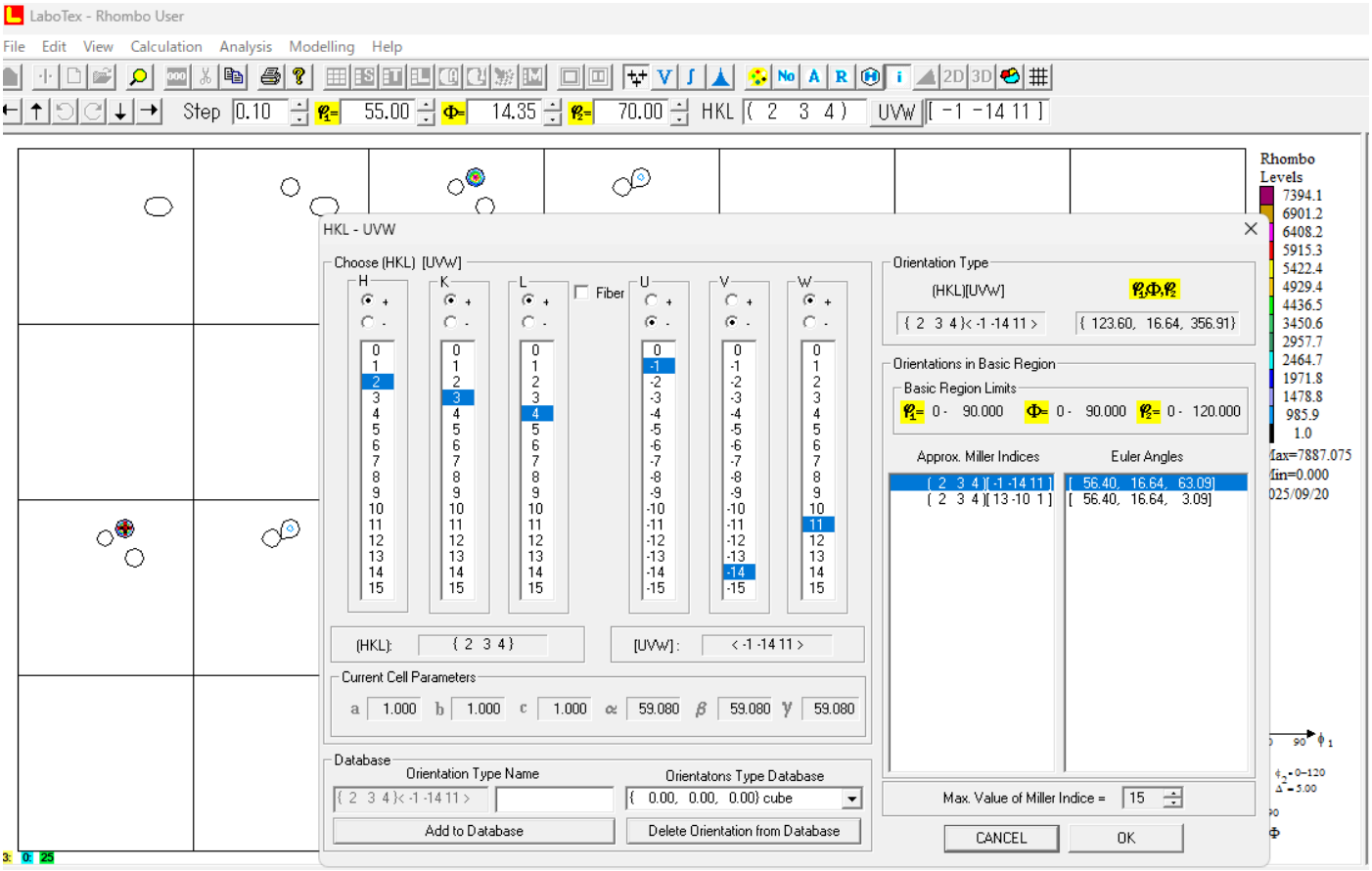
Ｒｈｏｍｂｏｈｅｄｒａｌに指数変換

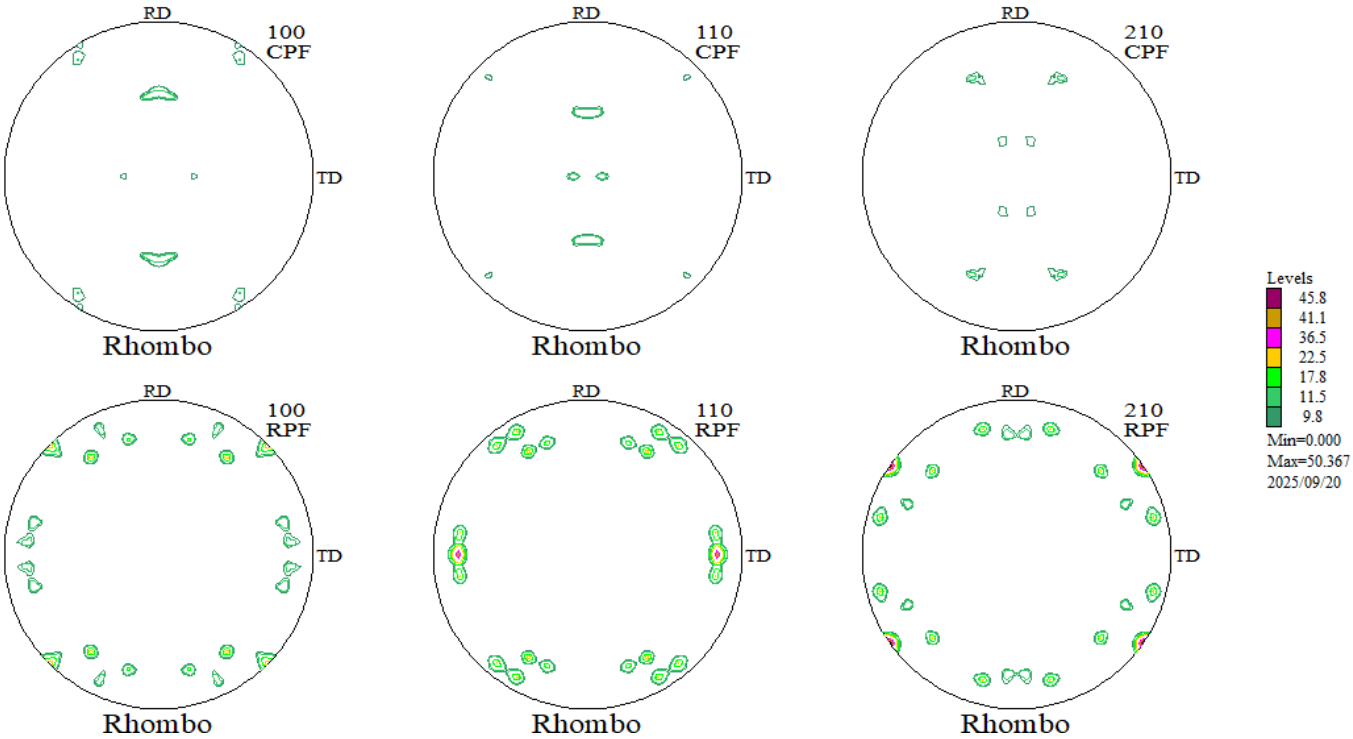


Ｒｈｏｍｂｏｈｅｄｒａｌによる解析



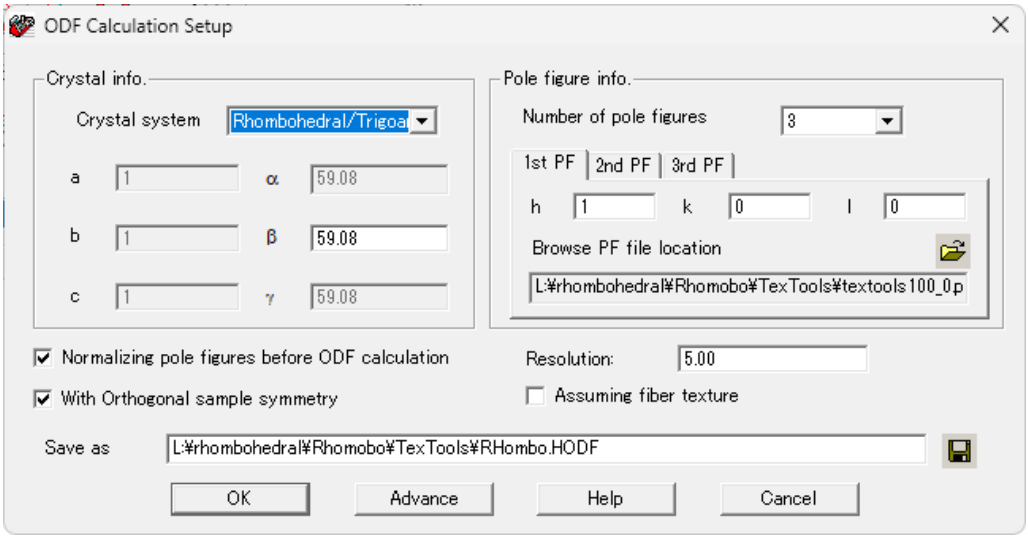
Ｌａｂｏ Ｔｅｘ

