

E B S D (O I M) データの O D F 解析

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HelperTexOffice

山田 義行

odftex@ybb.ne.jp

概要

最近、XRD の ODF 解析として、LaboTex, TexTools, StandardODF を購入され、各種解析を行うケースがあります。ODF 解析の手法により、解析結果が異なる事から、複数の ODF 解析を試されるケースが増えてきています。

LaboTex と TexTools は同じ ADC 解析手法を採用されているが、解析結果は異なります。

LaboTex は入力データのままで、あるが、TexTools は ADC+Hermonic のような結果になります。

今回、TSL 様から供給して頂いた EBSD 測定データ (Ang) を LaboTex、TexTools に入力しその比較を行ってみます。

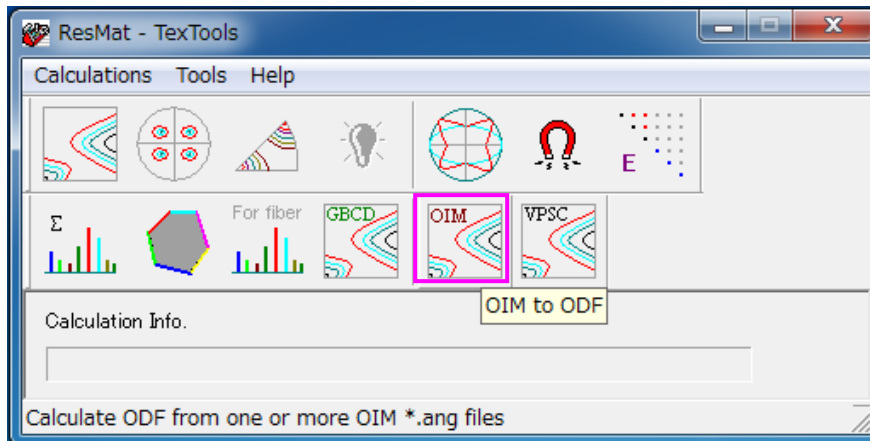
入力は、TexTools は直接読み込み、LaboTex は、CTR パッケージの EBSDtoLaboTex ソフトウェアを紹介して行う。

入力データ

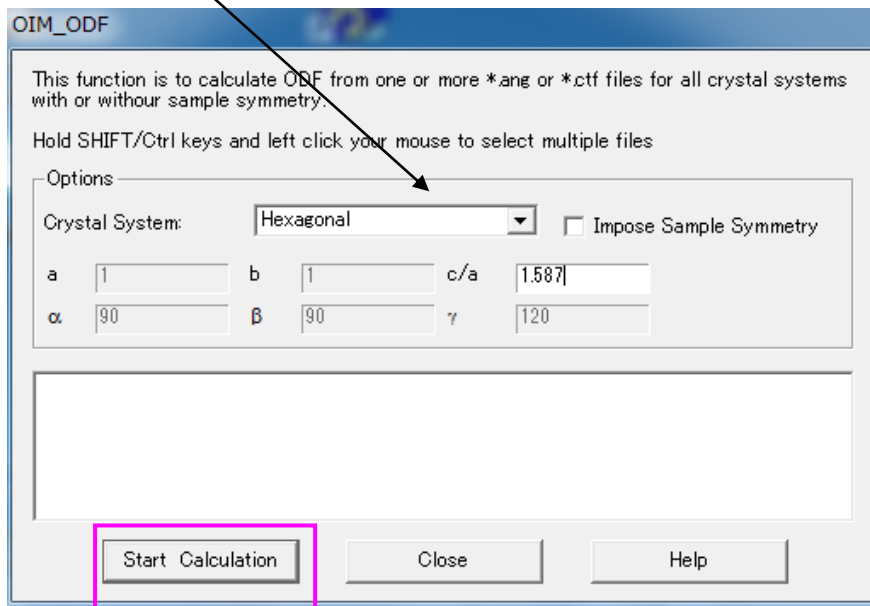
TSL 社、ANG データ、25,145KB データ

```
# TEM_PIXperUM      1.000000
# x-star             0.481100
# y-star             0.647000
# z-star             0.564700
# WorkingDistance    15.000000
#
# Phase 1
# MaterialName       Titanium (Alpha)
# Formula            Ti
# Info
# Symmetry            62
# LatticeConstants    2.950 2.950 4.680 90.000 90.000 120.000
# NumberFamilies      8
# hklFamilies         1 0 0 1 0.000000 1
# hklFamilies         0 0 2 1 0.000000 1
# hklFamilies         1 0 1 1 0.000000 1
# hklFamilies         1 0 2 1 0.000000 1
# hklFamilies         1 1 0 1 0.000000 1
# hklFamilies         1 0 3 1 0.000000 1
# hklFamilies         1 1 2 1 0.000000 1
# hklFamilies         2 0 1 1 0.000000 1
# Categories0 0 0 0 0
#
# GRID: HexGrid
# XSTEP: 2.000000
# YSTEP: 1.732051
# NCOLS_ODD: 501
# NCOLS_EVEN: 500
# NROWS: 578
#
# OPERATOR:      Administrator
#
# SAMPLEID:
#
# SCANID:
#
3.93910 1.84910 4.91315 0.00000 0.00000 377.4 0.006 0 1 1.973
1.48585 0.98494 5.63135 2.00000 0.00000 356.9 0.006 0 32767 2.446
3.83560 0.94878 3.65601 4.00000 0.00000 350.2 0.012 0 15859 2.173
3.05284 0.94230 1.30465 6.00000 0.00000 1393.3 0.794 0 12933 0.652
3.04085 0.94468 1.31030 8.00000 0.00000 1220.0 0.721 0 8999 0.901
3.04811 0.93653 1.30866 10.00000 0.00000 953.5 0.782 0 9258 0.679
2.89880 0.81277 0.95428 12.00000 0.00000 566.7 0.261 0 17246 1.689
0.88750 2.33078 0.00287 14.00000 0.00000 857.8 0.739 0 18139 0.915
4.04228 0.80403 1.04755 16.00000 0.00000 1258.6 0.642 0 22267 0.600
```

