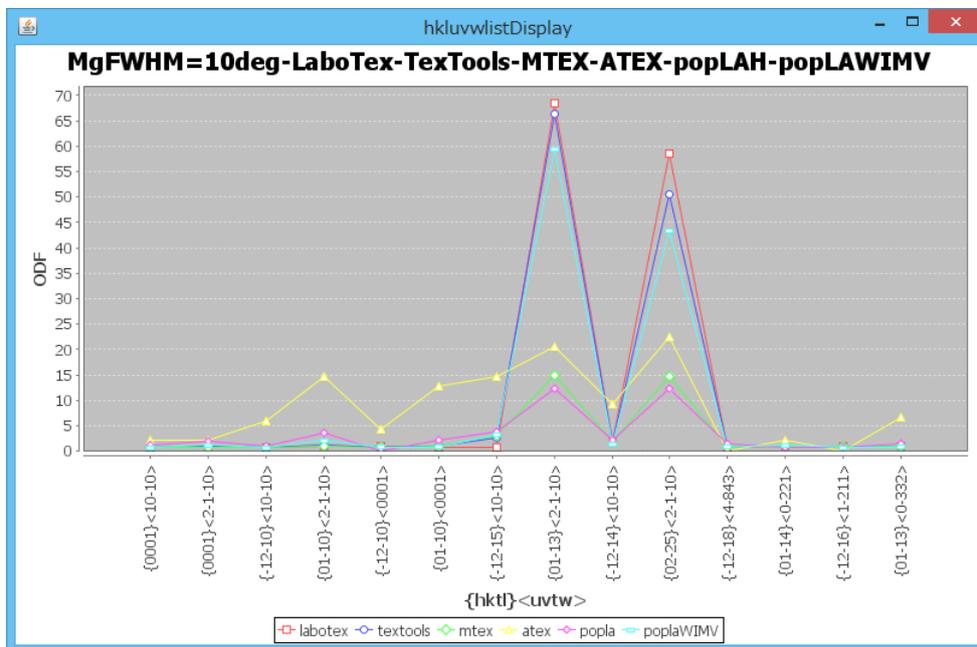


Mg-TD-split による

LaboTeX-TeXTools-MTEX-ATEX-ODF解析比較

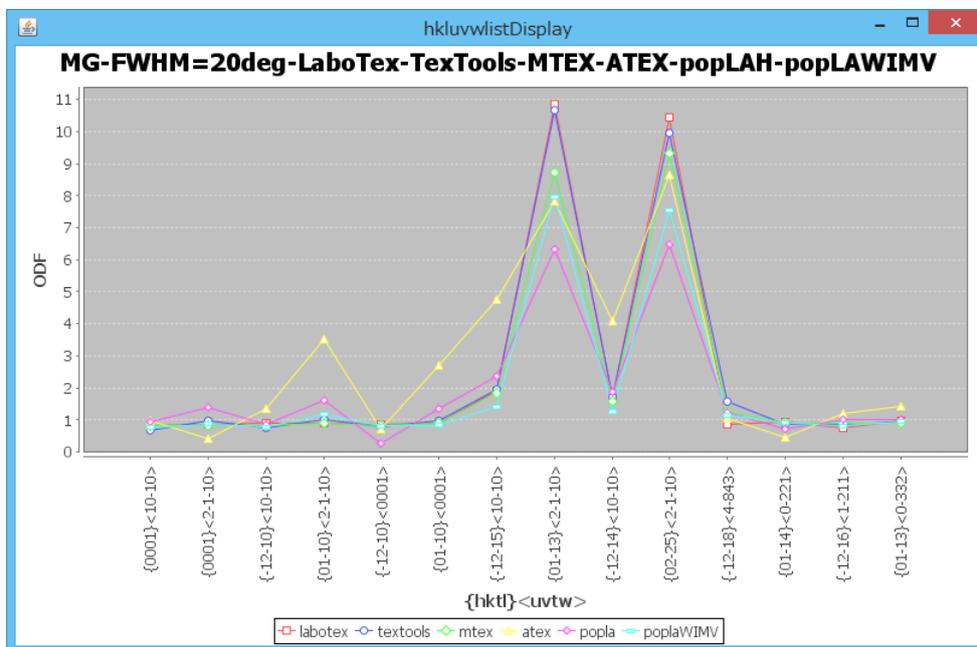
+ ATEX+popLA比較

FWHM=10deg では一致しないが



LaboTeX=TexTools=popLAWIMV

FWHM=20deg



LaboTeX=TexTools=MTEX=popLA