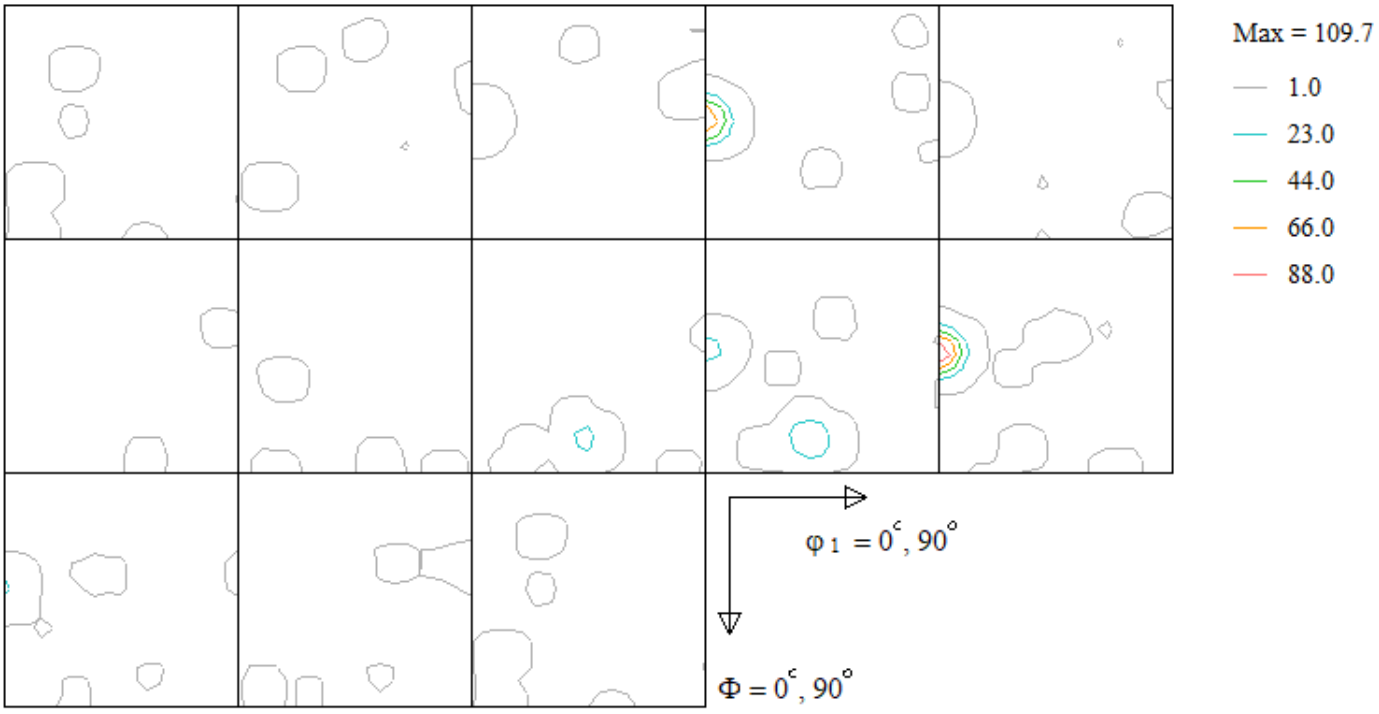


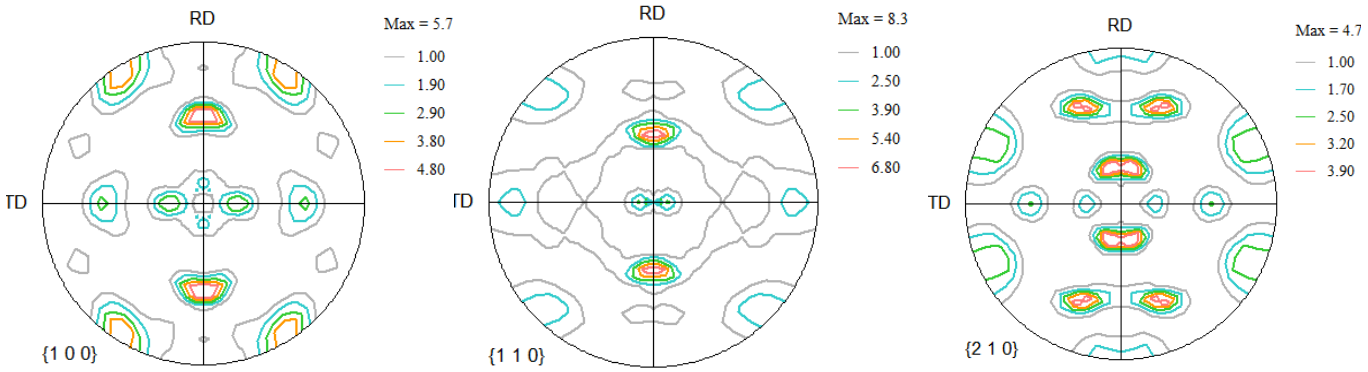


計算で来ていない

Ｔｅｘ Ｔｏｏｌｓ

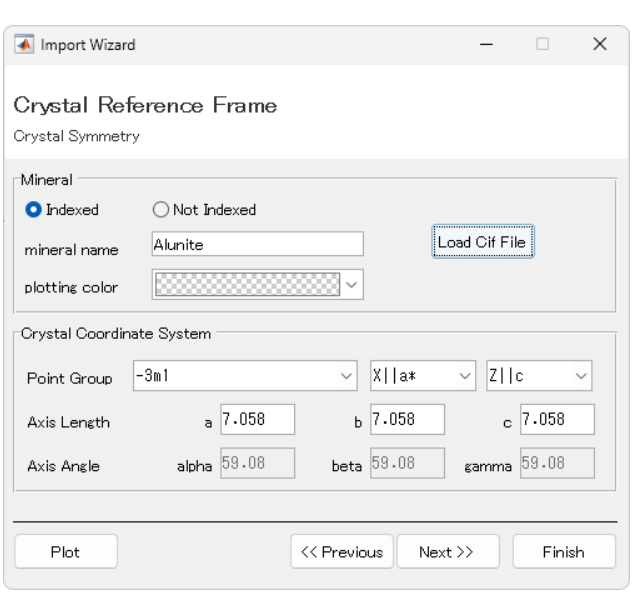


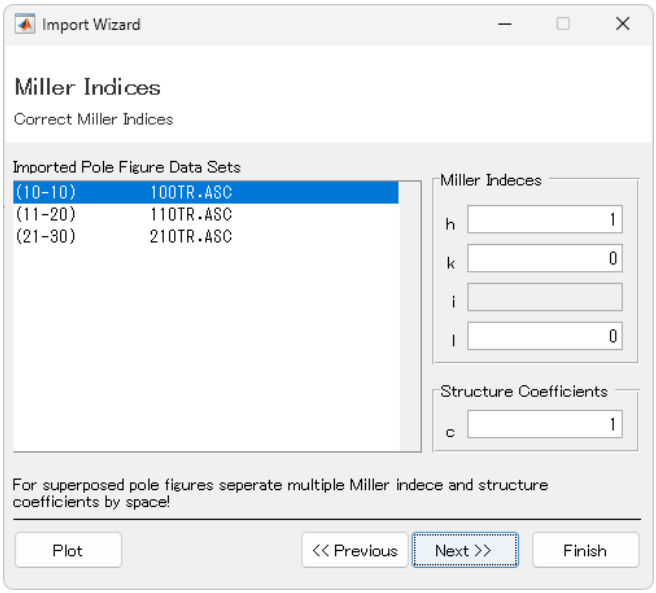


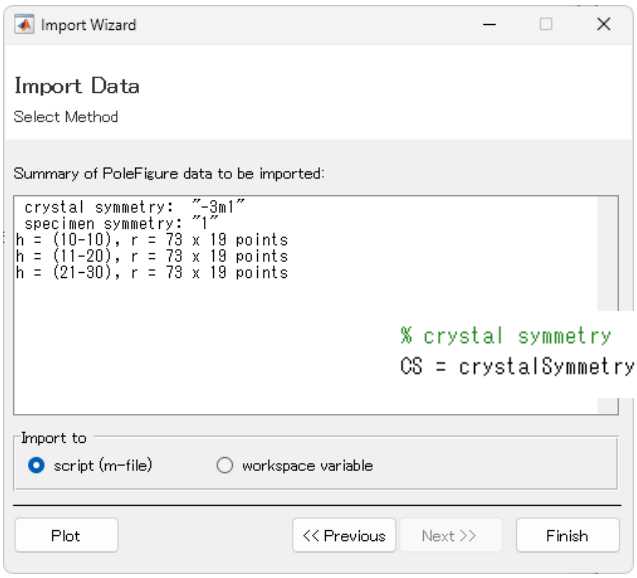