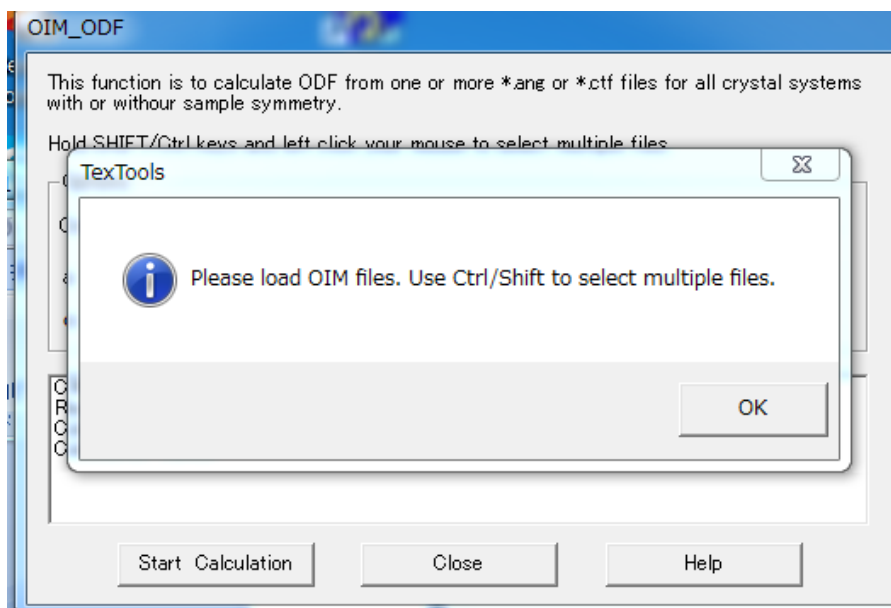
TexTools のデータ読み込み



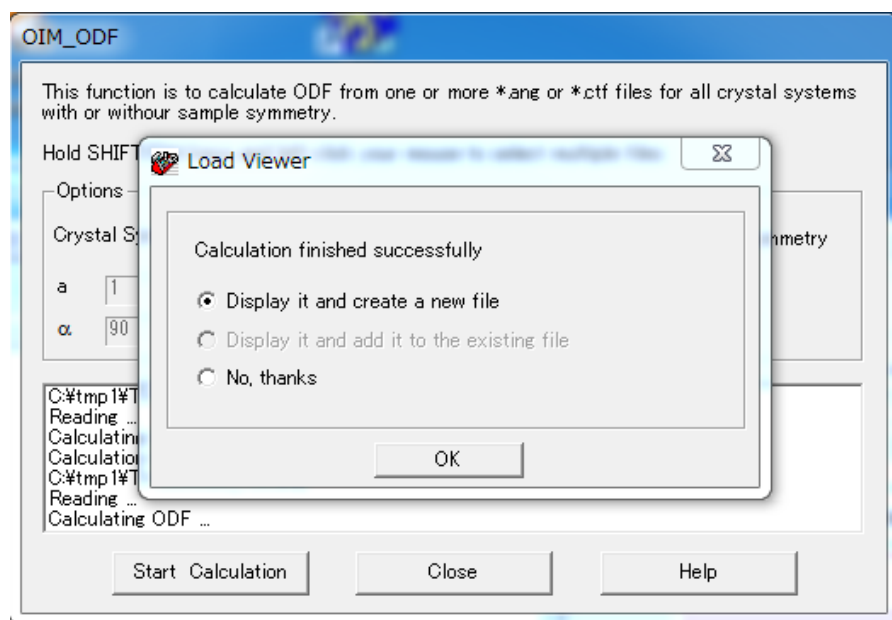
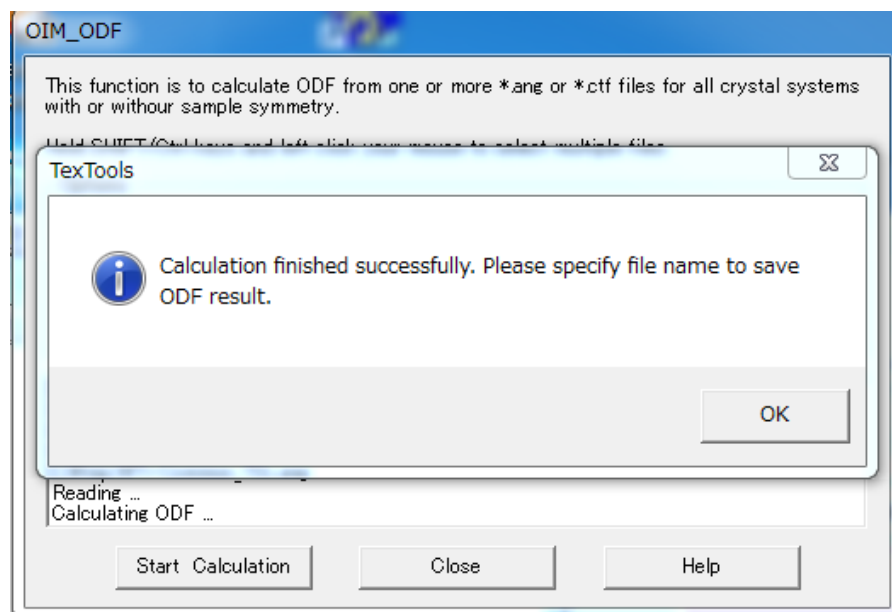
Titanium の格子定数を入力



