

ODF図から r a n d o m の定量をシュミレーションと実データ解析

2021年08月11日

HelperTex Office

概要

ODFの方位として代表的な方位をL a b o T e xで作成しr a n d o mレベルのシミュレーションを行う。

データ

 brass-FW10-20%.TXT	2021/08/10 18:54	テキスト文書	275 KB
 brass-FW20-20%.TXT	2021/08/10 18:54	テキスト文書	275 KB
 copper-FW10-20%.TXT	2021/08/10 18:53	テキスト文書	275 KB
 copper-FW20-20%.TXT	2021/08/10 18:52	テキスト文書	275 KB
 goss-FW10-20%.TXT	2021/08/10 18:55	テキスト文書	275 KB
 goss-FW20-20%.TXT	2021/08/10 18:58	テキスト文書	275 KB
 s-FW10-20%.TXT	2021/08/10 18:53	テキスト文書	275 KB
 s-FW20-20%.TXT	2021/08/10 18:53	テキスト文書	275 KB

方位に対してFWHMとVolumeFractionを与える。

b r a s s - F W 1 0 - 2 0 % . t x t では

b r a s s 方位のFWHM=10deg、VF%=20%を表す。

残りがr a n d o mでVF%=80%である。

r a n d o mは、本来最小値であるが、オーバシュートやばらつきが発生し、一致しないことがある。

5度ステップのODFでは18x19x19のデータ点に対しr a n d o m位置は

数多く存在する。よって、方位密度1.0以下にピーク状に現れると考えられる。

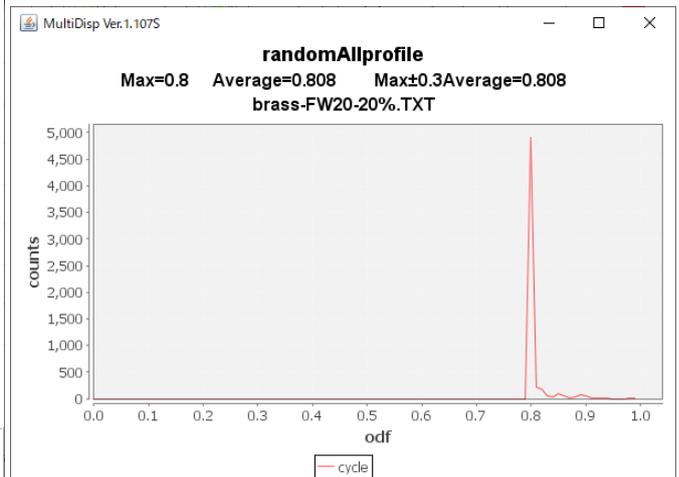
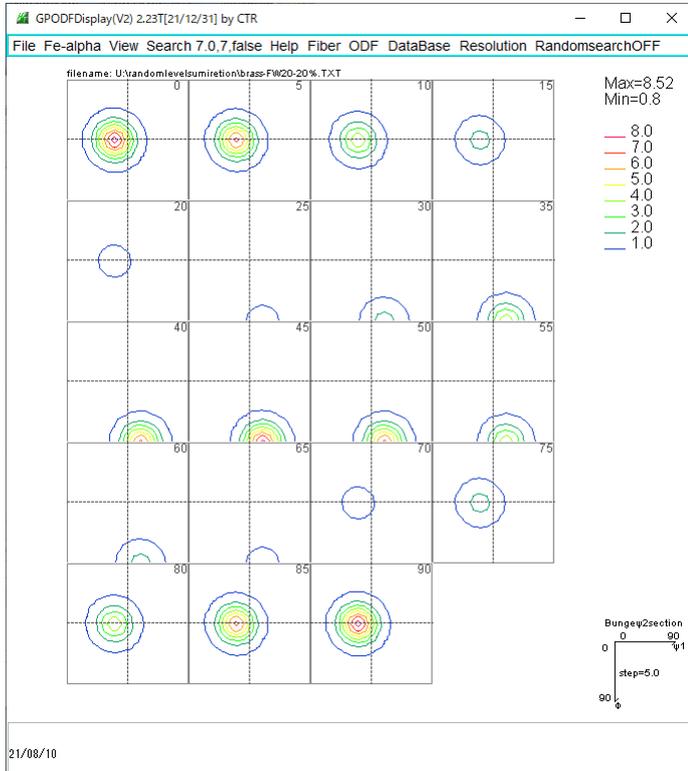
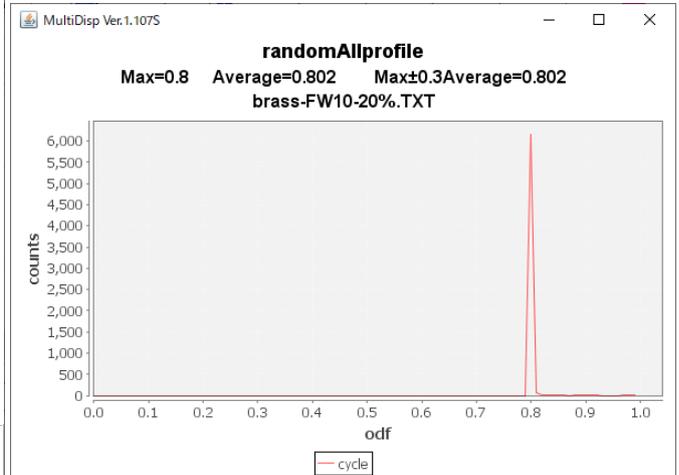
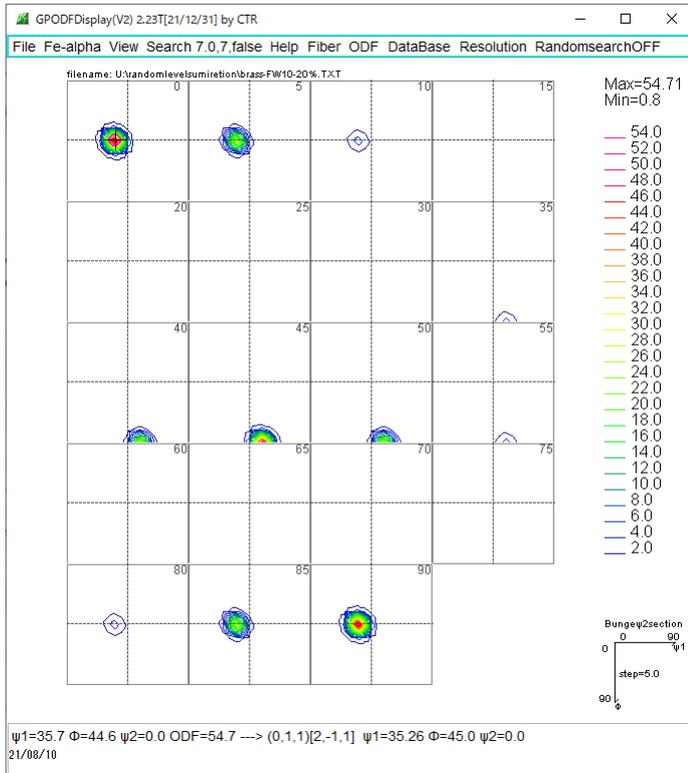
全てr a n d o mであれば、方位密度は1.0、20%が他の方位であればr a n d o m方位は

0.8に下がり、その0.8が80%で計算される。

検証結果

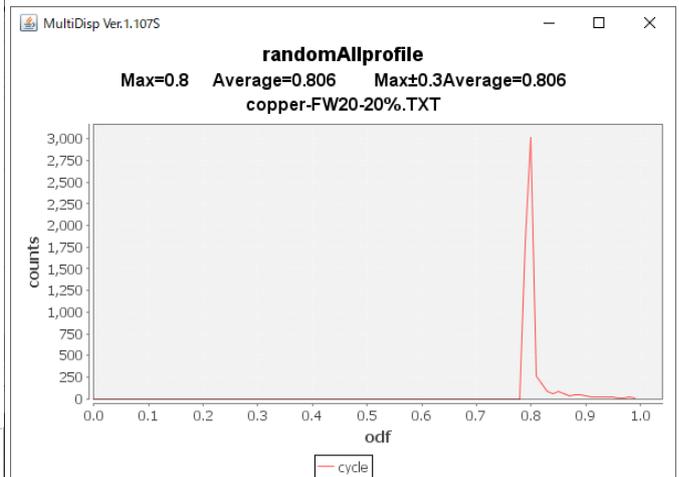
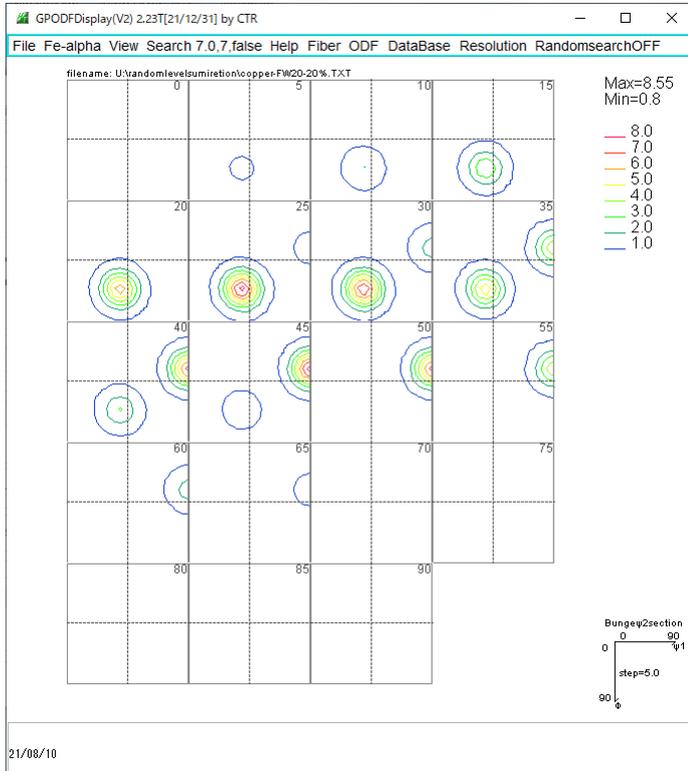
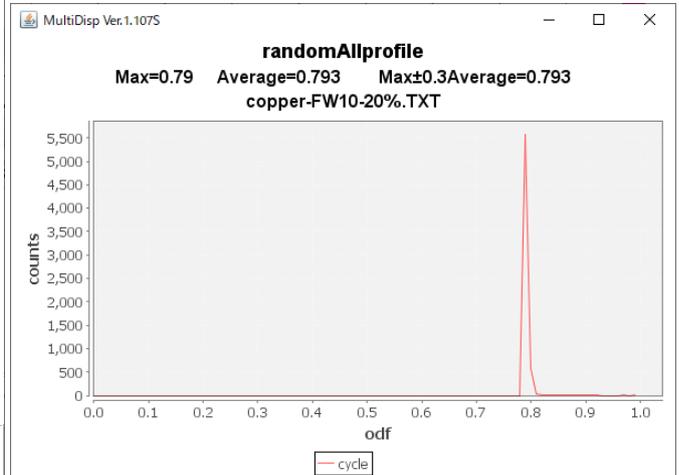
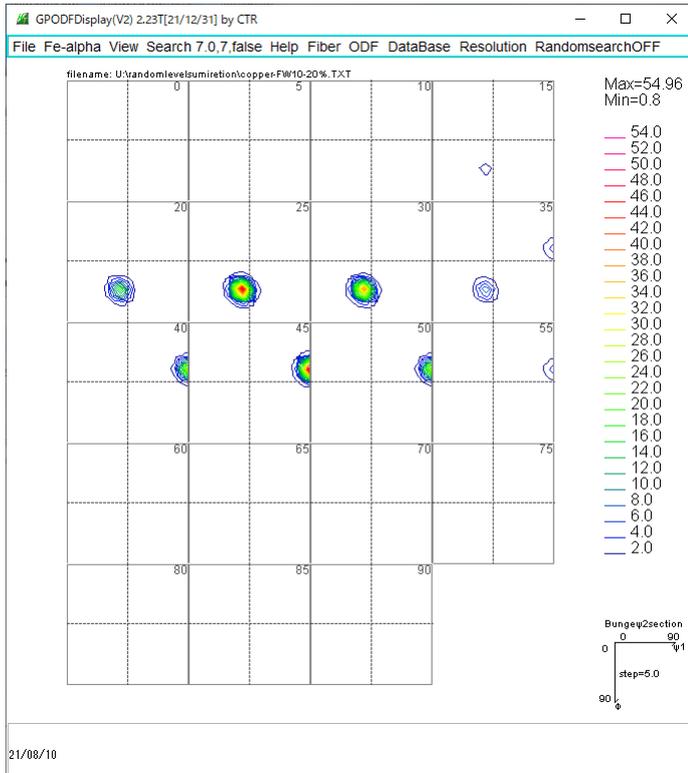
L a b o T e xでは他のODFに比べ、r a n d o mレベルがシャープに計算され正確なr a n d o m%が得られます。