ゴーストが発生

ＭＴＥＸ







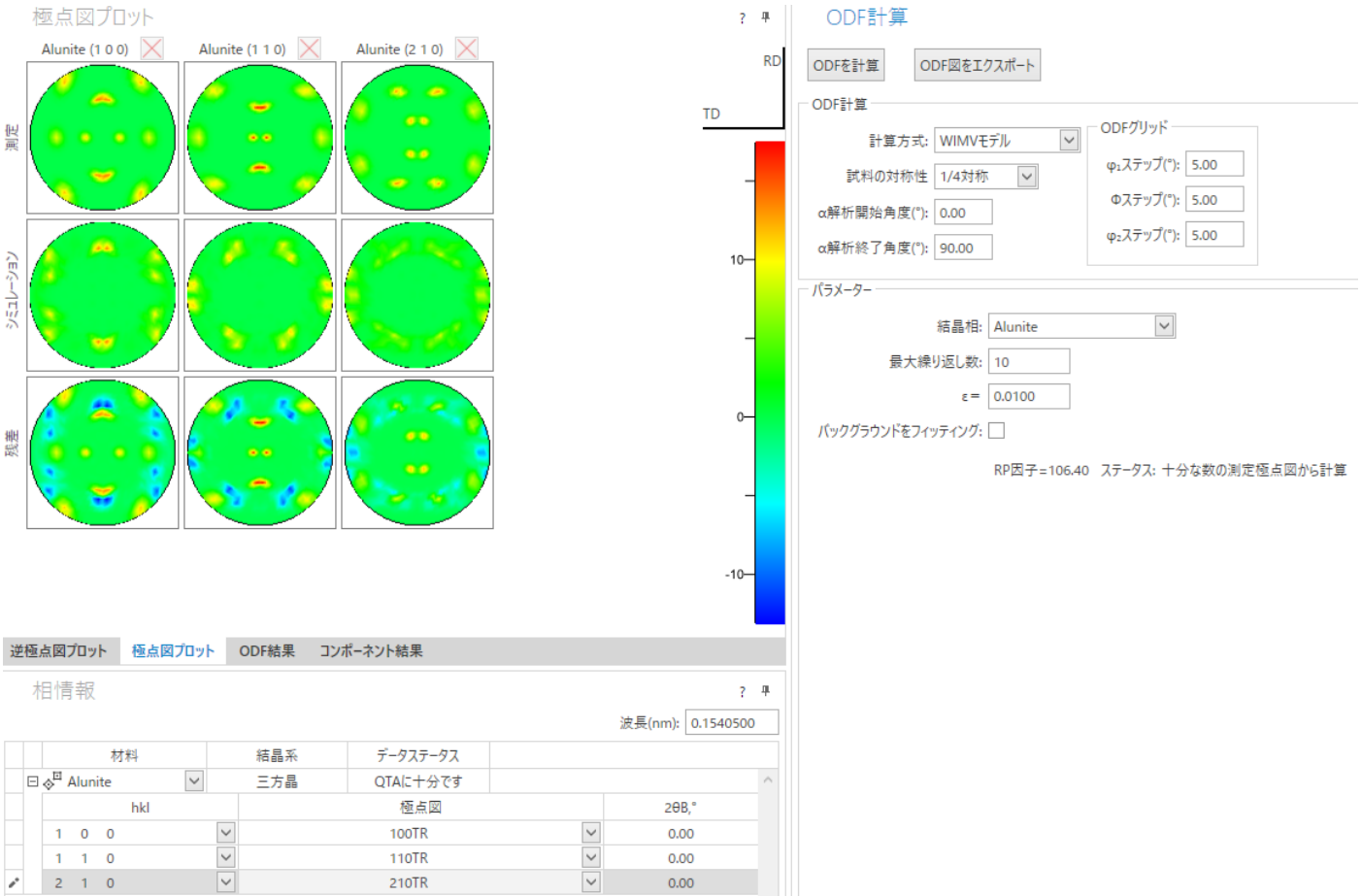

```
% crystal symmetry
CS = crystalSymmetry('-3m1', [7.1 7.1 7.1], 'X||a*', 'Z||c', 'mineral', 'Alunite');
```