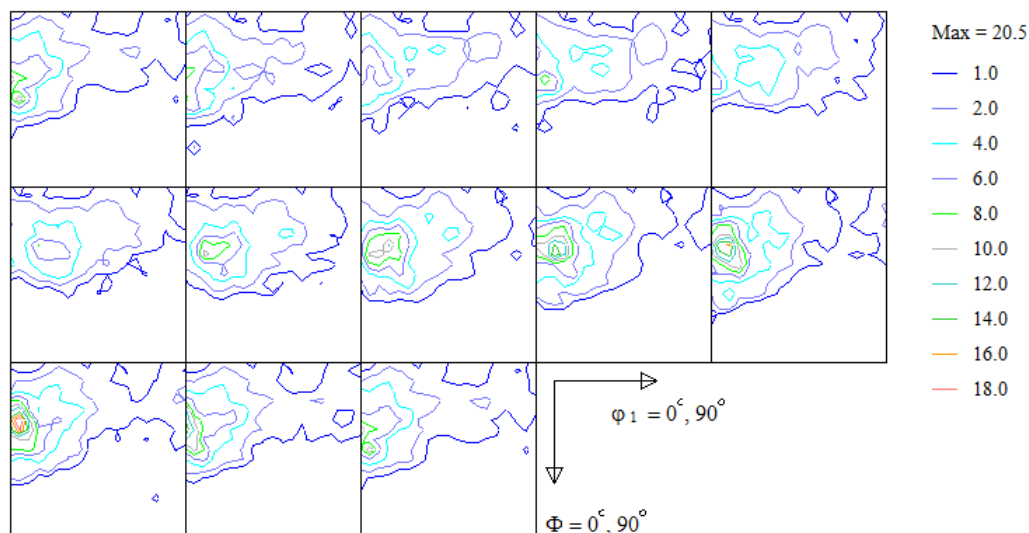
Ang ファイルを選択



ODF 解析結果ファイルを指定



ODF 解析結果が表示される

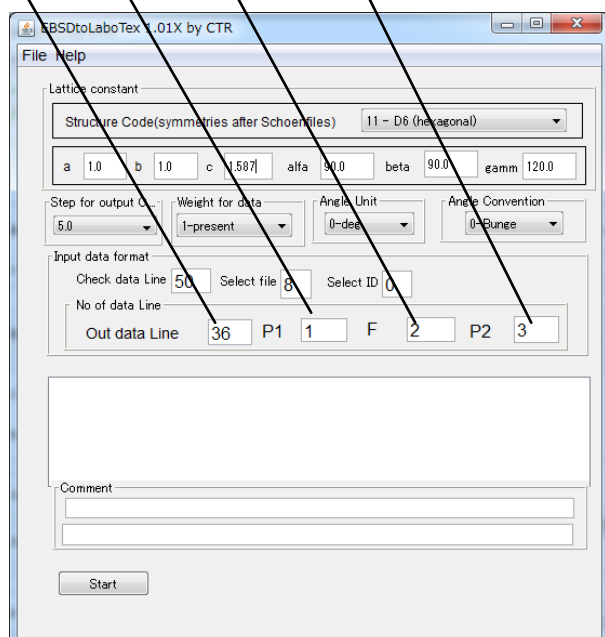


laboTex のデータの扱い

LaboTex では、Ang データを Sor データに変換を行って LaboTex で読み込む
Ang データの Format を調べる

```
1 | # TEM_PIXperUM          1.000000↓
2 | # x-star                0.481100↓
3 | # y-star                0.647000↓
4 | # z-star                0.564700↓
5 | # WorkingDistance       15.000000↓
6 | #↓
7 | # Phase 1↓
8 | # MaterialName          Titanium (Alpha)↓
9 | # Formula               Ti↓
10 | # Info                  ↓
11 | # Symmetry              62↓
12 | # LatticeConstants      2.950 2.950 4.680 90.000 90.000 120.000↓
13 | # NumberFamilies        8↓
14 | # hklFamilies           1 0 0 1 0.000000 1↓
15 | # hklFamilies           0 0 2 1 0.000000 1↓
16 | # hklFamilies           1 0 1 1 0.000000 1↓
17 | # hklFamilies           1 0 2 1 0.000000 1↓
18 | # hklFamilies           1 1 0 1 0.000000 1↓
19 | # hklFamilies           1 0 3 1 0.000000 1↓
20 | # hklFamilies           1 1 2 1 0.000000 1↓
21 | # hklFamilies           2 0 1 1 0.000000 1↓
22 | # Categories0 0 0 0 0 ↓
23 | #↓
24 | # GRID: HexGrid↓
25 | # XSTEP: 2.000000↓
26 | # YSTEP: 1.732051↓