brass 方位



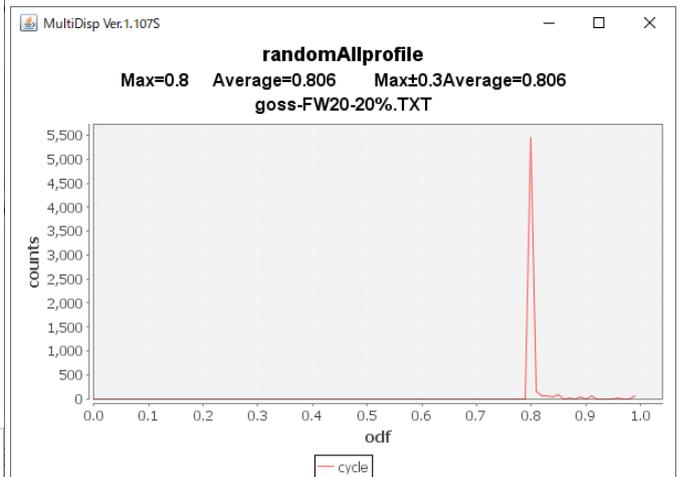
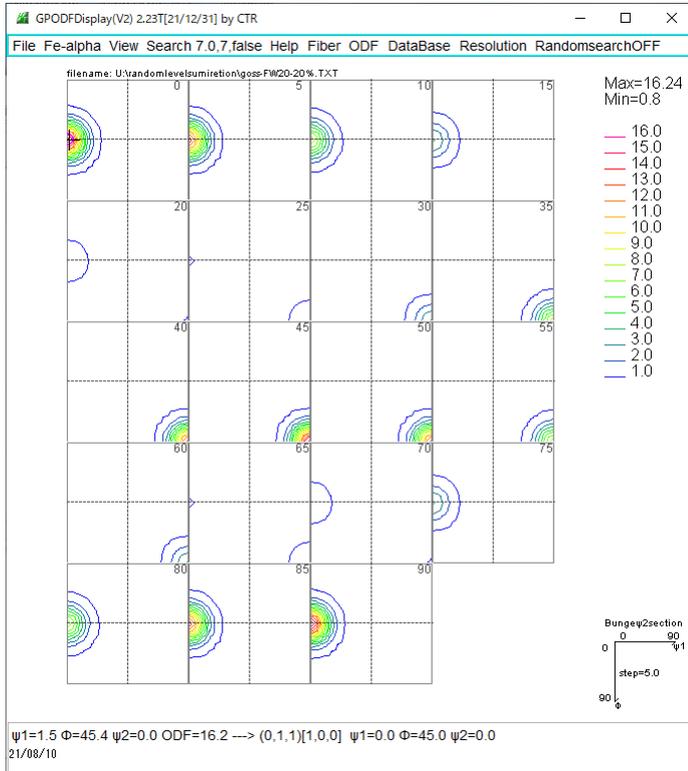
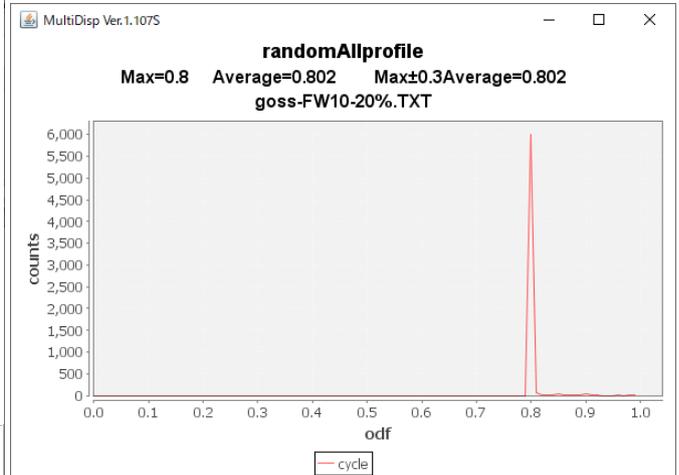
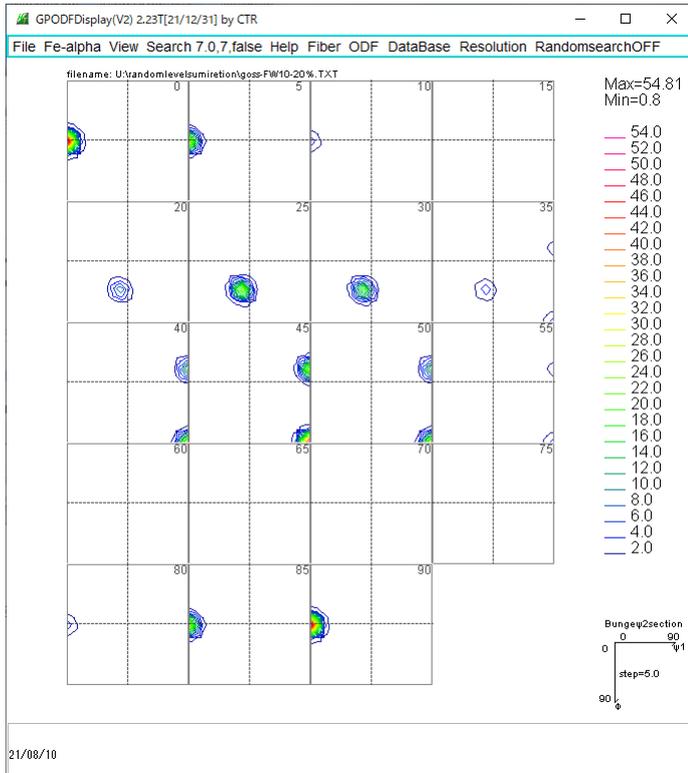
Brass 方位 VF%=20%ではFWHMを変えるとMax方位密度は変わるが最小値は変わらず randomlevel=0.8→random=80%と考えられます。

c o p p e r 方位



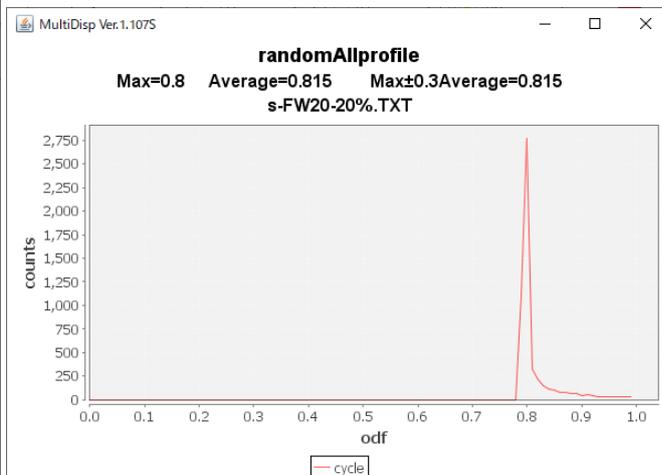
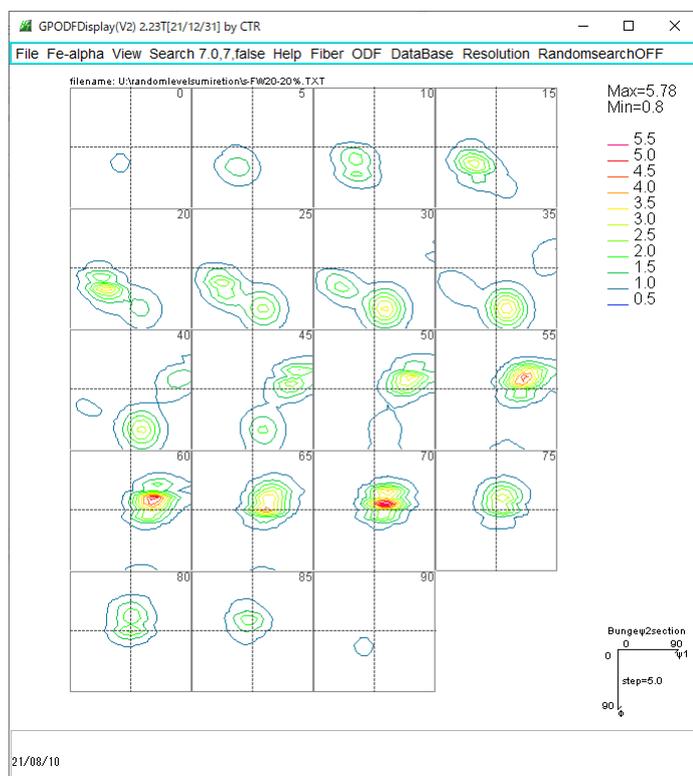
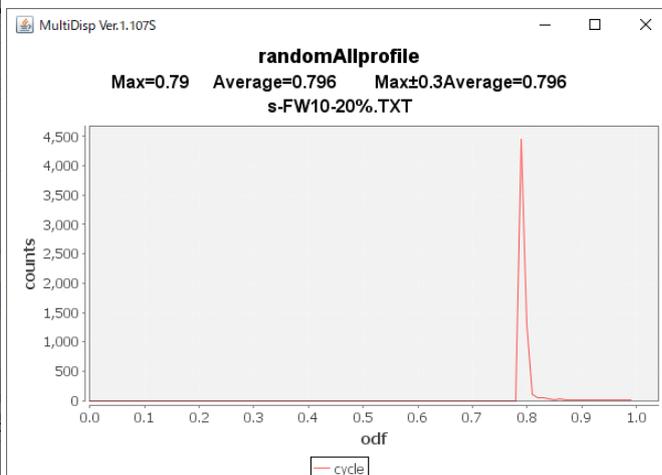
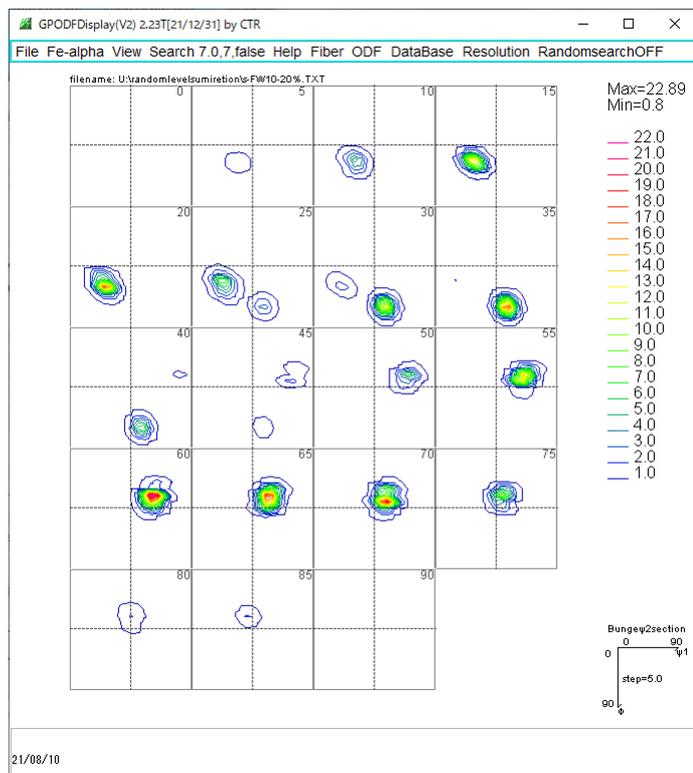
同じように r a n d o m = 8 0 % が得られます。

g o s s 方位



random = 80%が得られます。

S 方位



random = 80%が得られます。

MT EXでc o p p e r 2 0%の極点図作成

```
cs = crystalSymmetry('cubic')
```

```
ss = specimenSymmetry('orthorhombic')
```

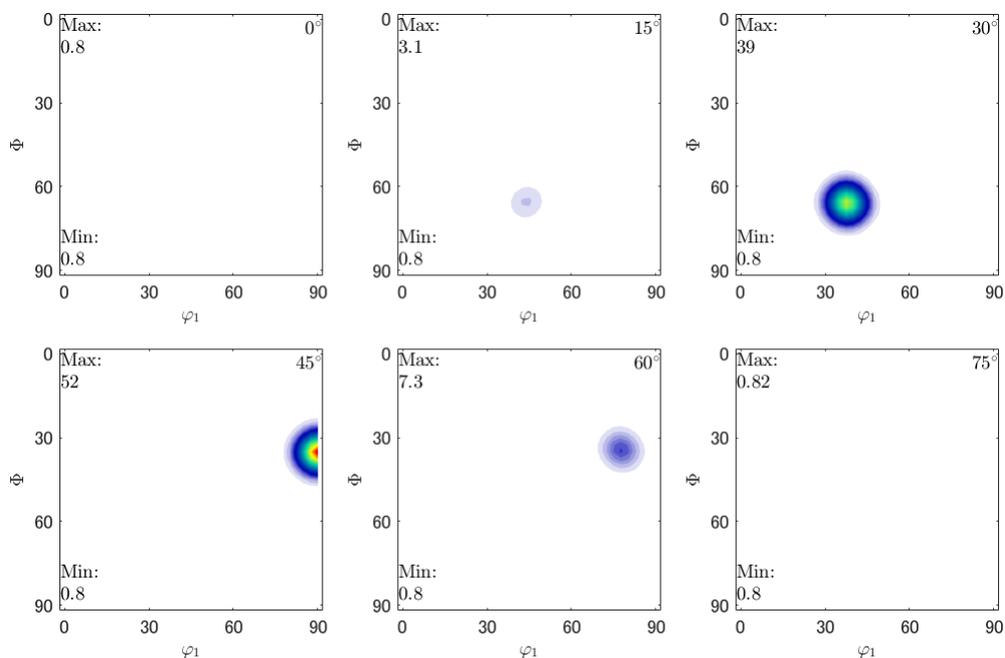
```
ori=orientation.byMiller([1,1,2],[-1,-1,1],cs,ss)
```

```
psi = vonMisesFisherKernel('HALFWIDTH',5*degree)
```

```
odfc=unimodelODF(cs,ori)
```

```
random=uniformODF(cs,ss)
```

```
odf=0.2*odfc+0.8*random
```

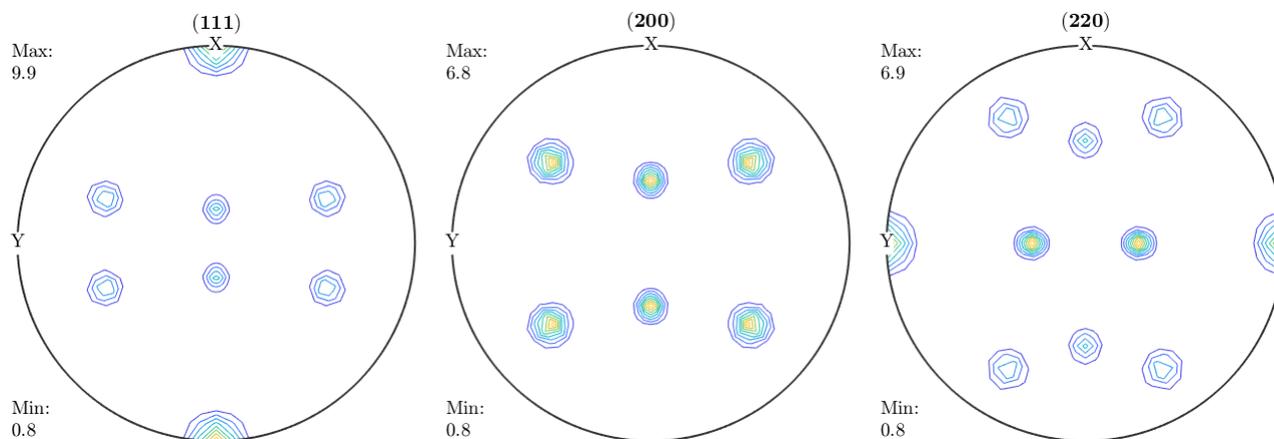


Min=0.8 random=80%が得られる。

```
h = { Miller(1,1,1,cs), Miller(2,0,0,cs), Miller(2,2,0,cs) }
```

```
rpf=calcPoleFigure(odf,h)
```

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



この極点図をE x p o r t し、各種ODFで比較する。



PFtoODF3 8.53T[21/12/31] by CTR
 File Option Symmetric Software Data Help

Lattice constant

Material: Aluminum.txt

Structure Code(Symmetries after Schoenfiles): cif 7 - O (cubic)

a: 1.0 <=b: 1.0 <=c: 1.0 alpha: 90.0 beta: 90.0 gamma: 90.0

Initialize: Start

getHKL<-Filename (selected)

AllFileSelect

PF Holder: U#randomlevelsumiretion#MTEX

PF Data

SelectFile(TXT(b,intens),TXT2(a,b,intens))	h,k,l	2Theta	Alpha scope	AlphaS	AlphaE	Select
111_txt-rp_2.TXT	1,1,1	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>
200_txt-rp_2.TXT	2,0,0	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>
220_txt-rp_2.TXT	2,2,0	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>
	2,1,0	0.0		0.0	0.0	<input type="checkbox"/>
	2,1,1	0.0		0.0	0.0	<input type="checkbox"/>
	3,1,1	0.0		0.0	0.0	<input type="checkbox"/>
	4,0,0	0.0		0.0	0.0	<input type="checkbox"/>
	3,3,1	0.0		0.0	0.0	<input type="checkbox"/>
	4,2,2	0.0		0.0	0.0	<input type="checkbox"/>
	5,1,1	0.0		0.0	0.0	<input type="checkbox"/>
	5,2,1	0.0		0.0	0.0	<input type="checkbox"/>
	5,3,1	0.0		0.0	0.0	<input type="checkbox"/>