読み込んだｃｉｆ

```
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↓
```

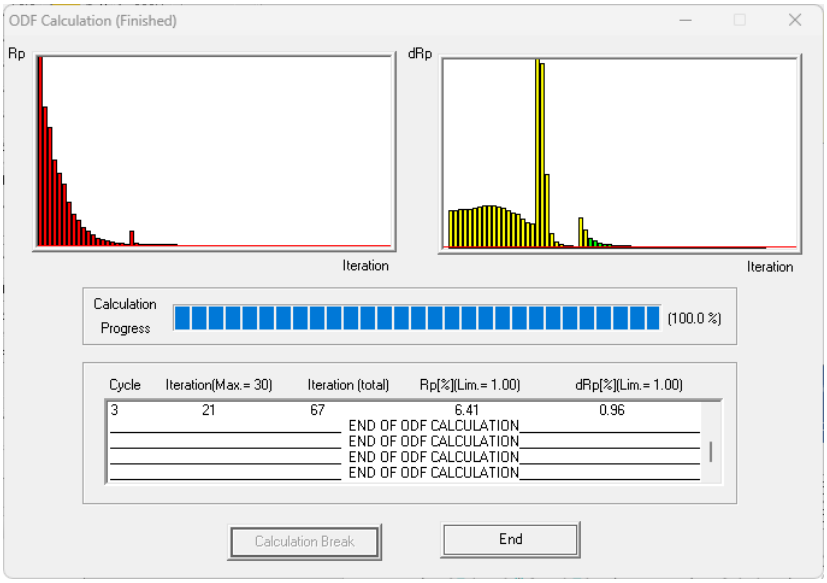
しかし、Ｈｅｘａｇｏｎａｌとして４指数変換されてします。

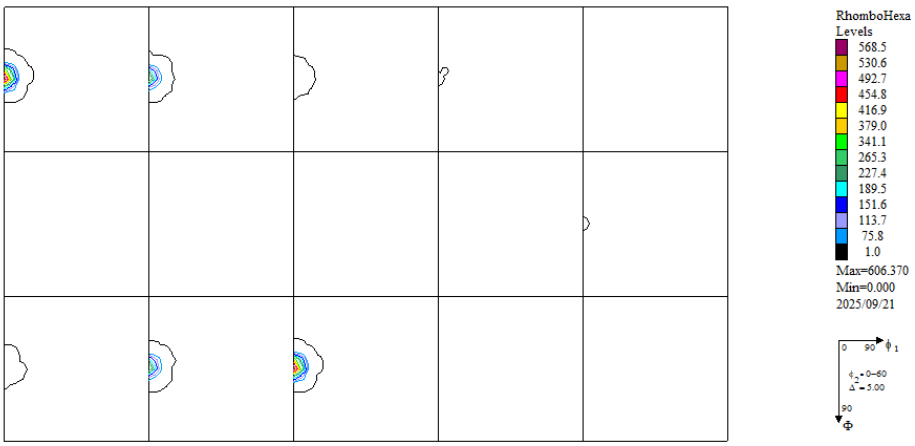
ｎｅｗＯＤＦ

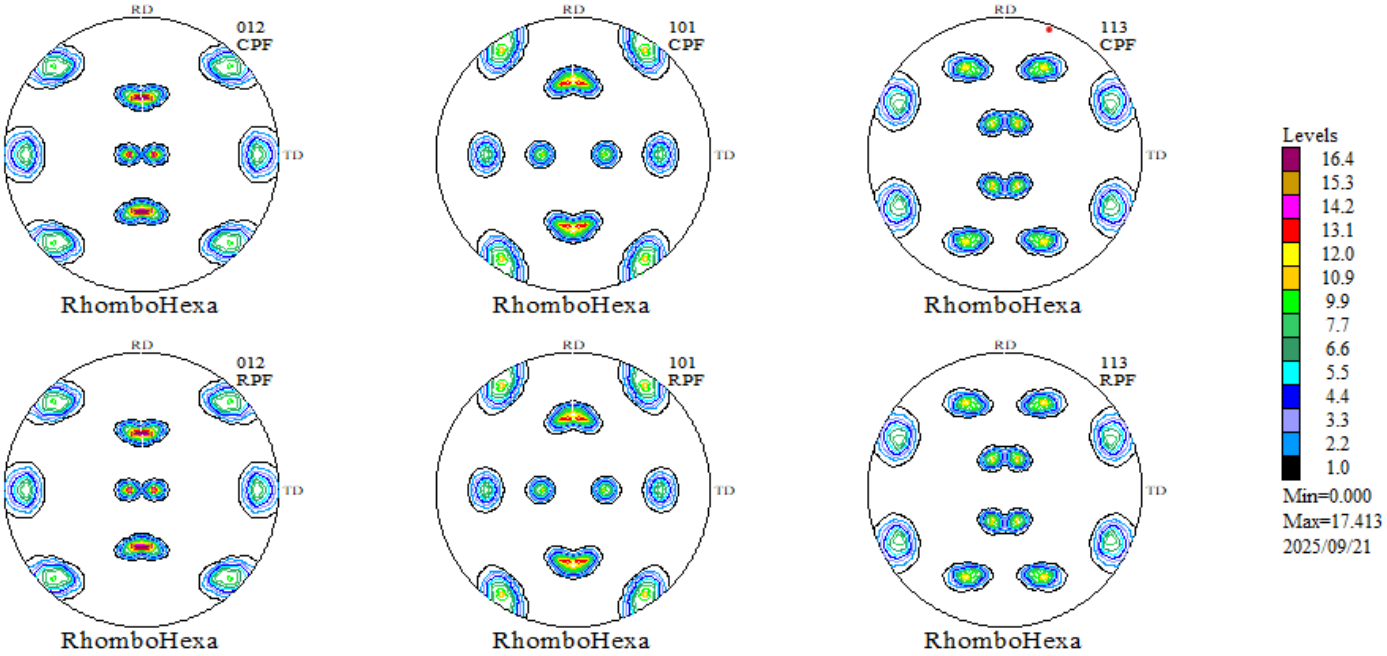


解析できない

Ｈｅｘａｇｏｎａｌで解析

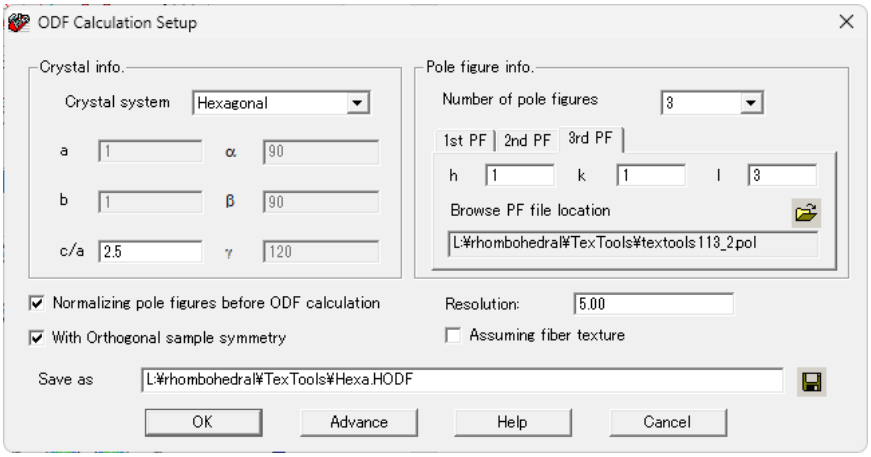


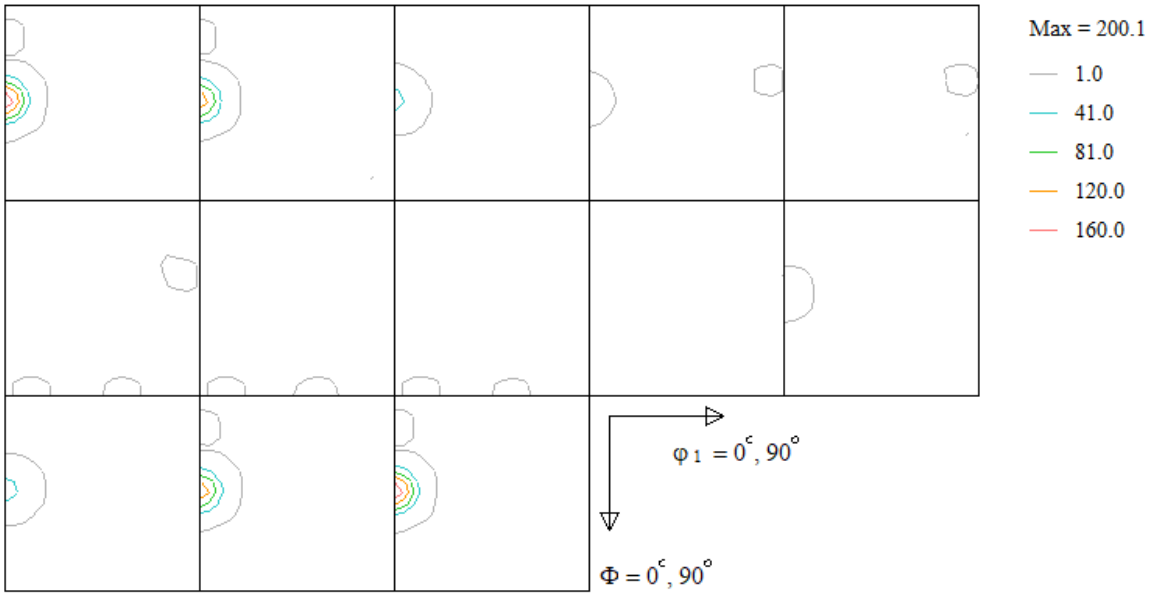


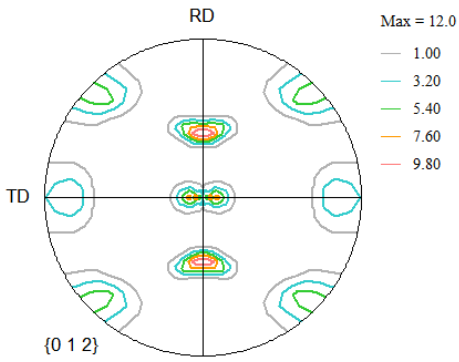


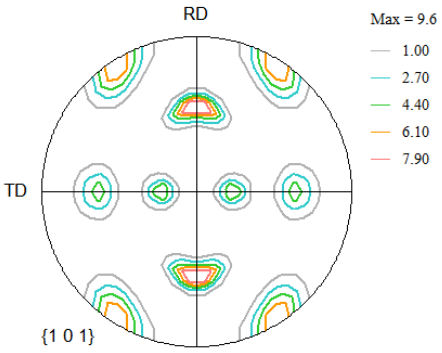
正常

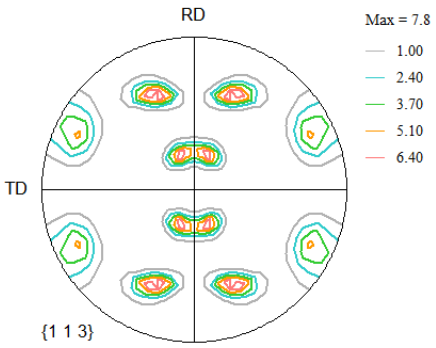
T e x T o o l s


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
2nd PF
3rd PF
h
1
k
1
l
3
Browse PF file location
L:¥rhombohedral¥TexTools¥textools113_2pol
Normalizing pole figures before ODF calculation
With Orthogonal sample symmetry
Resolution:
5.00
Assuming fiber texture
Save as
L:¥rhombohedral¥TexTools¥Hexa.HODF
OK
Advance
Help
Cancel