MTEX,ATEX は Hermonic と考えられる

2019年01月30日

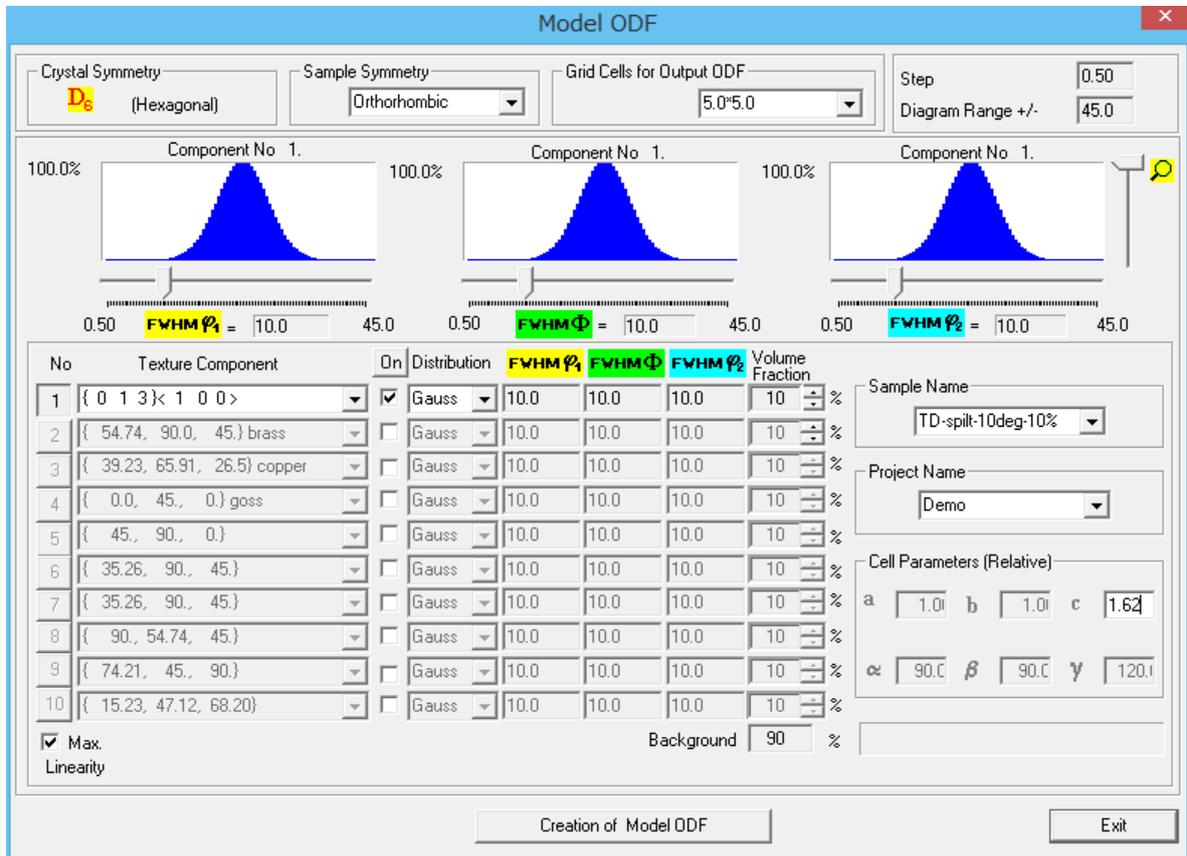
HelperTex Office

概要

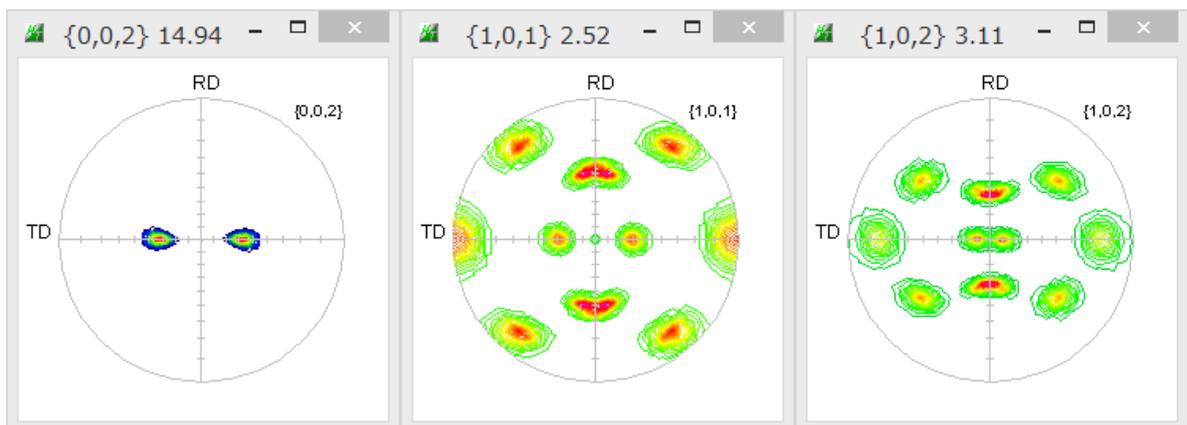
TD-splitに関し、ODFの半価幅が10degの場合、LaboTexとMTEXの解析結果が異なり半価幅が20degの場合、一致する事が確認されている。又、ODF解析結果の結晶方位位置がずれる事が確認されている。