Comment: 111_txt-rp_2.TXT 200_txt-rp_2.TXT 220_txt-rp_2.TXT

Symmetric type: Full

CenterData: Average

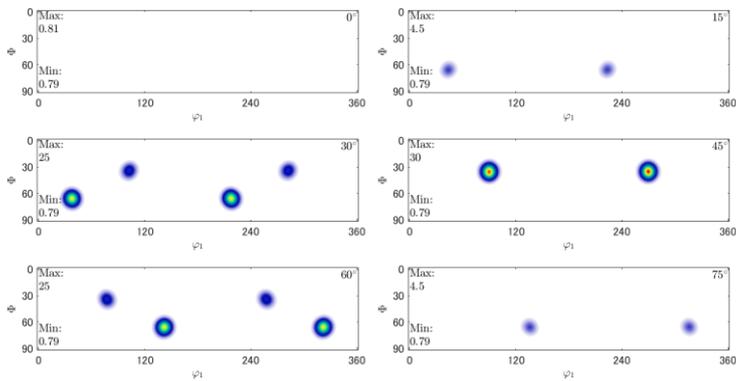
Epf file save

Labotex(EPF),popLA(RAW) filename: MTEX

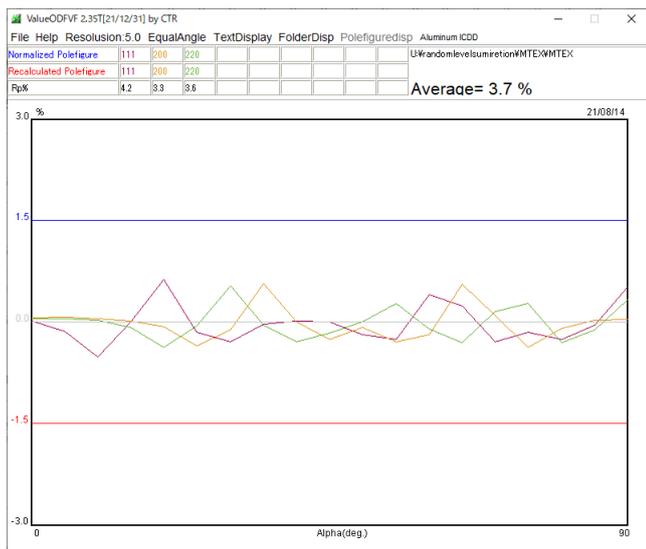
MT EXで解析

Radially symmetric portion:

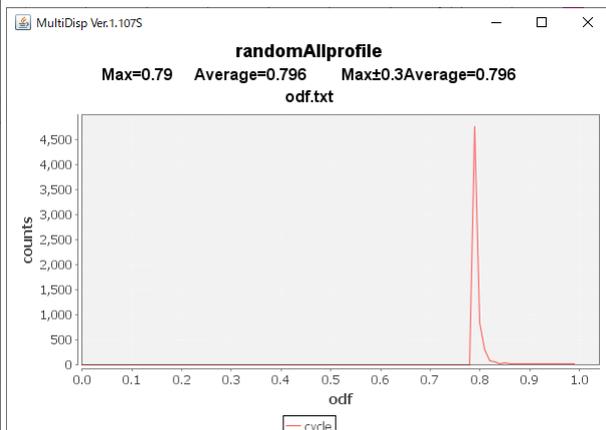
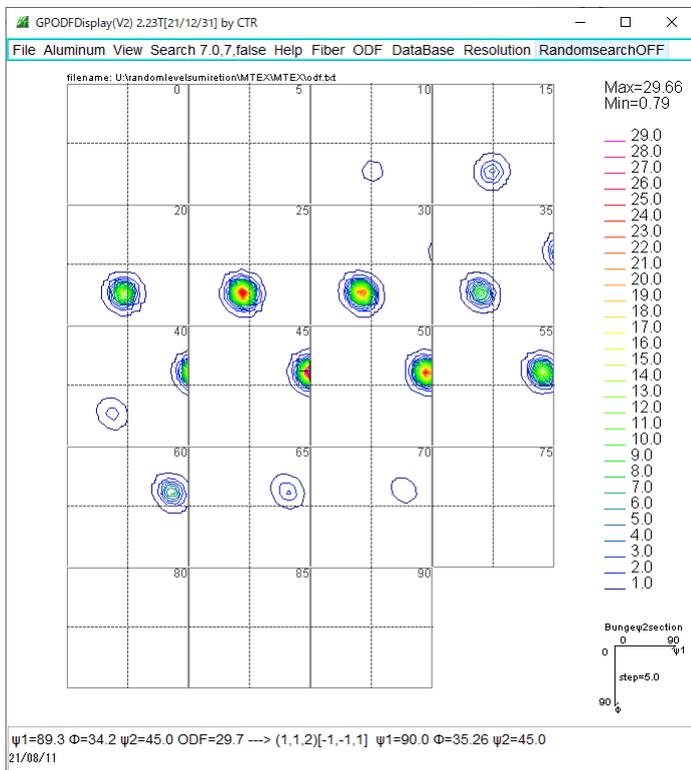
kernel: de la Vallee Poussin, halfwidth 5° |
 center: 4903 orientations, resolution: 5°
 weight: 0.20855



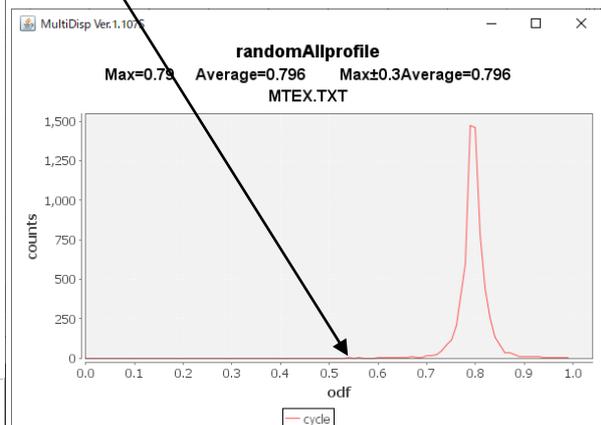
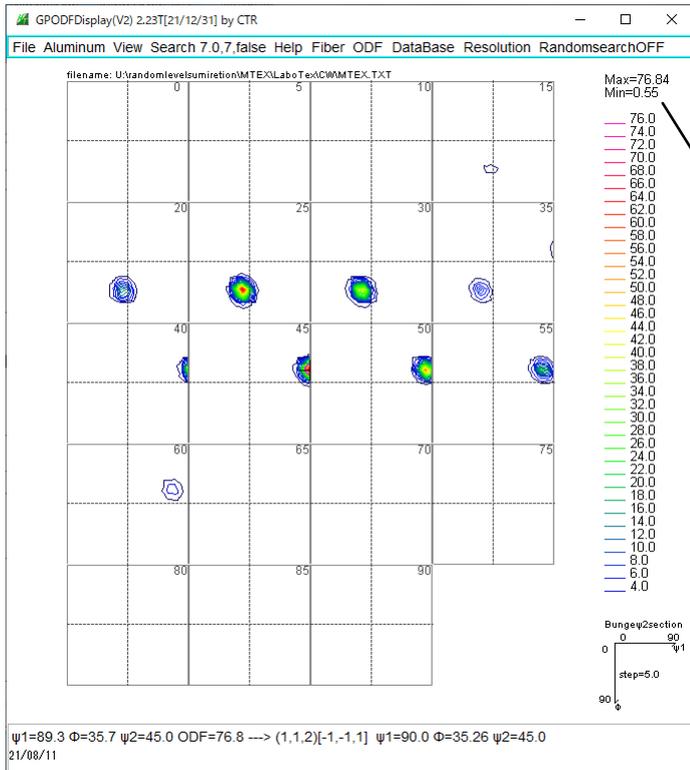
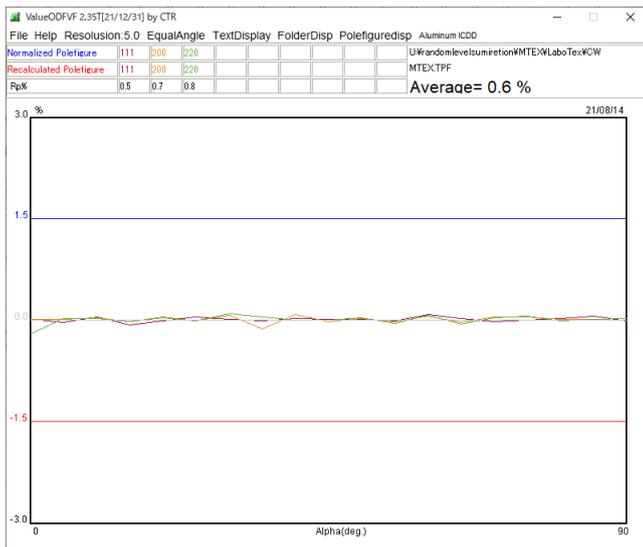
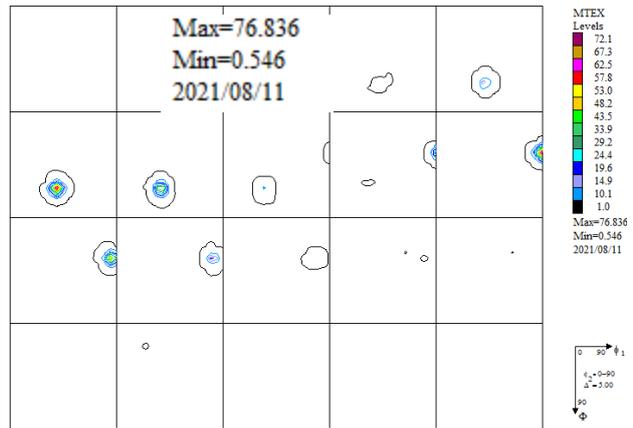
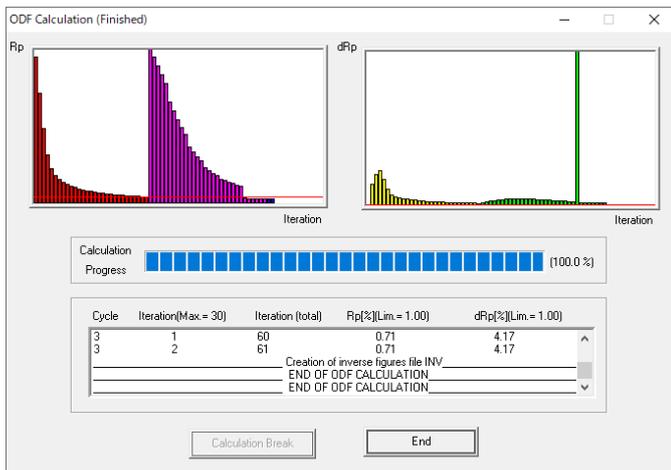
Min=0.79



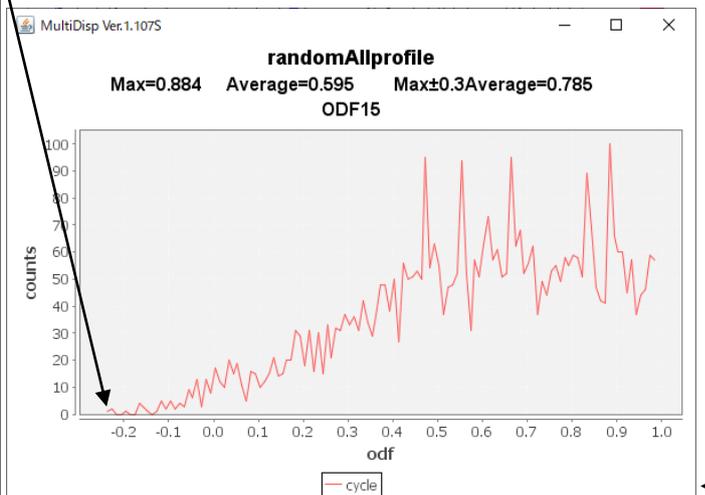
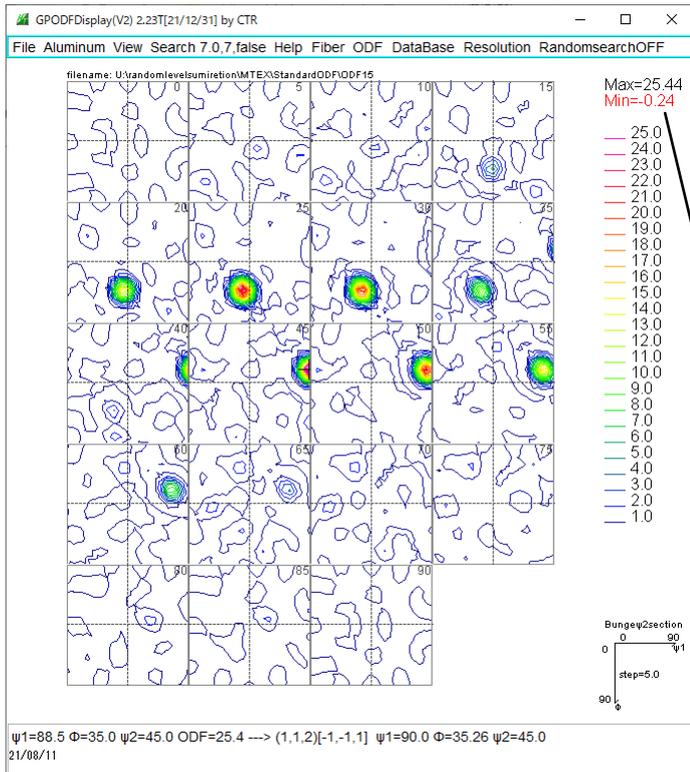
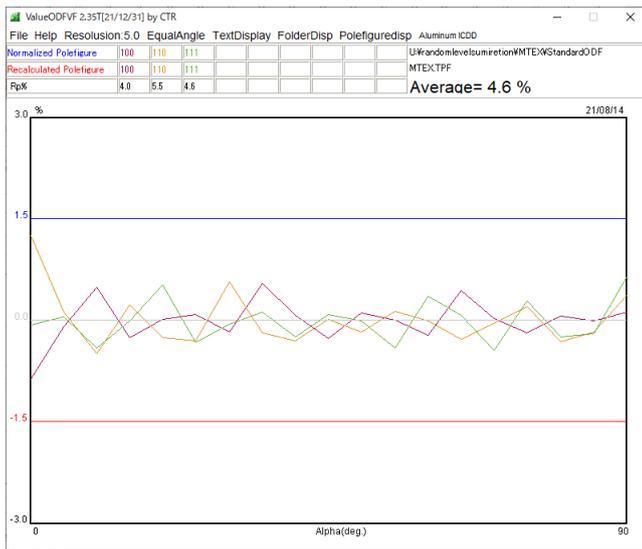
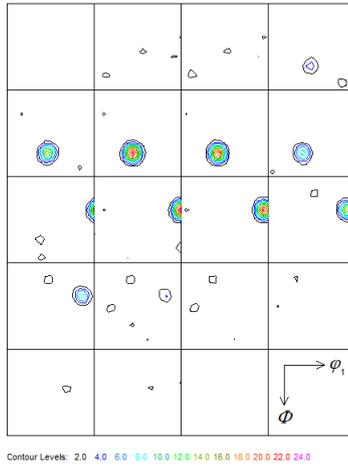
Triclinic->Orthorhombic