Max = 200.1
1.0
41.0
81.0
120.0
160.0
φ1 = 0°, 90°
Φ = 0°, 90°

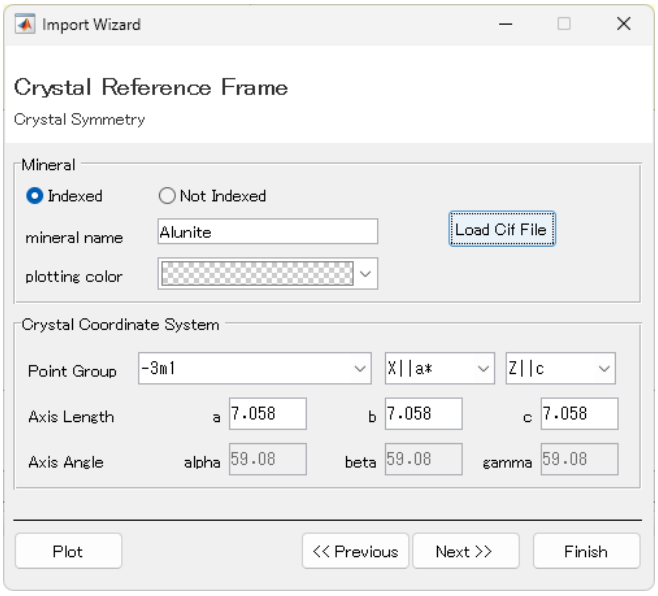

RD
TD
{0 1 2}
Max = 12.0
1.00
3.20
5.40
7.60
9.80

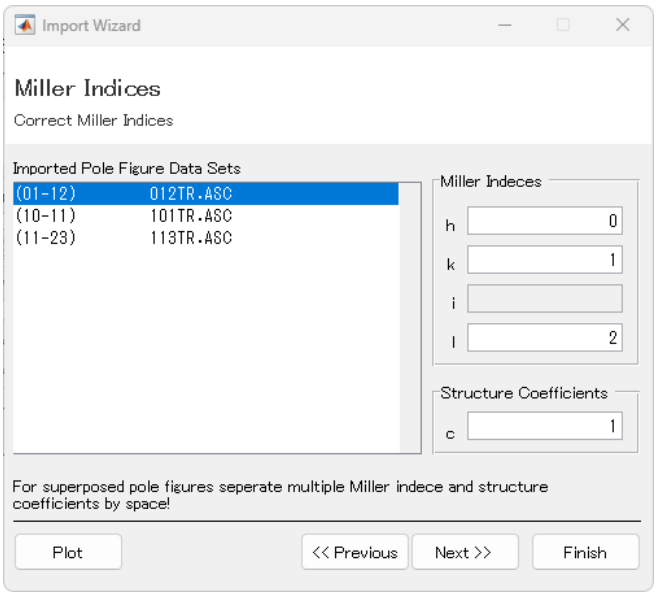

RD
TD
{1 0 1}
Max = 9.6
1.00
2.70
4.40
6.10
7.90


RD
TD
{1 1 3}
Max = 7.8
1.00
2.40
3.70
5.10
6.40

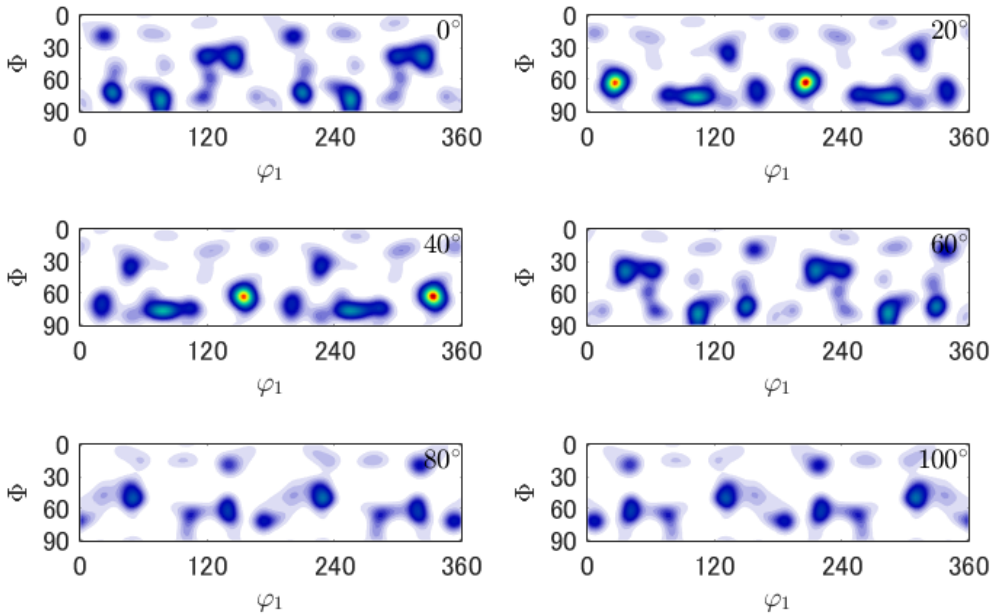
正常

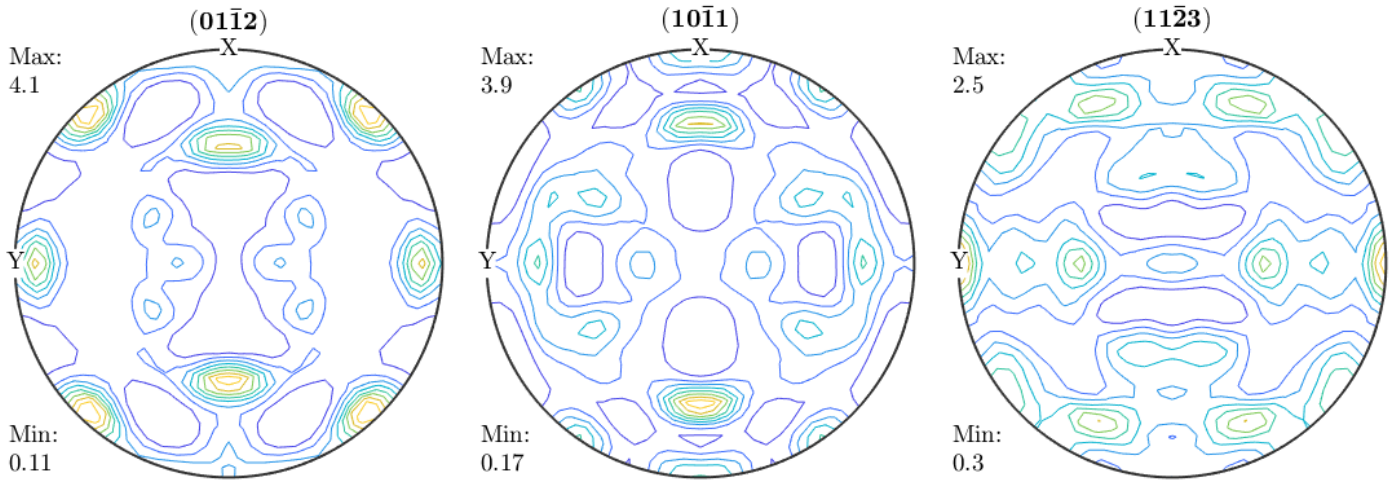
ＭＴＥＸ（ｃｉｆにＲｈｏｍｂｏｈｅｄｒａｌを指定）





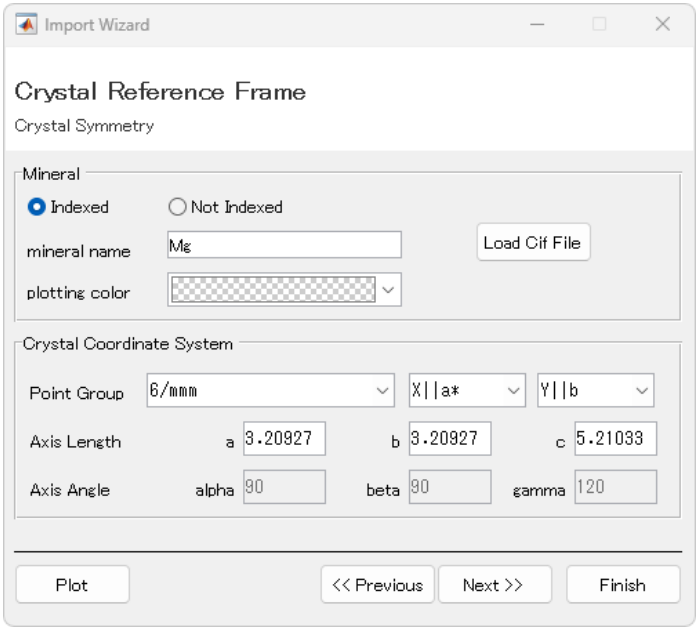
解析結果





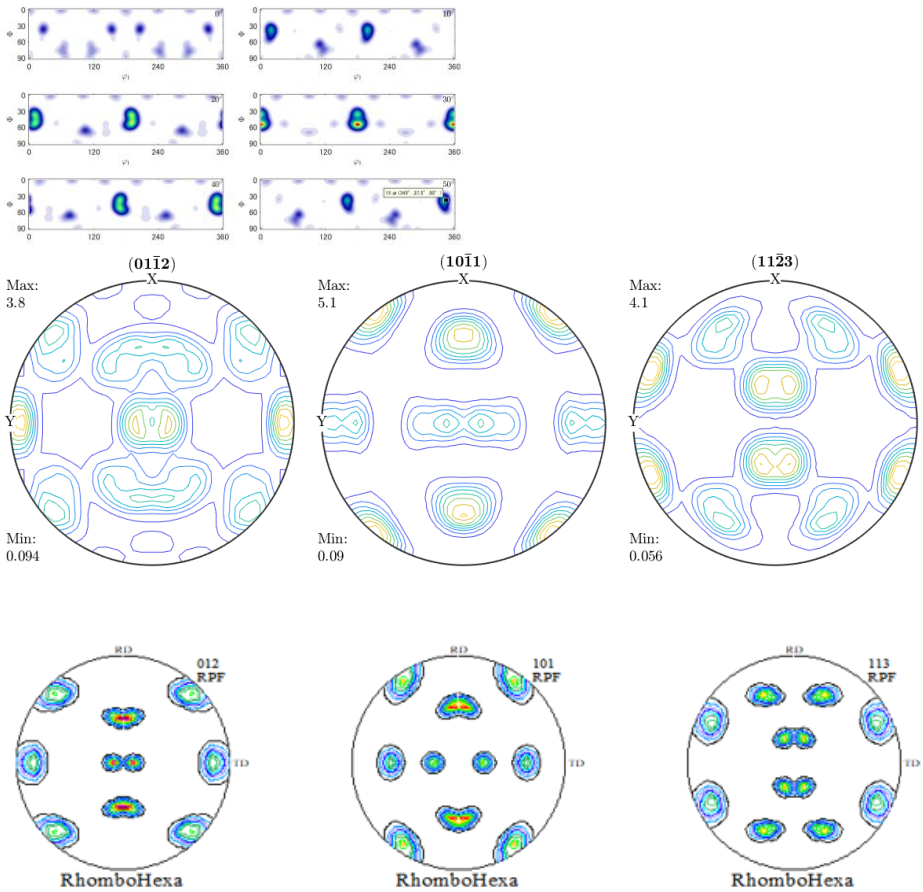
解析できない

ＭＴＥＸ（ｃｉｆにＭｇを指定し、変数の変更）