今回、TexToolsも比較してみました。

極点図作成

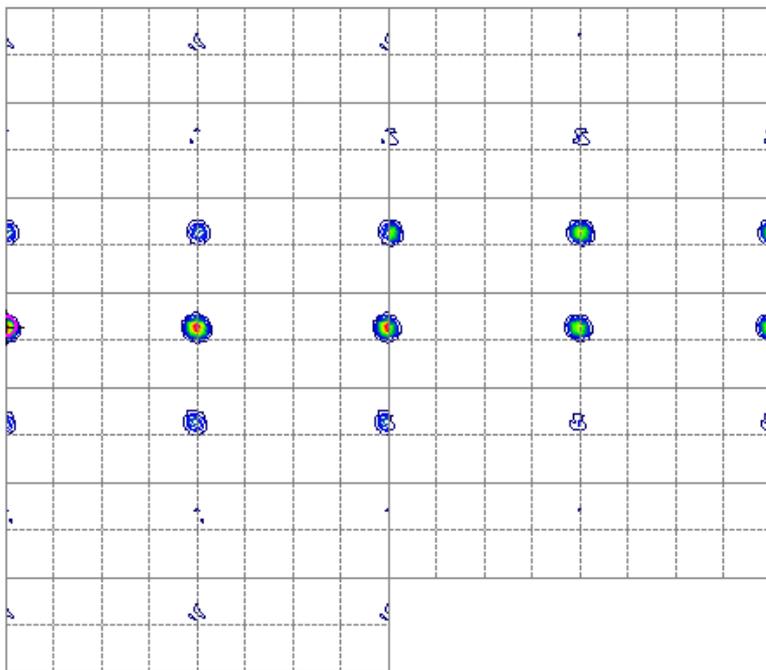


作成される極点図



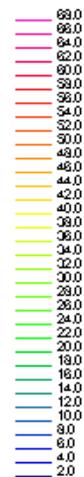
LaboTex 解析結果

filename: U:\TD-spilt-10deg-10%\LaboTex\CW\90ODFExport.TXT



Max=68.42

Min=0.47



BType X=[10-10]