LaboTexで解析

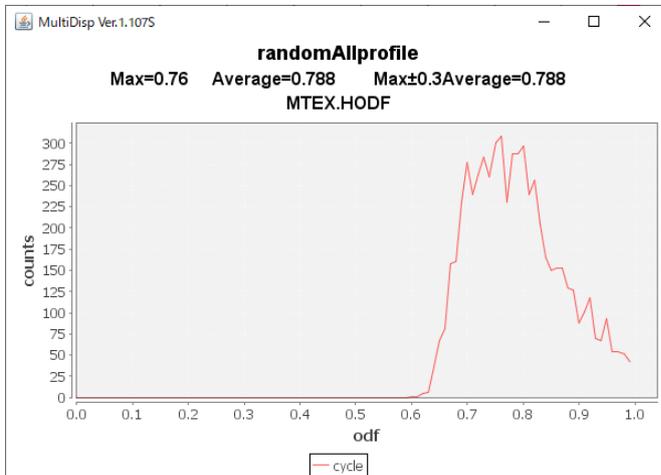
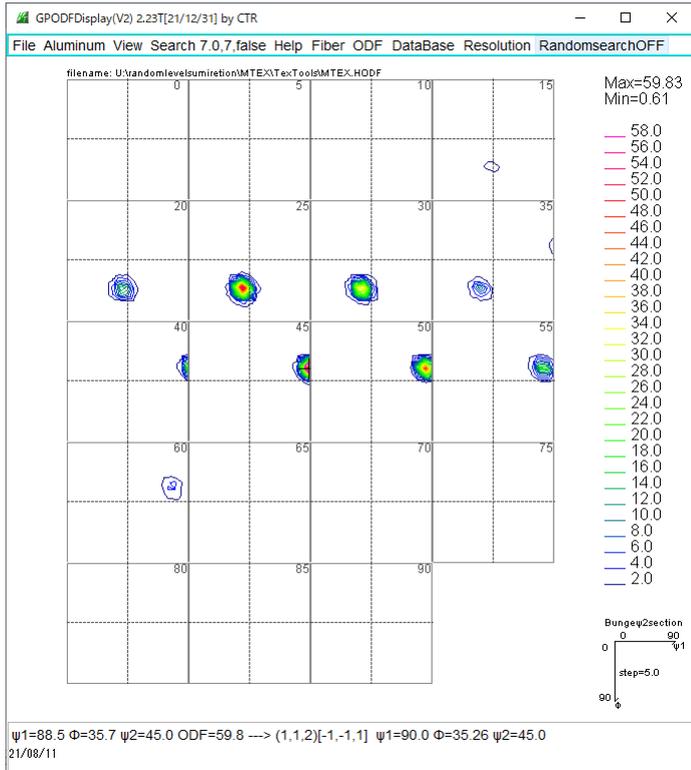
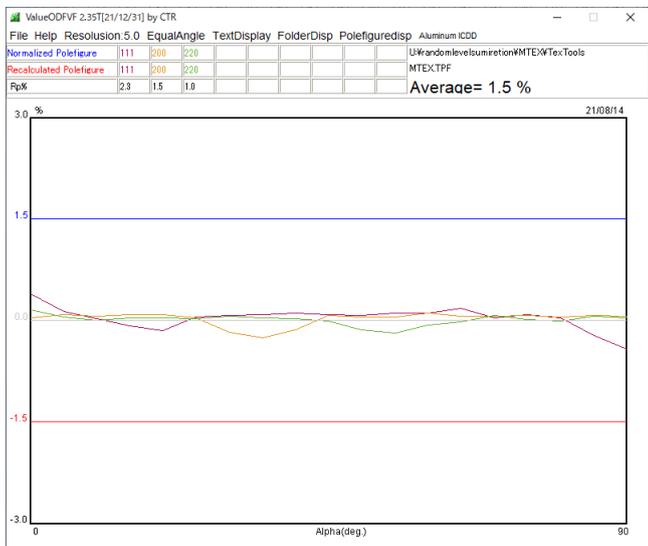
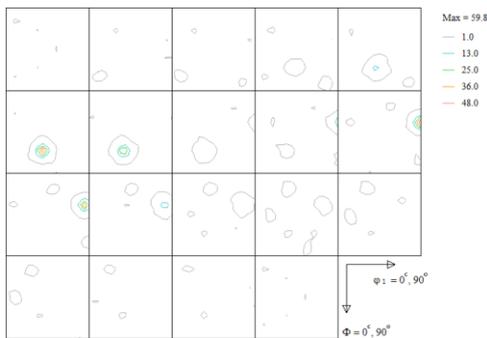
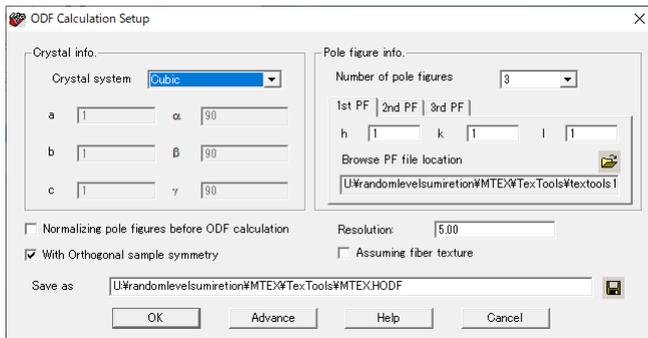


StandardODFで解析



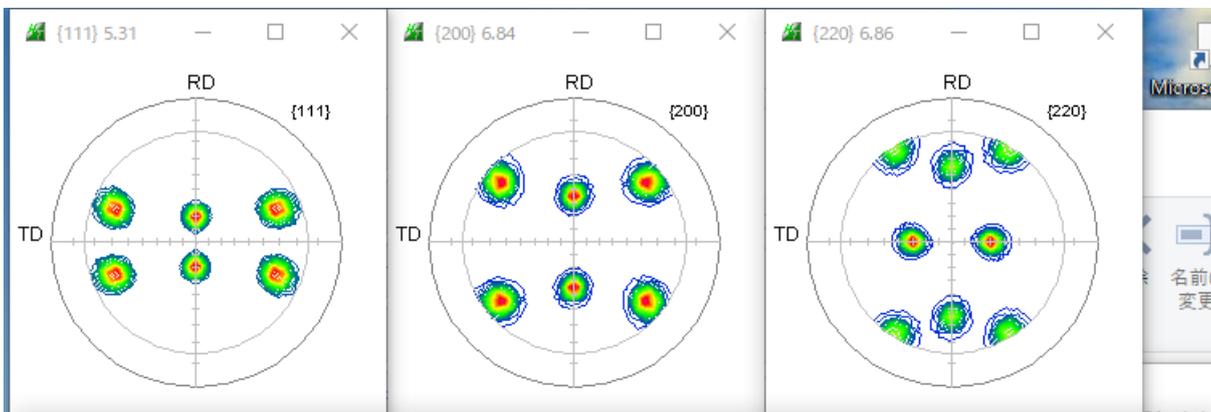
StandardODF ではオーバシュートが激しく、定量は難しい。

TexTools



LaboTex, MTEXに比べると、randomが広がる

では、測定範囲を75度とした場合を調べる



PfToODF3 8.53T[21/12/31] by CTR

File Option Symmetric Software Data Help

Lattice constant

Material: Aluminum.txt

Structure Code(Symmetries after Schoenfiles): cif 7 - O (cubic)

a: 1.0 <=b: 1.0 <=c: 1.0 alpha: 90.0 beta: 90.0 gamm: 90.0

Initialize: Start

getHKL<-Filename

AllFileSelect

PF Holder: U:\randomlevelsumiretion\MTEX\A75

PF Data

SelectFile(TXT(b,intens),TXT2(a,b,intens))	h,k,l	2Theta	Alpha scope	AlphaS	AlphaE	Select
111_txt-rp75_2.TXT	1,1,1	0.0	0.0->75.0	0.0	75.0	<input checked="" type="checkbox"/>
200_txt-rp75_2.TXT	2,0,0	0.0	0.0->75.0	0.0	75.0	<input checked="" type="checkbox"/>
220_txt-rp75_2.TXT	2,2,0	0.0	0.0->75.0	0.0	75.0	<input checked="" type="checkbox"/>
	2,1,0	0.0		0.0	0.0	<input type="checkbox"/>
	2,1,1	0.0		0.0	0.0	<input type="checkbox"/>
	3,1,1	0.0		0.0	0.0	<input type="checkbox"/>
	4,0,0	0.0		0.0	0.0	<input type="checkbox"/>
	3,3,1	0.0		0.0	0.0	<input type="checkbox"/>
	4,2,2	0.0		0.0	0.0	<input type="checkbox"/>
	5,1,1	0.0		0.0	0.0	<input type="checkbox"/>
	5,2,1	0.0		0.0	0.0	<input type="checkbox"/>
	5,3,1	0.0		0.0	0.0	<input type="checkbox"/>

Comment: 111_txt-rp75_2.TXT 200_txt-rp75_2.TXT 220_txt-rp75_2.TXT

Symmetric type: Full

CenterData: Average

EpF file save

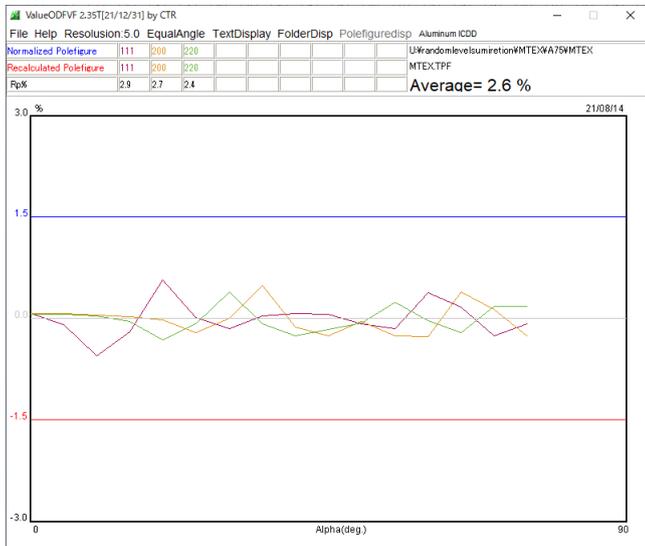
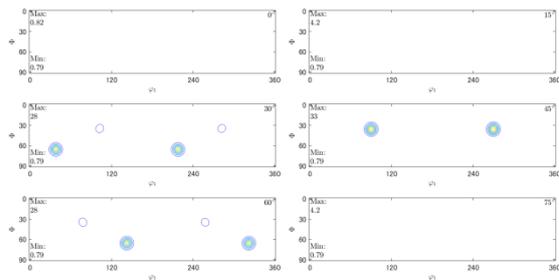
Labotex(EPF),popLA(RAW) filename: MTEX75

MTEXで解析

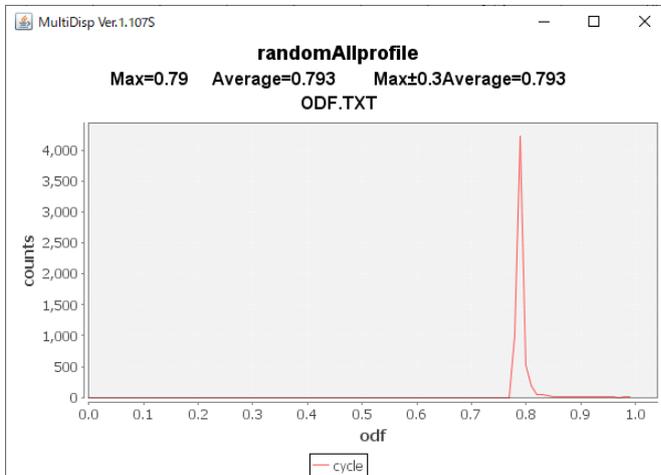
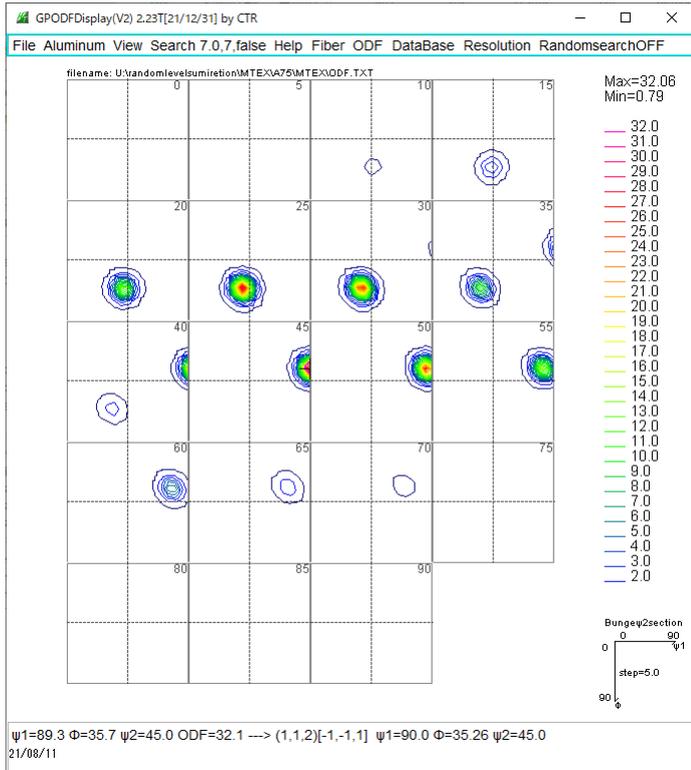
U: randomlevelsumiretion MTEX A75 MTEX