27 | # NCOLS_ODD: 501↓
28 | # NCOLS_EVEN: 500↓
29 | # NROWS: 578↓
30 | #↓
31 | # OPERATOR: Administrator↓
32 | #↓
33 | # SAMPLEID: ↓
34 | #↓
35 | # SCANID: ↓
36 | #↓
37 | 3.93910 1.84910 4.91315 0.00000 0.00000 377.4 0.006 0 1
38 | 1 973 ↓
```

Out dataline に読み飛ばす行数を指定、 ϕ 1、 Φ 、 ϕ 2 の並びを指定する。



入力 Ang データを選択

EBSDtoLaboTex 1.01X by CTR

File Help

Condition save

Load

End

Step for output O... 5.0

Weight for data 1-present

Angle Unit 0-deg

Angle Convention 0-Bunge

Input data format

Check data Line 50 Select file 8 Select ID 0

No of data Line

Out data Line 36 P1 1 F 2 P2 3

Comment

Start

EBSDtoLaboTex 1.01X by CTR

File Help

Lattice constant

Structure Code(symmetries after Schoenflies) 11 - D6 (hexagonal)

a 1.0 b 1.0 c 1.587 alfa 90.0 beta 90.0 gamm 120.0

Step for output O... 5.0

Weight for data 1-present

Angle Unit 0-deg

Angle Convention 0-Bunge

Input data format

Check data Line 50 Select file 8 Select ID 0

No of data Line

Out data Line 36 P1 1 F 2 P2 3

33: #

34: # SCANID:

35: #

36:	3.93910	1.84910	4.91315	0.00000	0.00000
37:	1.48585	0.98494	5.63135	2.00000	0.00000

Comment

C:\tmp\1#Ti-Common_TSLang

Start

Complete !!!