Bungeψ2section

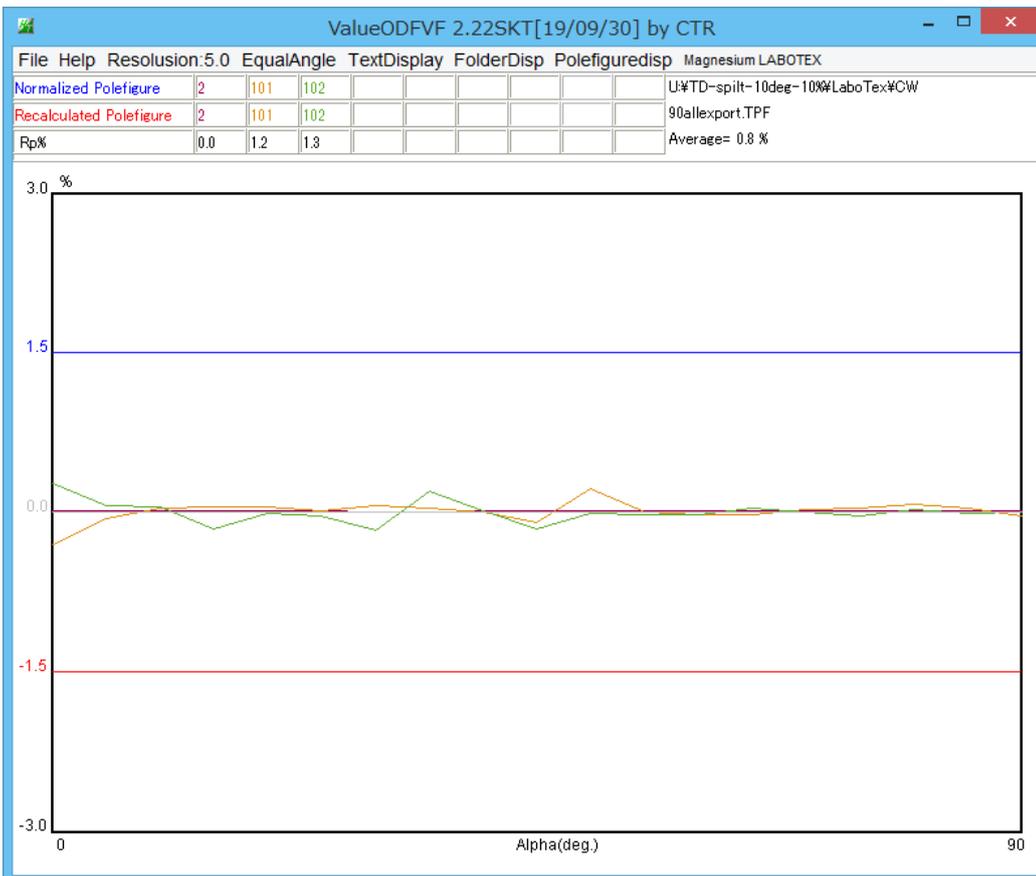
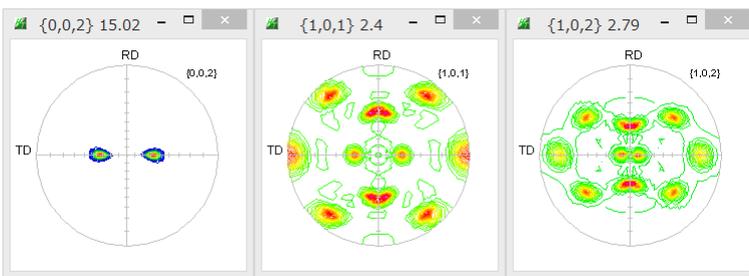
0 360