Uniform portion:
weight: 0.78888

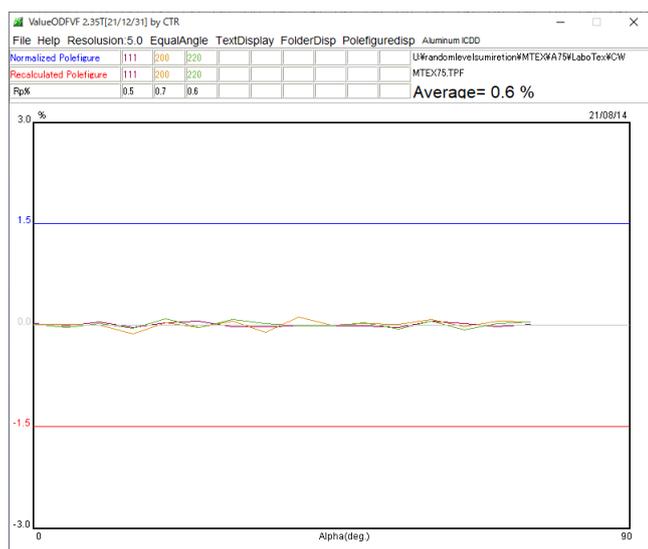
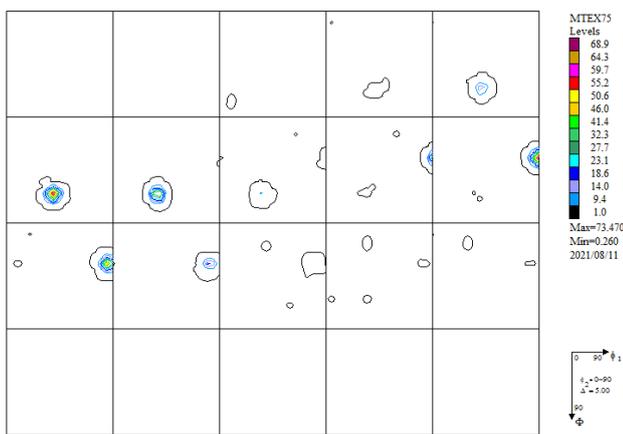
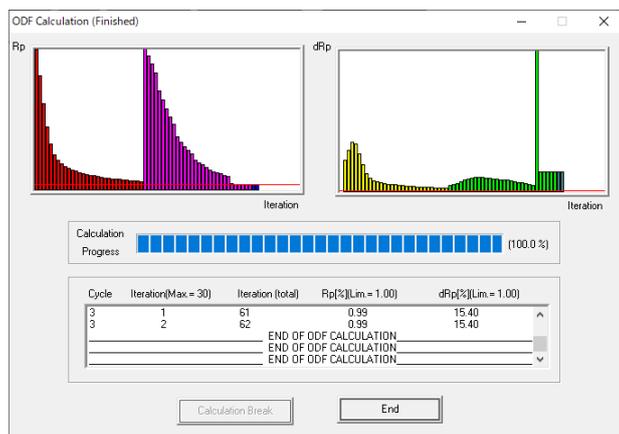
Radially symmetric portion:
kernel: de la Vallee Poussin, halfwidth 5°
center: 4903 orientations, resolution: 5°
weight: 0.21112



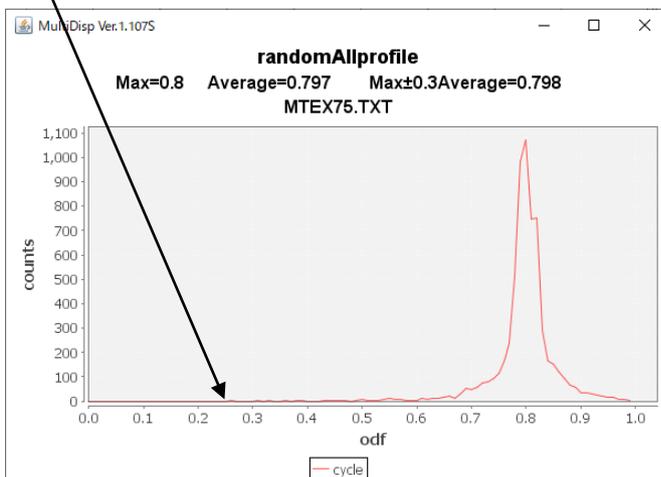
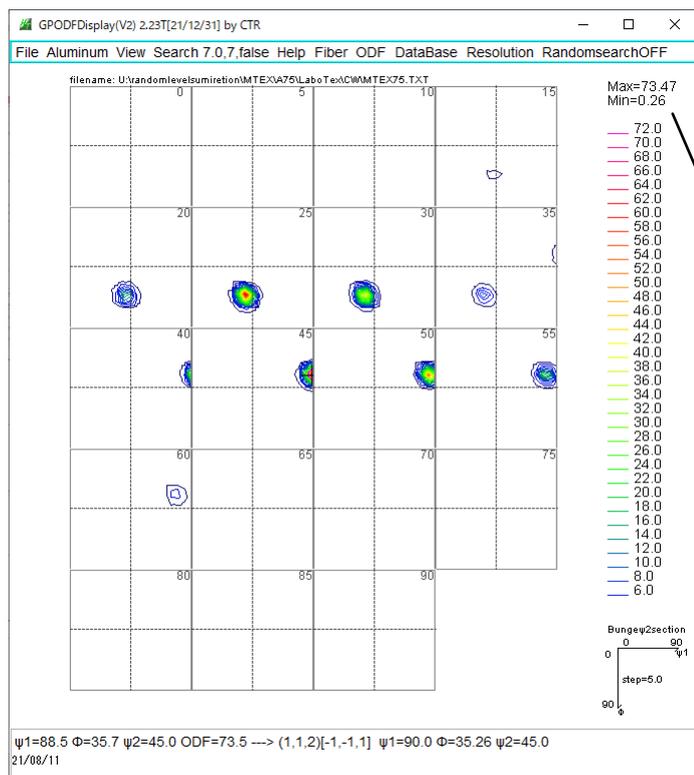
完全極点図 3. 7 → 2. 6% (範囲が狭いため)



LaboTexで解析



完全極点図0.6%と変わらず



StandardODFで解析

ODF Calculation

種点図データ

面指数 重み

ファイル名(フルパス)

計算結果

完全ODFの最大強度: 24.14
 係数ODFの最大強度: 21.32
 再計算極点図の最大強度: 6.65
 逆極点図の最大強度: 6.65

Standard ODF
 for Windows XP/Me/2000/98SE/98/NT4.0/95 Ver.2.4 解析法について

結晶方位分布関数

展開次数 22

ゼロ密度補填のしきい値 0.3

表示断面 Phi1断面 Phi2断面

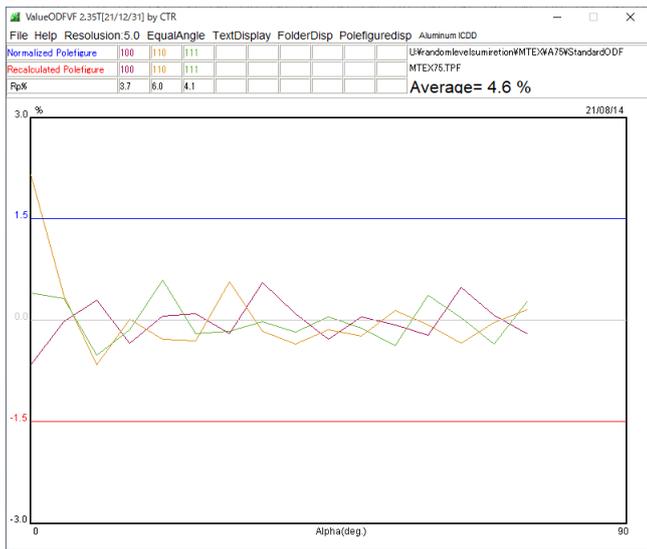
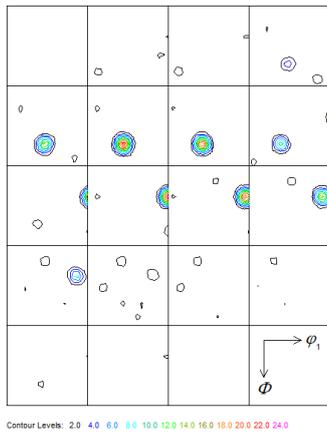
再計算極点図

1 100 2 110
 3 111 4

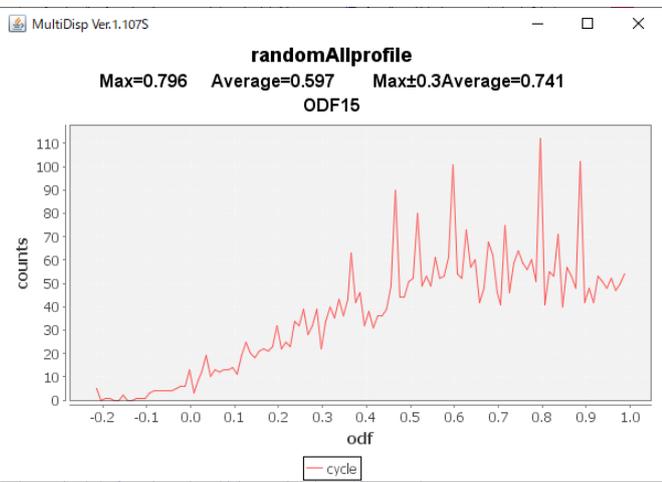
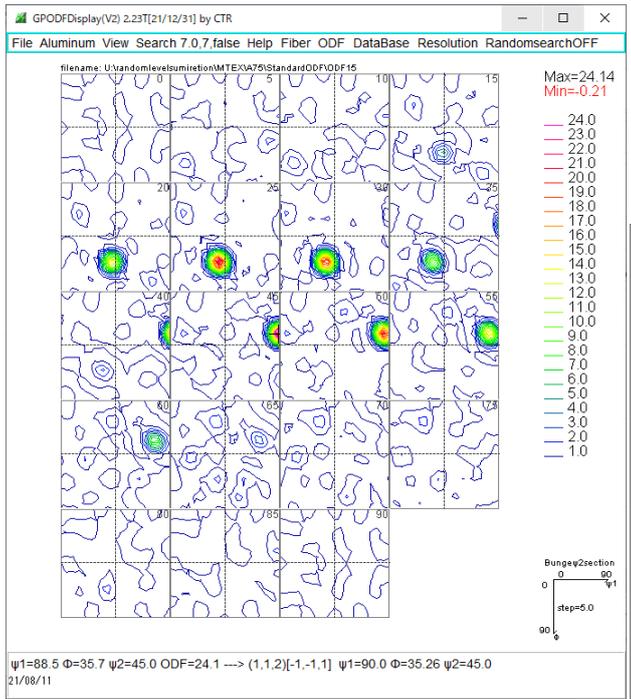
1/4極点図 C係数 偶数項 奇数項

0% 100%

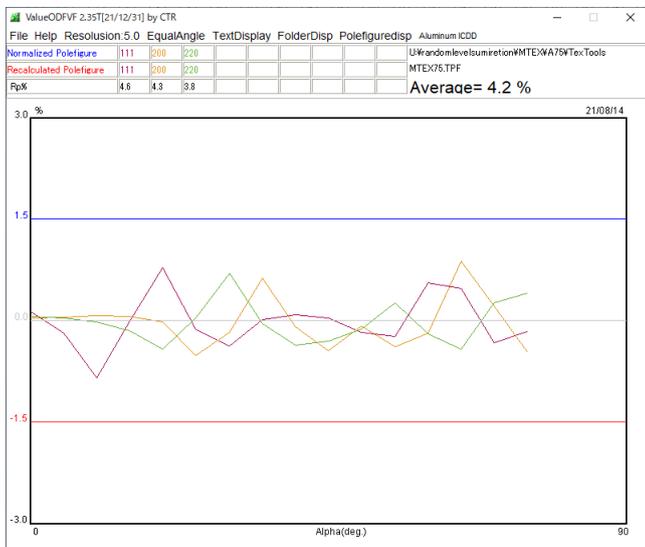
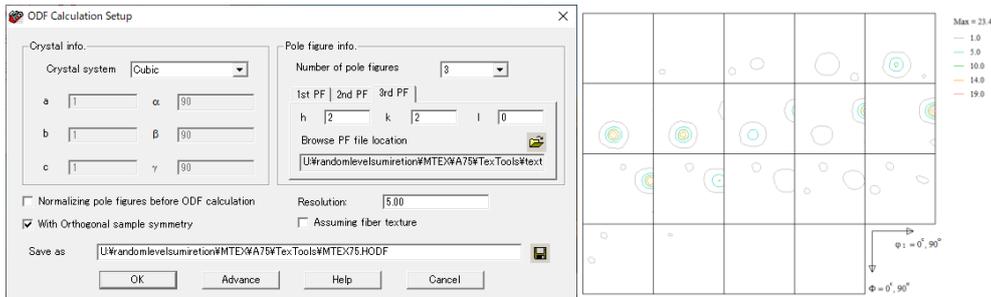
実行(G) 終了(E)



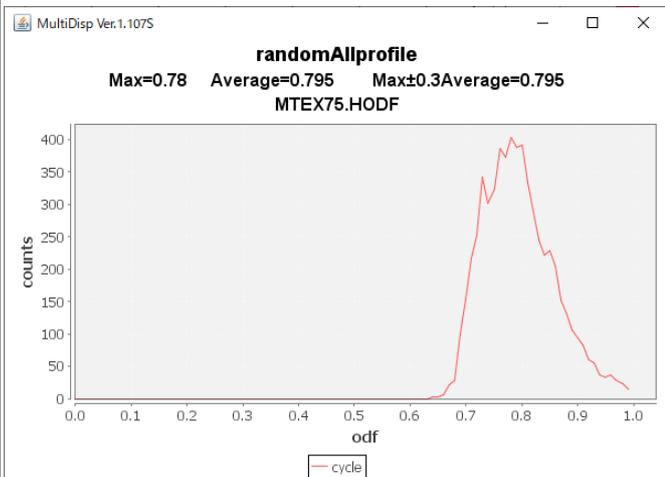
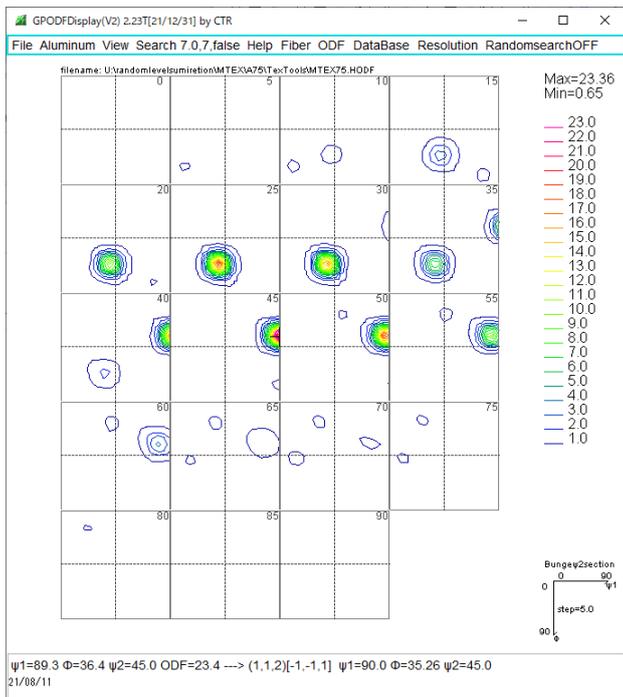
完全極点図と同一