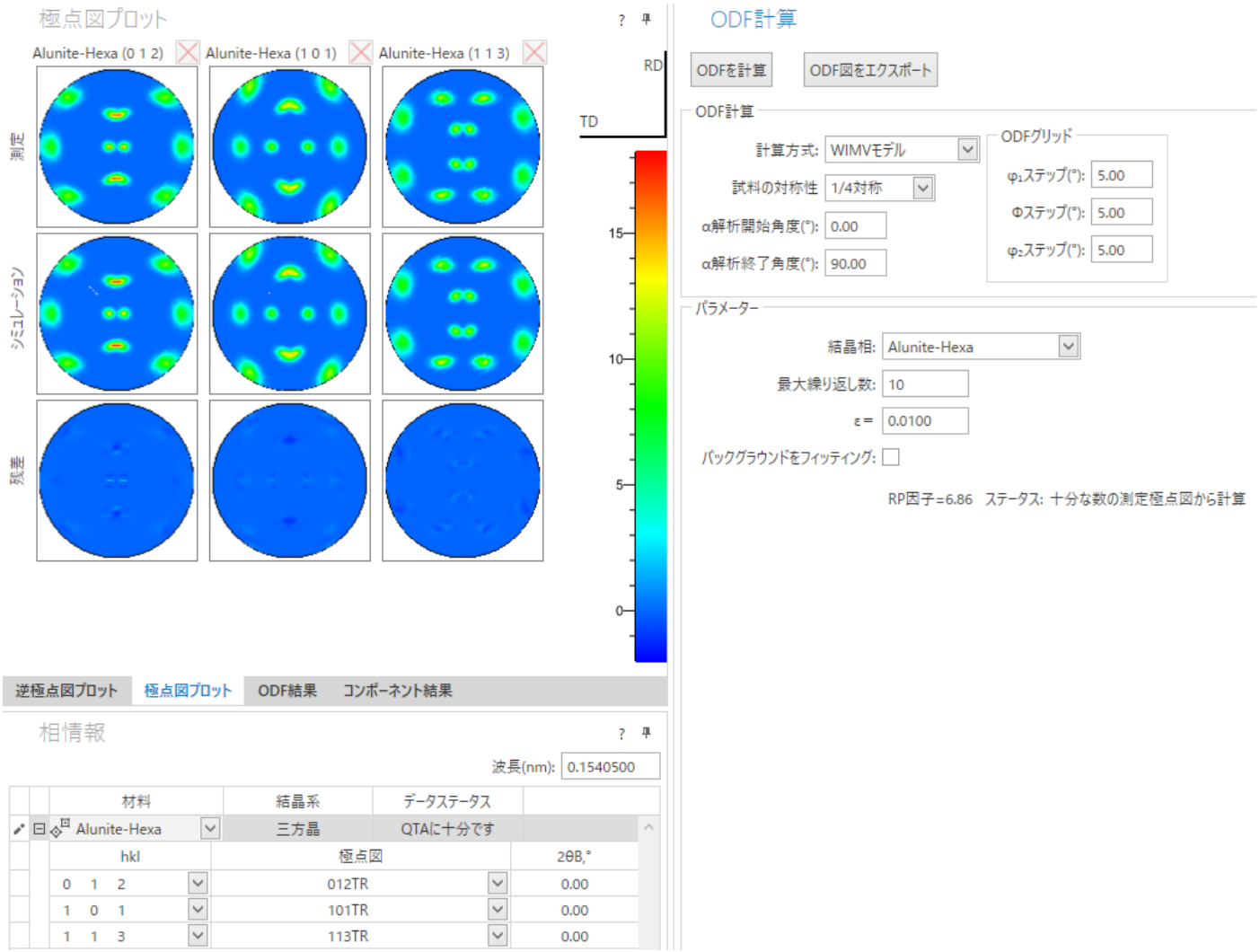

```
CS = crystalSymmetry('6/mmm', [3.2 3.2 5.2], 'X||a*', 'Y||b', 'Z||c*', 'mineral', 'Mg');
```

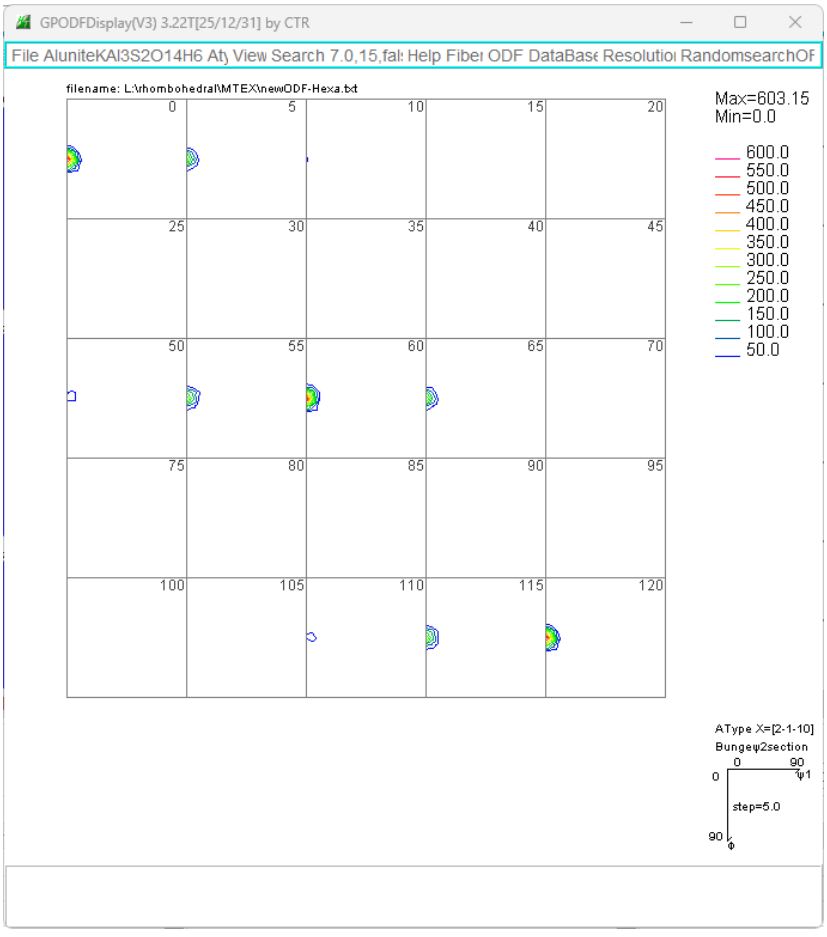
```
CS = crystalSymmetry('6/mmm', [6.9 6.9 17.4], 'X||a*', 'Y||b', 'Z||c*', 'mineral', 'Mg');
```



解析結果はずれている。

ｎｅｗＯＤＦ


極点図プロット
Alunite-Hexa (0 1 2)
Alunite-Hexa (1 0 1)
Alunite-Hexa (1 1 3)
測定
シミュレーション
残差
RD
TD
15
10
5
0
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
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の解析開始角度(°): 0.00
αの解析終了角度(°): 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-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


GPODFDisplay(V3) 3.22T[25/12/31] by CTR
File AluniteKAl3S2O14H6 At) View Search 7.0,15,fal: Help Fiber ODF DataBase Resolutio Randomsearch OF
filename: L:\rhombohedral\MTEX\newODF-Hexa.txt
Max=603.15
Min=0.0
600.0
550.0
500.0
450.0
400.0
350.0
300.0
250.0
200.0
150.0
100.0
50.0
AType X=[2-1-10]
Bungeψ2section
step=5.0

まとめ

Ｒｈｏｍｂｏｈｅｄｒａｌの指定方法が悪いのか？解析できない。

Ｒｈｏｍｂｏｈｅｄｒａｌ材料のＯＤＦ解析はＨＥｘａｇｏｎａｌ変換で行うこと