LaboTex で SOR データ読み込み

New Sample

Choose Experimental Data (LaboTex Single Orientations Files)

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

Ti-Common_TSL.SOR

Path C:\tmp1\ Ti-Common_TS

Info C:\tmp1\Ti-Common_TSL.ang

Choose Defocussing Correction

☒ Correction (On/Off)


☒ Correction Data from File ☐ Correction Data from Formula

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

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

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

Info

Crystal Symmetry  (Hexagonal)

Project Name

Demo
EBSDANG

Project Name : EBSDANG

Sample Name

Ti-Common_TSL

Sample Name : Ti

Cancel Create of ODF from Single Orientations Data

ODF Calculations from a Set of Single Orientations

Project EBSDANG Sample Ti

Crystal Symmetry D6-Hexagonal

Cell Parameters (Relative)

a 1.0i b 1.0i c 1.5i

Angle Convention for Data Bunge

Grid Cells for Output ODF 5.0*5.0

Angle Unit Degrees

Weight Yes

Phase 0

Descriptions

C:\tmp1\Ti-Common_TSL.ang

Single Orientations Files

Ti-Common_TSL.SOR

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

ODF Calculations from a Set of Single Orientations

Project EBSDANG Sample Ti

Crystal Symmetry D6-Hexagonal

Cell Parameters (Relative)

a 1.0i b 1.0i c 1.5i

Angle Convention for Data Bunge

Grid Cells for Output ODF 5.0*5.0

Angle Unit Degrees

Weight Yes

Phase 0

Descriptions

C:\tmp1\Ti-Common_TSL.ang

Single Orientations Files

Ti-Common_TSL.SOR

Calculations Progress

Merge (files) 1/1



No of single orien. 289289

100.0% Calculation Finished

'SOR' Output File Options

Add (HKL)<UVW> ☐ Max. Value of Miller Indices = 15

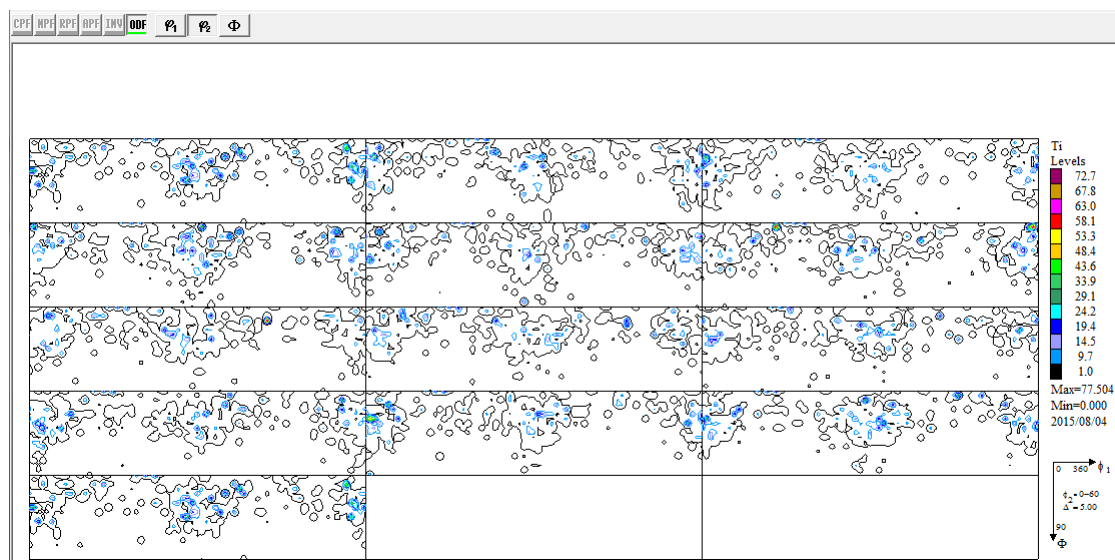
Hexagonal Axis Convention of Data (important only in Hexagonal C.S.)

☒  ☐ 

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

BREAK END

ODF 解析結果



ODF Triclinic->Orthorombic