TexToolsで解析



完全極点図1. 5%より一致度が悪化



random 80%が保たれてる

以下に実サンプルを比較

アルミニウム H 材

(111) 7.02

(200) 3.99

(220) 7.48

PF to MTEX by CTR PftoODF3 8.53T[21/12/31] by CTR

File Option Symmetric Software Data Help

Lattice constant

Material: Aluminum.txt

Structure Code(Symmetries after Schoenfiles): cif 7 - O (cubic)

a: 1.0 <=b: 1.0 <=c: 1.0 alpha: 90.0 beta: 90.0 gamma: 90.0

Initialize: Start

getHKL<-Filename

PF Holder: C:\CTR\DATA\Aluminum-H-O\Aluminum-H

SelectFile(TXT(b,intens),TXT2(a,b,intens))	h,k,l	2Theta	Alpha scope	AlphaS	AlphaE	Select
<input type="button" value="111_chB00D1S_2.TXT"/>	1,1,1	0.0	0.0->75.0	0.0	75.0	<input checked="" type="checkbox"/>
<input type="button" value="200_chB00D1S_2.TXT"/>	2,0,0	0.0	0.0->75.0	0.0	75.0	<input checked="" type="checkbox"/>
<input type="button" value="220_chB00D1S_2.TXT"/>	2,2,0	0.0	0.0->75.0	0.0	75.0	<input checked="" type="checkbox"/>
<input type="button" value=""/>	2,1,0	0.0		0.0	0.0	<input type="checkbox"/>
<input type="button" value=""/>	2,1,1	0.0		0.0	0.0	<input type="checkbox"/>
<input type="button" value=""/>	3,1,1	0.0		0.0	0.0	<input type="checkbox"/>
<input type="button" value=""/>	4,0,0	0.0		0.0	0.0	<input type="checkbox"/>
<input type="button" value=""/>	3,3,1	0.0		0.0	0.0	<input type="checkbox"/>
<input type="button" value=""/>	4,2,2	0.0		0.0	0.0	<input type="checkbox"/>
<input type="button" value=""/>	5,1,1	0.0		0.0	0.0	<input type="checkbox"/>
<input type="button" value=""/>	5,2,1	0.0		0.0	0.0	<input type="checkbox"/>
<input type="button" value=""/>	5,3,1	0.0		0.0	0.0	<input type="checkbox"/>

Comment: 111_chB00D1S_2.TXT 200_chB00D1S_2.TXT 220_chB00D1S_2.TXT

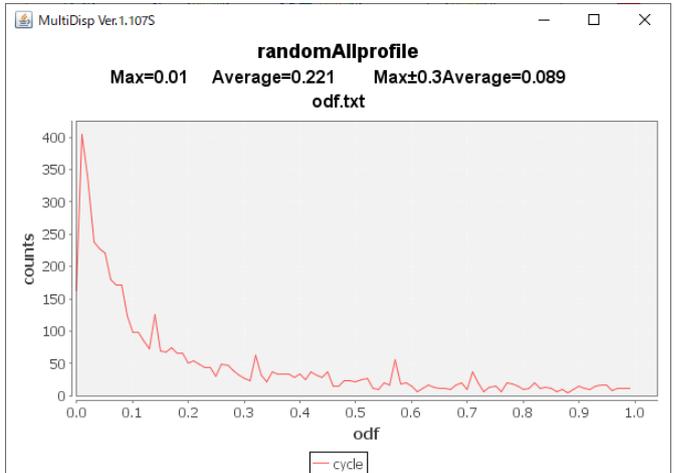
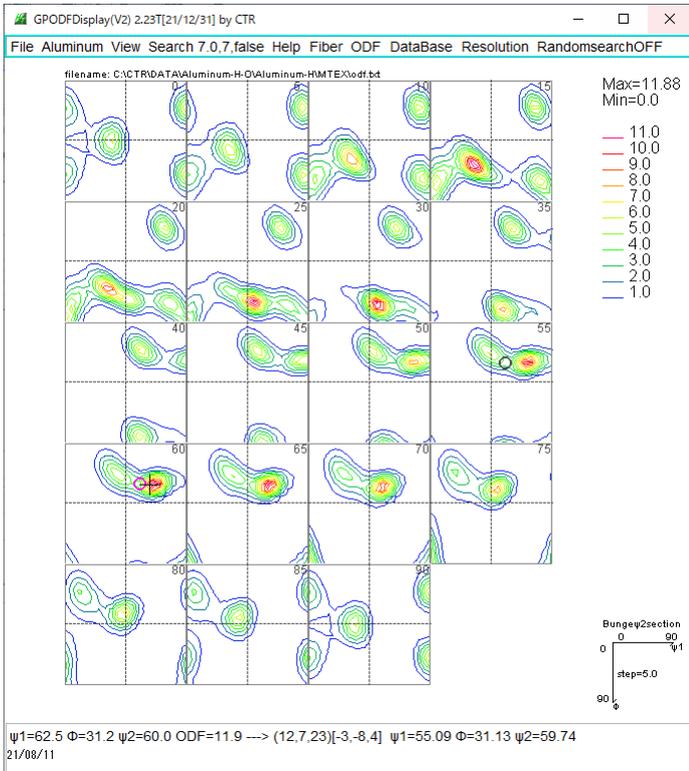
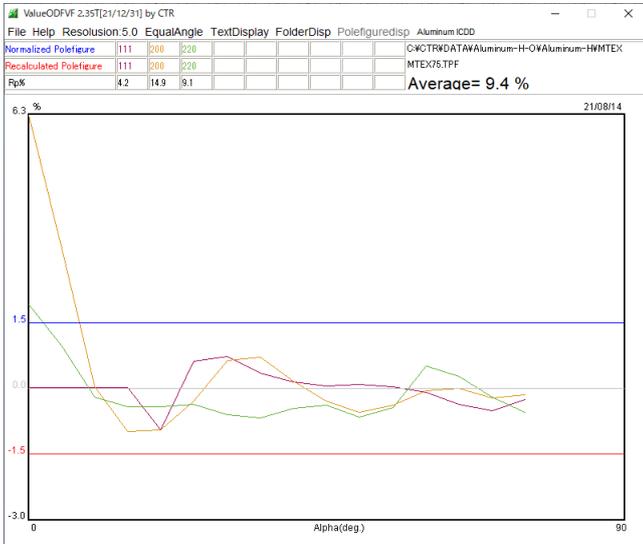
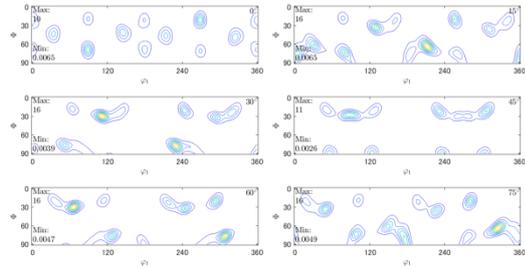
Symmetric type: Full

CenterData: Average

Labotex(EPF),popLA(RAW) filename: ASC

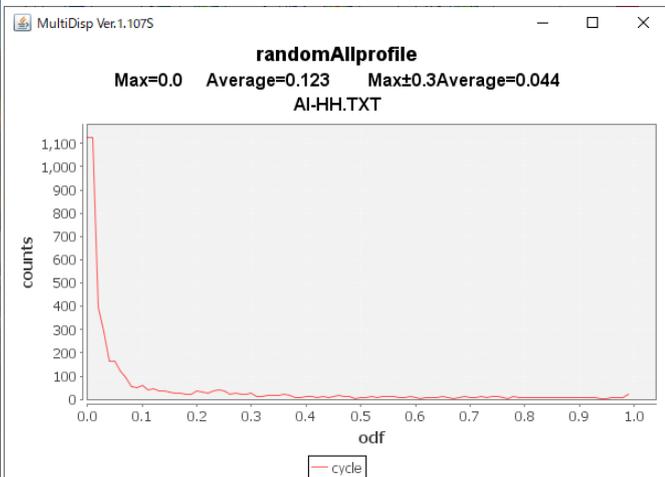
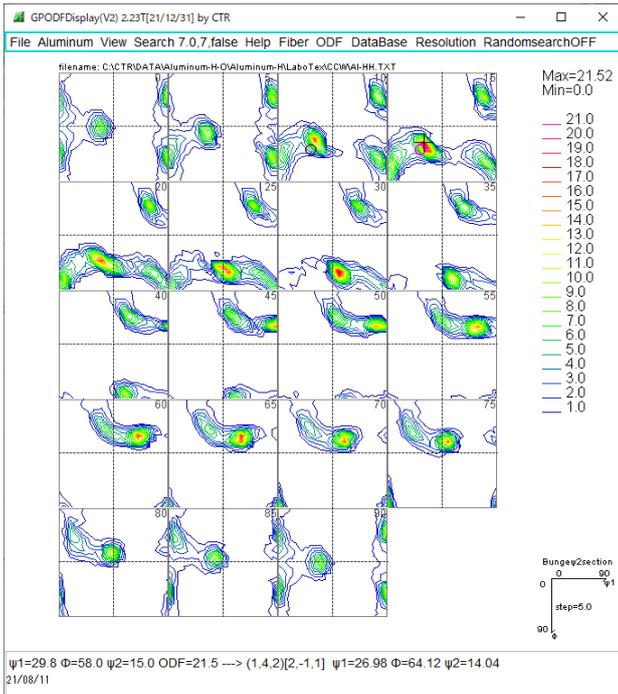
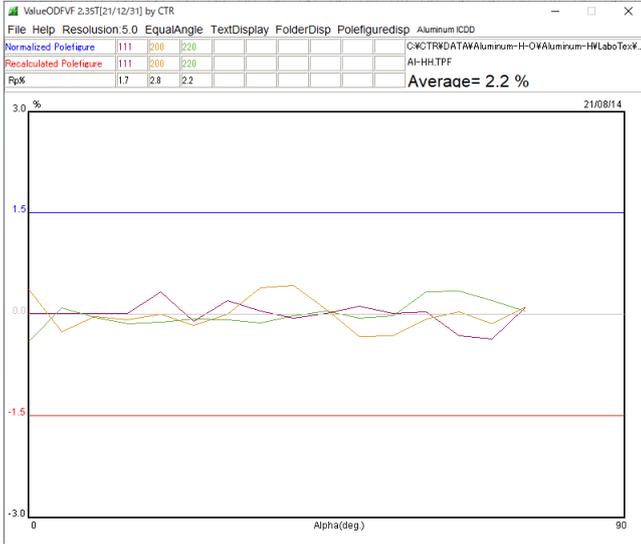
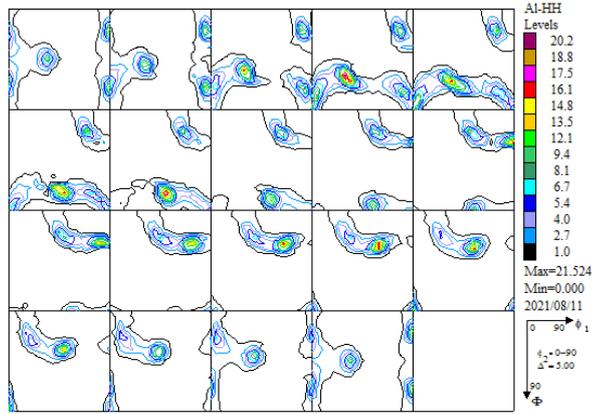
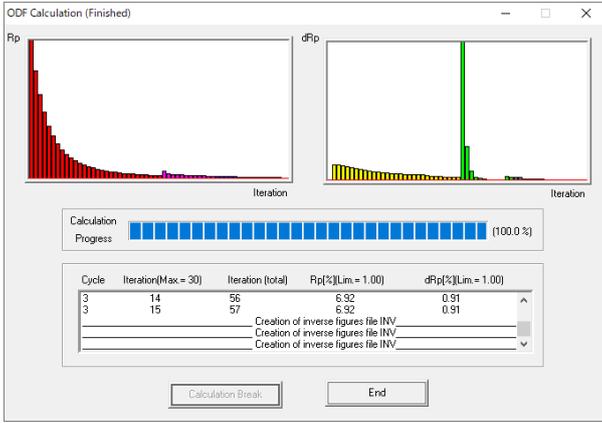
MTEXで解析

Radially symmetric portion:
 kernel: de la Vallee Poussin, halfwidth 5°
 center: 4952 orientations, resolution: 5°
 weight: 1



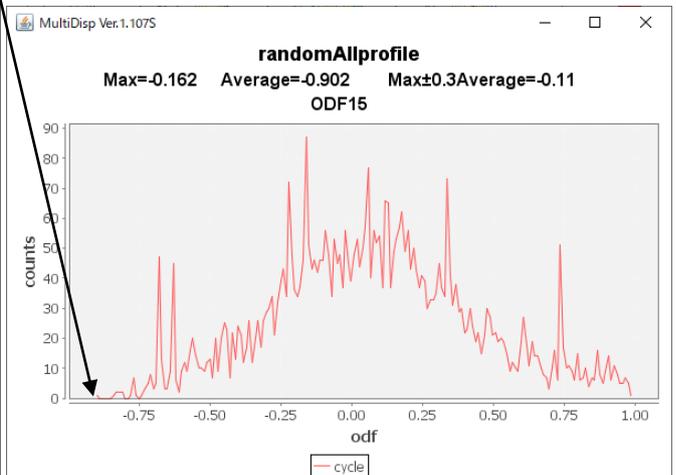
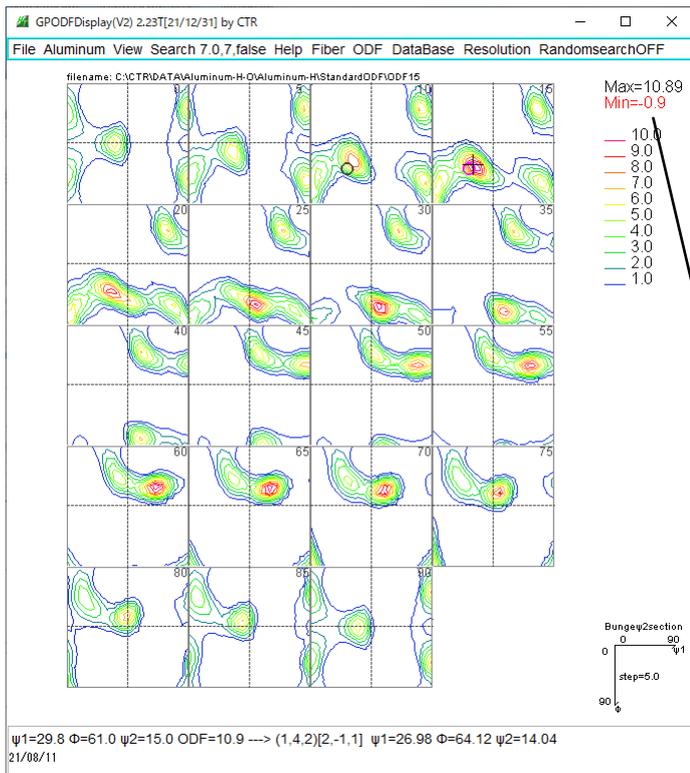
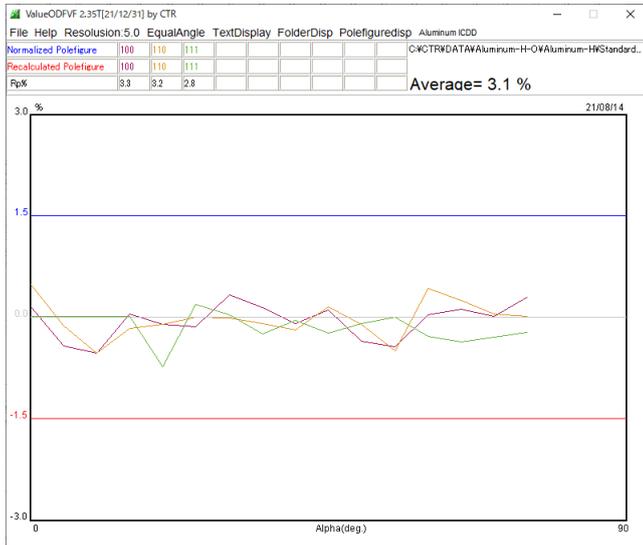
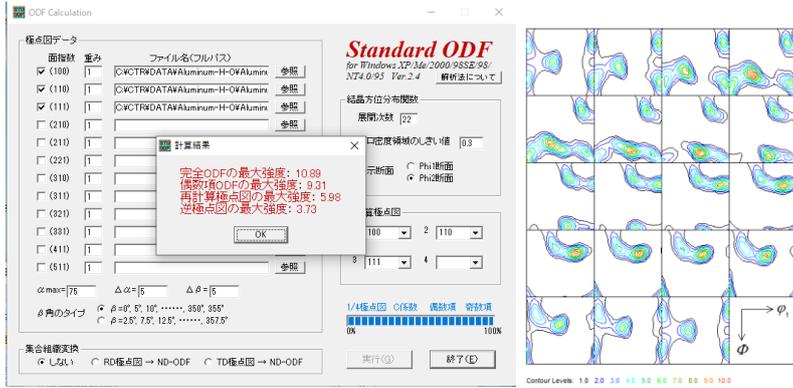
random成分は、1%程度

LaboTexで評価



random=0%

Standard ODFで解析



random level プロファイルの分散が大きすぎます。

TextToolsで解析

ODF Calculation Setup

Crystal info.
 Crystal system: Cubic
 a: 1, α : 90
 b: 1, β : 90
 c: 1, γ : 90

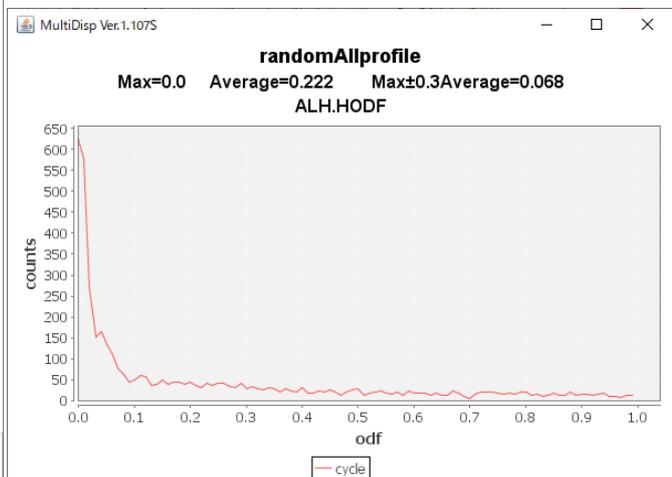
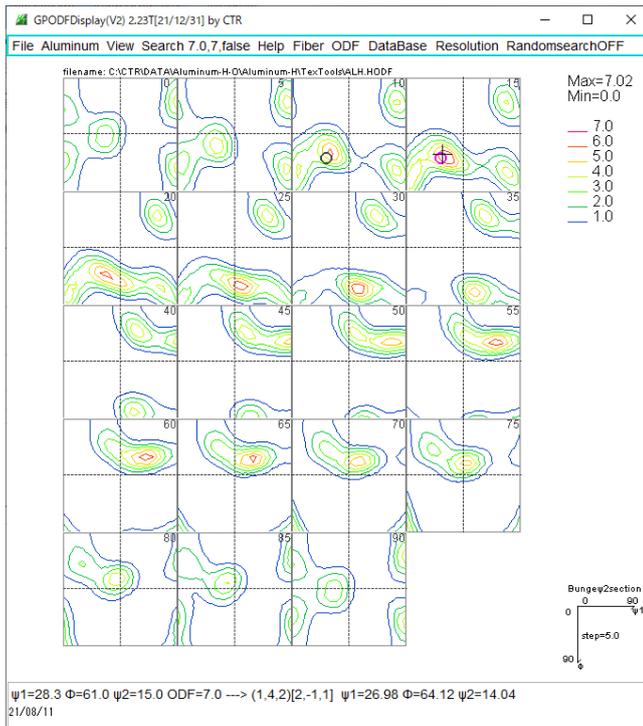
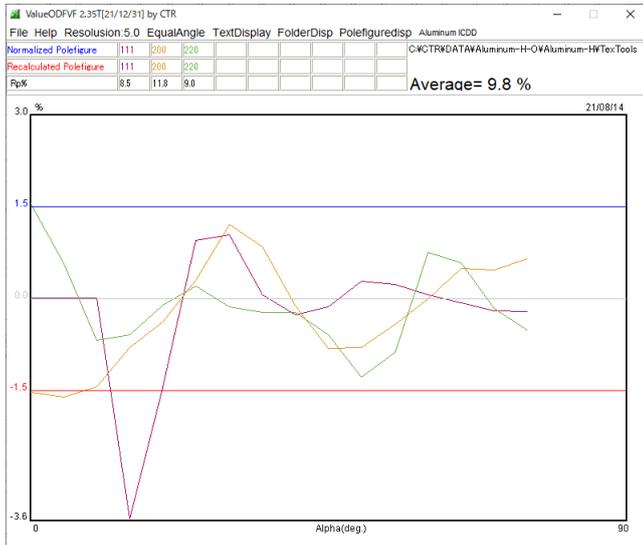
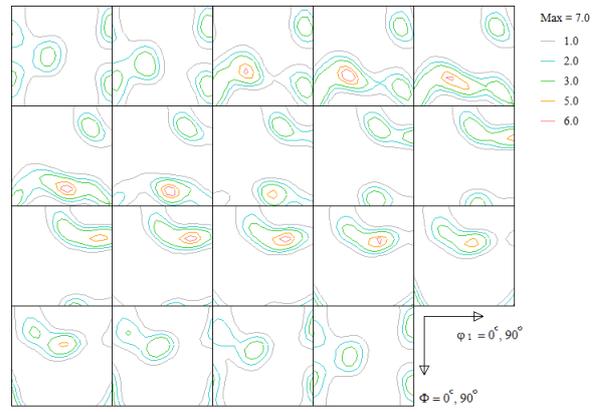
Pole figure info.
 Number of pole figures: 3
 1st PF | 2nd PF | 3rd PF
 h: 2, k: 2, l: 0
 Browse PF file location: C:\CTR\DATA\Aluminum-H-O\Aluminum-H\Tex\Toc

Normalizing pole figures before ODF calculation
 With Orthogonal sample symmetry
 Assuming fiber texture

Resolution: 5.00

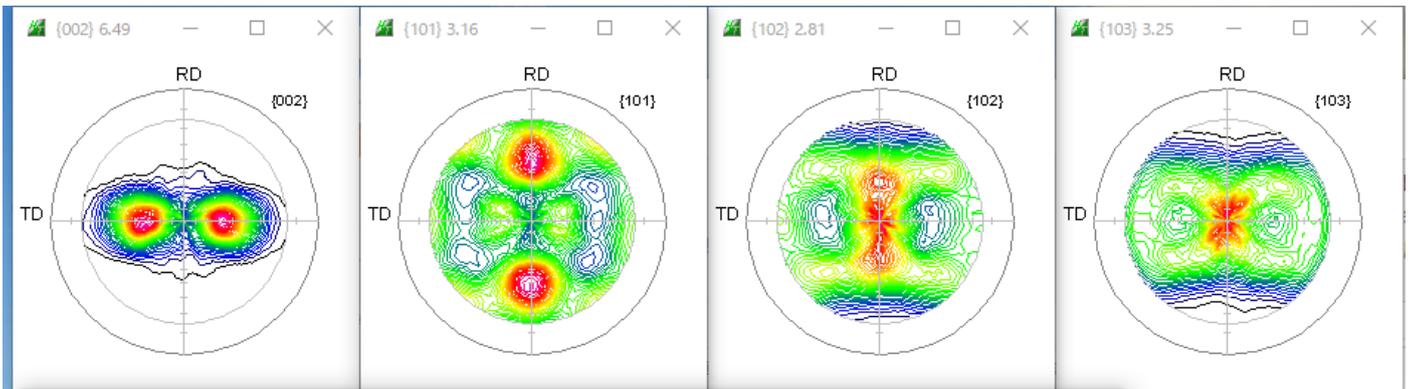
Save as: C:\CTR\DATA\Aluminum-H-O\Aluminum-H\Tex\Tools\ALH.HODF

OK Advance Help Cancel



random = 0%が得られます。

Titaniumへの応用



PfToODF3 8.53T[21/12/31] by CTR

File Option Symmetric Software Data Help

Lattice constant

Material: Titanium-alpha.txt

Structure Code(Symmetries after Schoenfiles): cif 11 - D6 (hexagonal)

a: 1.0, b: 1.0, c: 1.5885, alpha: 90.0, beta: 90.0, gamma: 120.0

Initialize: Start

getHKL<-Filename

AllFileSelect

PF Holder: U:\測定データ\材料-軽金属研究部会\2010-01-20-Standard-Ti-終了\解析\Ti-R\LaboTex\CW\calcdefocus\Newdata

SelectFile(TXT(b,intens),TXT2(ab,intens))	h,k,l	2Theta	Alpha scope	AlphaS	AlphaE	Select
002_DS0-25deg_chB02A56CAS_2.TXT	0,0,2	0.0	0.0->75.0	0.0	75.0	<input checked="" type="checkbox"/>
101_DS0-25deg_chB02A56CAS_2.TXT	1,0,1	0.0	0.0->75.0	0.0	75.0	<input checked="" type="checkbox"/>
102_DS0-25deg_chB02A56CAS_2.TXT	1,0,2	0.0	0.0->75.0	0.0	75.0	<input checked="" type="checkbox"/>
103_DS0-25deg_chB02A56CAS_2.TXT	1,0,3	0.0	0.0->75.0	0.0	75.0	<input checked="" type="checkbox"/>
	2,1,1	0.0		0.0	0.0	<input type="checkbox"/>
	3,1,1	0.0		0.0	0.0	<input type="checkbox"/>
	4,0,0	0.0		0.0	0.0	<input type="checkbox"/>
	3,3,1	0.0		0.0	0.0	<input type="checkbox"/>
	4,2,2	0.0		0.0	0.0	<input type="checkbox"/>
	5,1,1	0.0		0.0	0.0	<input type="checkbox"/>
	5,2,1	0.0		0.0	0.0	<input type="checkbox"/>
	5,3,1	0.0		0.0	0.0	<input type="checkbox"/>

Comment: 101_DS0-25deg_chB02A56CAS_2.TXT 102_DS0-25deg_chB02A56CAS_2.TXT 103_DS0-25deg_chB02A56CAS_2.TXT

Symmetric type: Full

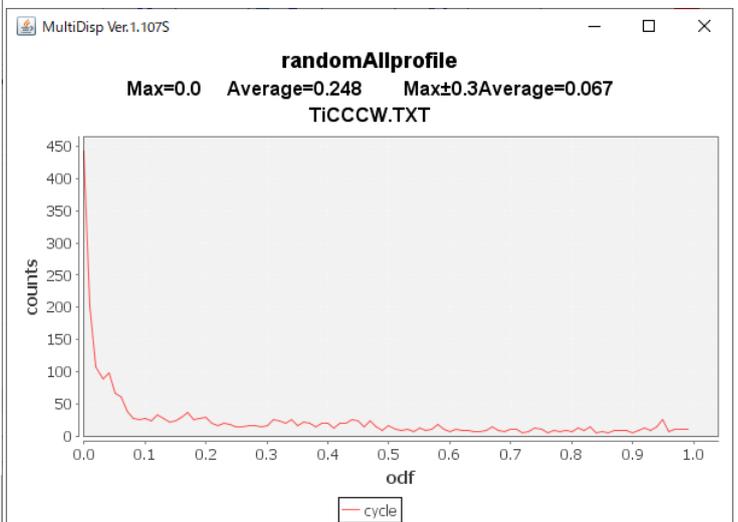
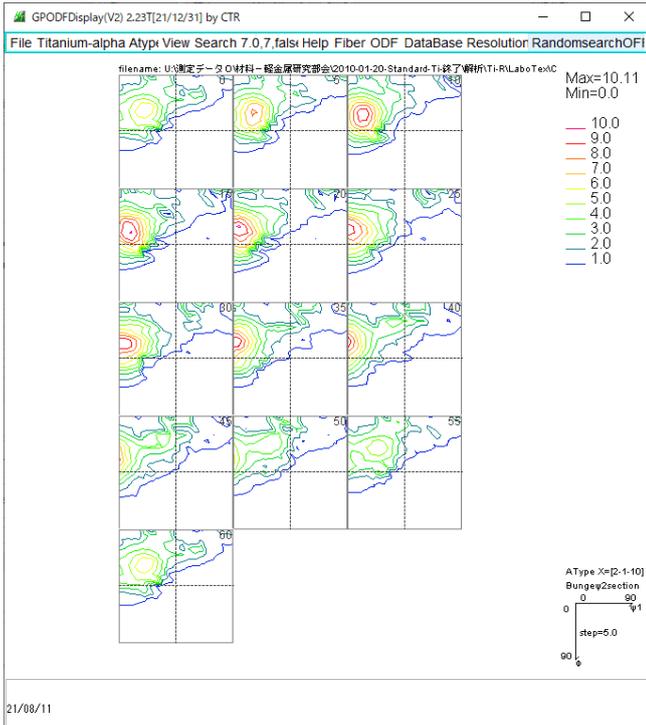
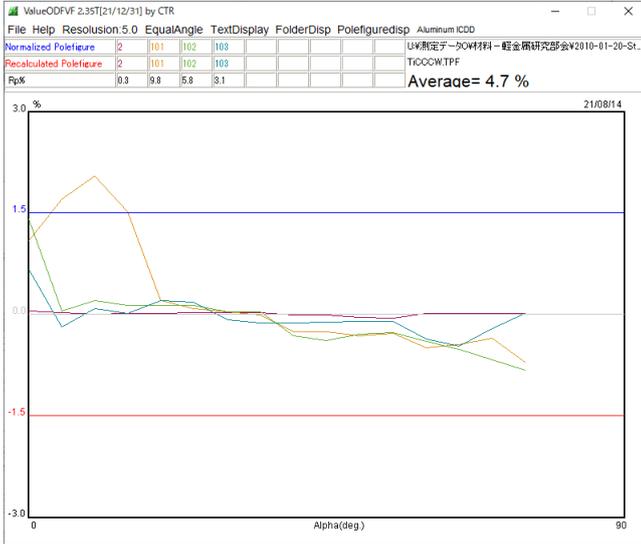
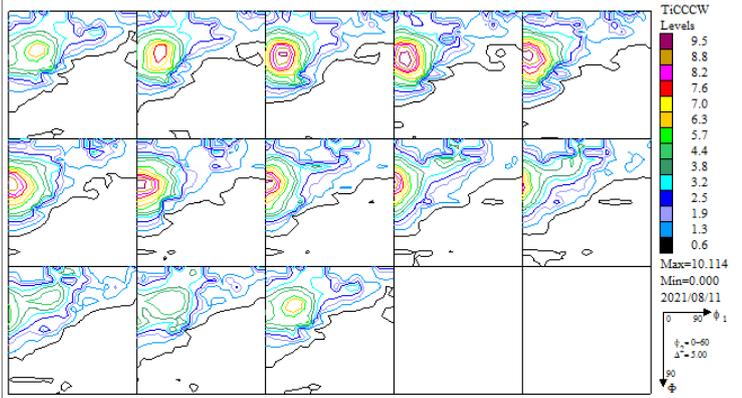
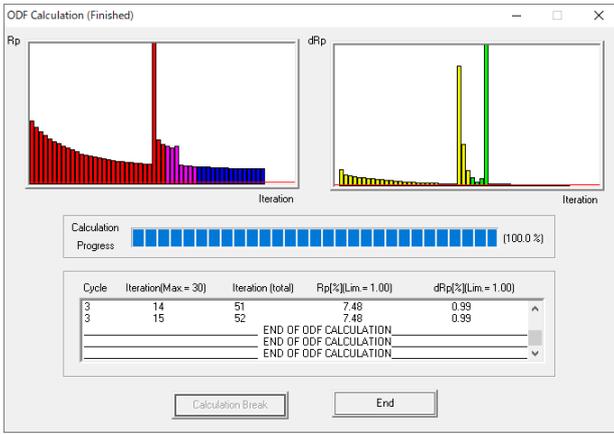
Center Data: Average

Epf file save: Ti

Labotex(EPF),popLA(RAW) filename

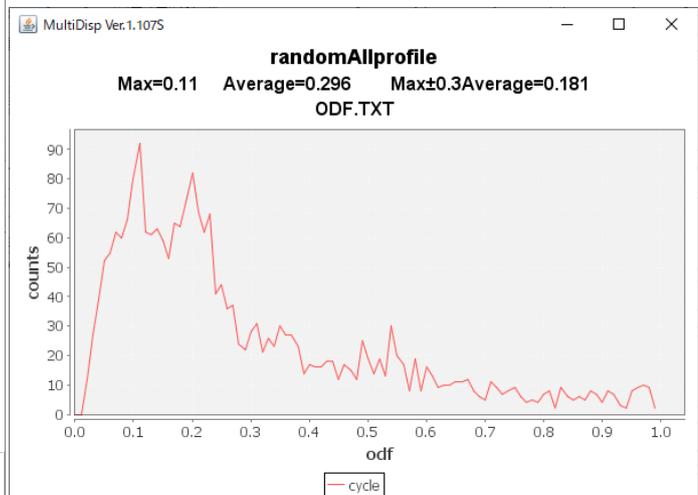
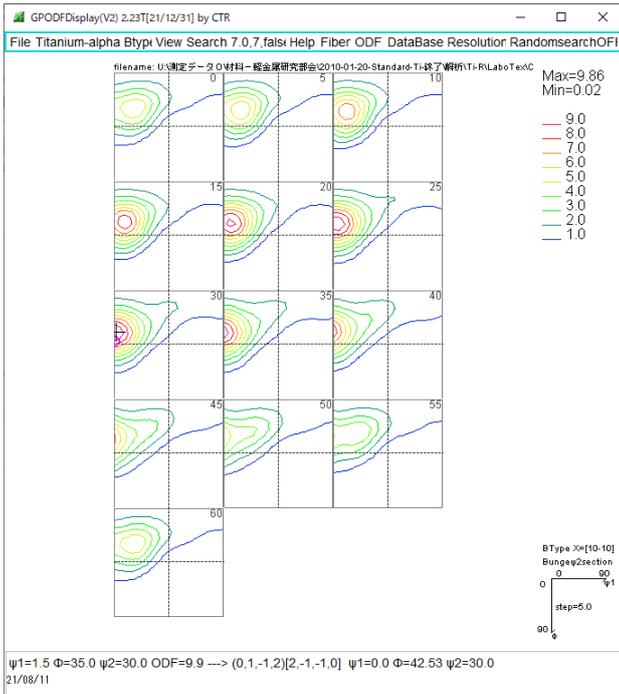
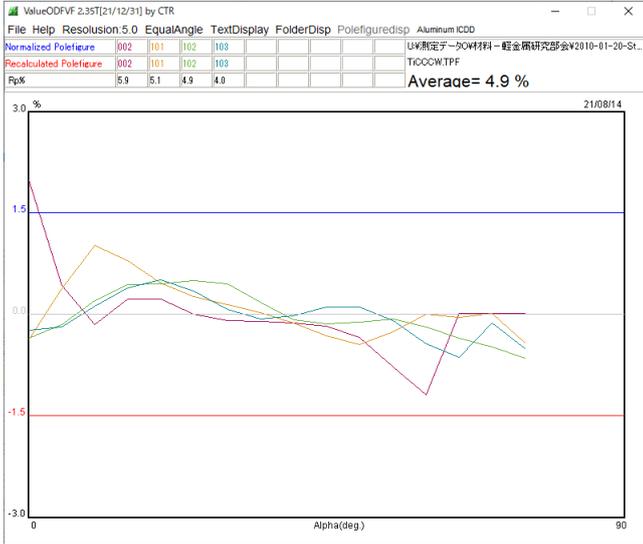
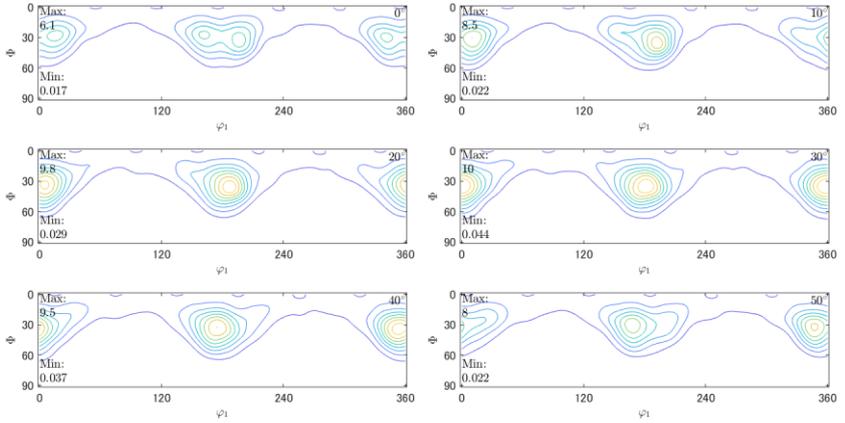
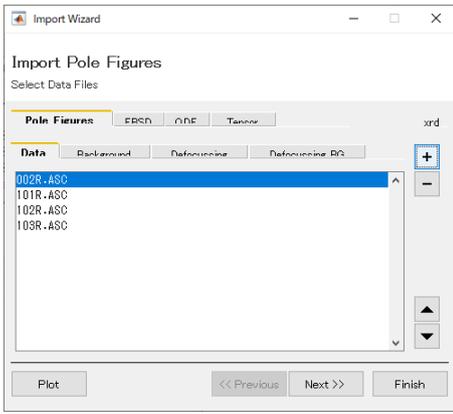
更新日時	種
2021/07/29 8:38	フ
2021/07/29 8:35	テ
2010/02/09 19:12	R

LaboTexで解析



random=0%

MT E Xで解析



randomの分散が大きくハッキリしない

TextToolsで解析

ODF Calculation Setup

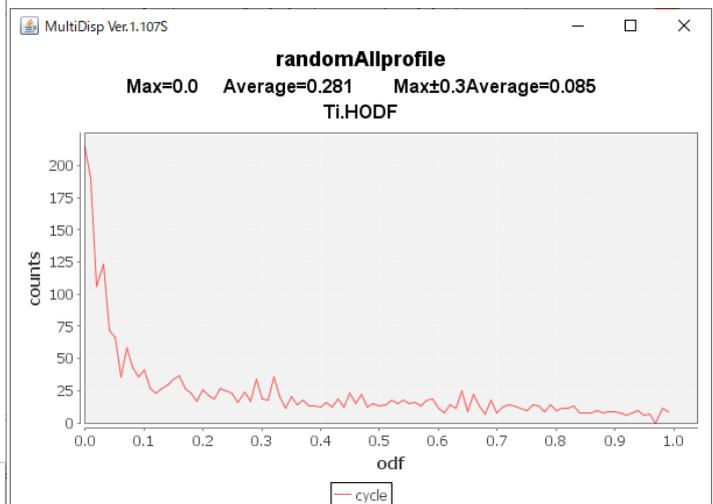
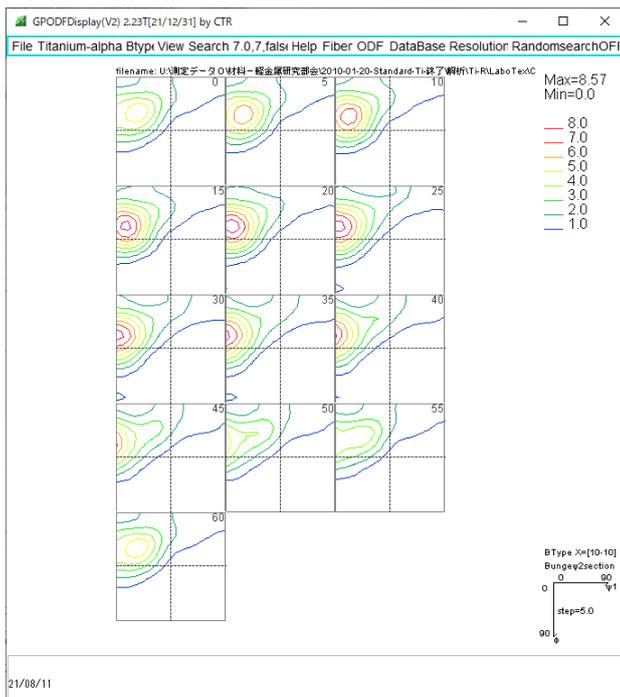
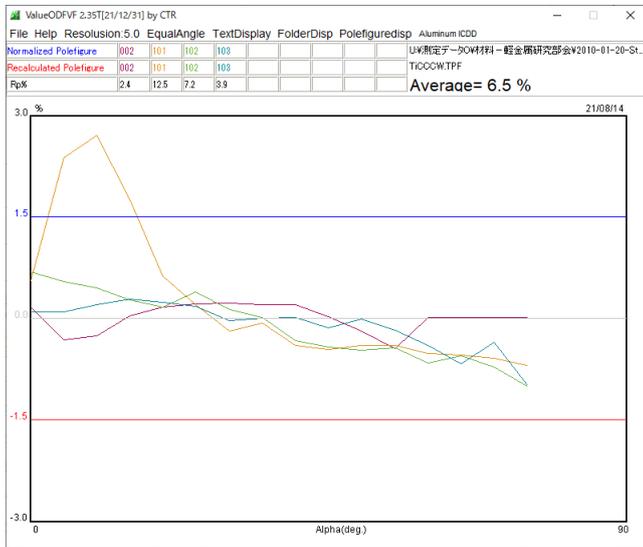
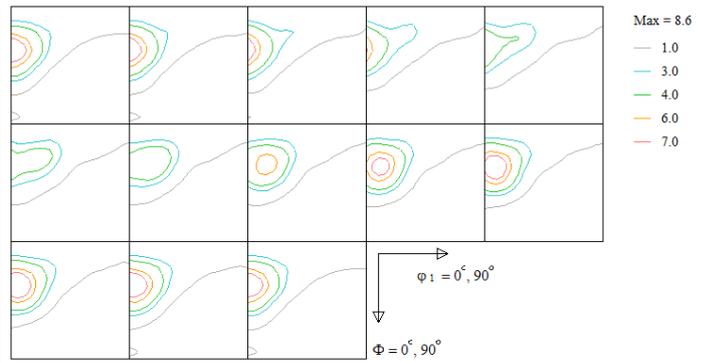
Crystal info.
 Crystal system: Hexagonal
 a: 1, α : 90
 b: 1, β : 90
 c/a: 1.58, γ : 120

Pole figure info.
 Number of pole figures: 4
 1st PF | 2nd PF | 3rd PF | 4th PF
 h: 1, k: 0, l: 3
 Browse PF file location: U:\測定データ\材料-軽金属研究部会\2010-01-20-

Normalizing pole figures before ODF calculation
 With Orthogonal sample symmetry
 Resolution: 5.00
 Assuming fiber texture

Save as: U:\測定データ\材料-軽金属研究部会\2010-01-20-Standard-Ti-終了解析\TI-R\LaboTex

OK Advance Help Cancel



random = 0%が得られる。

まとめ

r a n d o m 1 0 0 % の方位密度はすべて 1. 0 であるが、他に方位が存在すると r a n d o m 方位は 1. 0 以下になる。この 1. 0 以下を調べることで r a n d o m の定量が出来るとしてシミュレーションを行って見たが、M T E X , L a b o T e x , T e x T o o l s では良い結果が得られるが、S t a n d a r d O D F はオーバシュートの影響で正確な定量値は得られない。

従来、O D F 解析後の r a n d o m の定量は行われていないが、V o l u m e F r a c t i o n を計算する時、指定された方位以外は b a c k g r o u n d として評価されている。

この b a c k g r o u n d 値も定量の収束判断としている。

$b a c k g r o u n d = r a n d o m \text{ 定量値} + \text{指定以外の方位値}$ と考えれば

b a c k g r o u n d の収束値として考える事が出来ます。

最後に T i t a n i u m の解析を行ったが r a n d o m の分散から L a b o T e x , T e x T o o l s の結果が正しいと考えられます。

今後の r a n d o m 定量値の応用に期待します。

本資料はMTEX 5. 7. 0を使用

odfはcalcODF0で計算

Uniform portion:
weight: 0.79145

Radially symmetric portion:
kernel: de la Vallee Poussin, halfwidth 5°
center: 4903 orientations, resolution: 5°
weight: 0.20855

MTEX 5. 1. 1では

Uniform portion:
weight: 0.78816

Radially symmetric portion:
kernel: de la Vallee Poussin, halfwidth 5°
center: 4882 orientations, resolution: 5°
weight: 0.21184