ψ1

ψ2=0->60

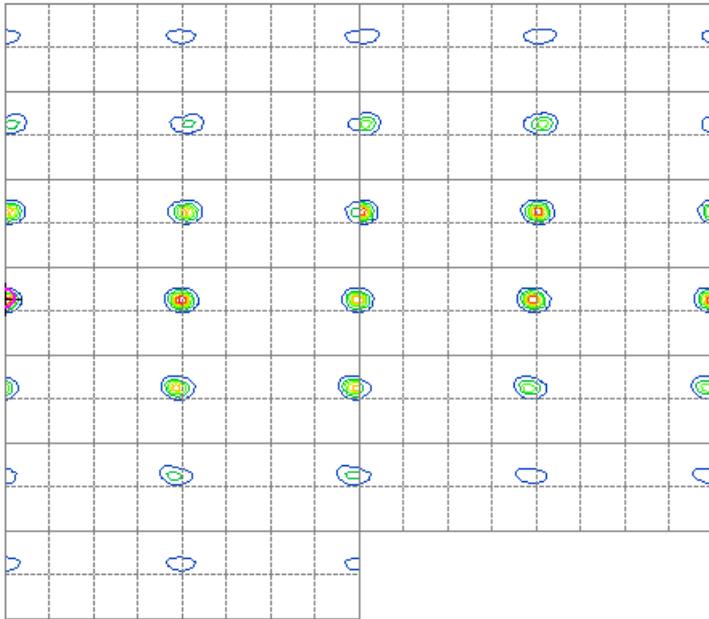
step=5.0

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=68.42



MTEXの解析結果

filename: U:\TD-spilt-10deg-10\MTEX\od90.txt

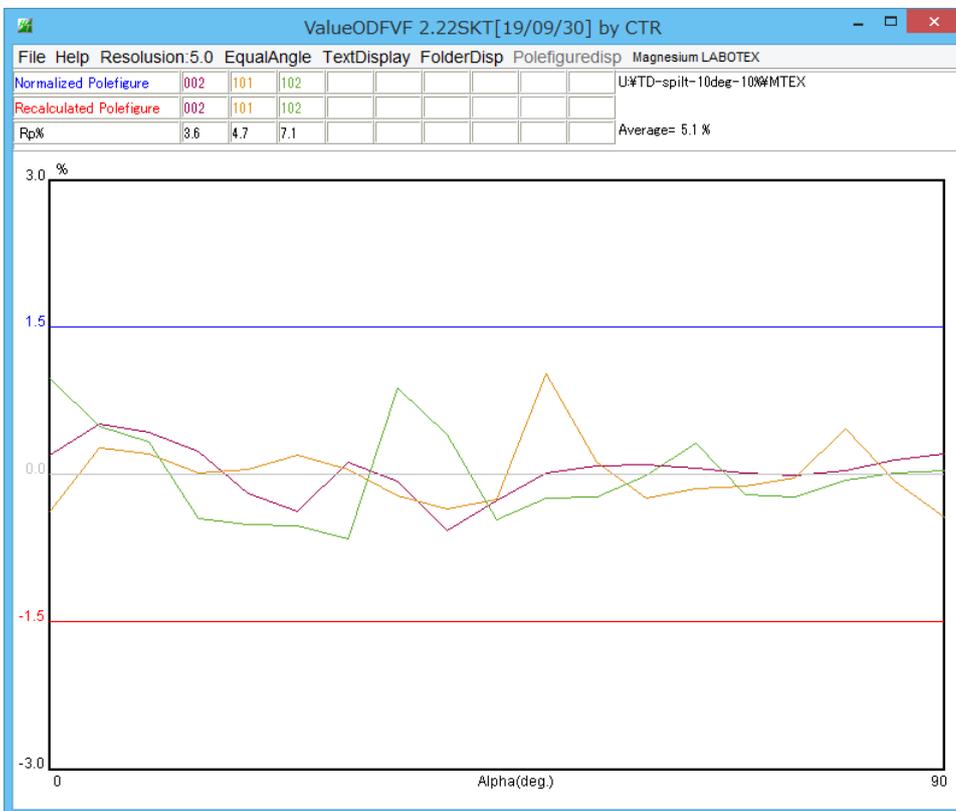
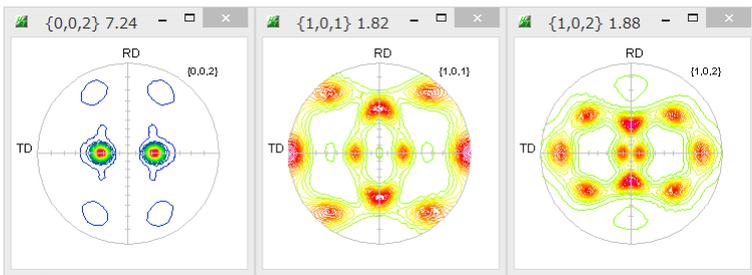


Max=15.24
Min=0.82



BType X=[10-10]
Bungeψ2section
0 360
ψ1
0 ψ2=0->80
step=5.0
90
φ

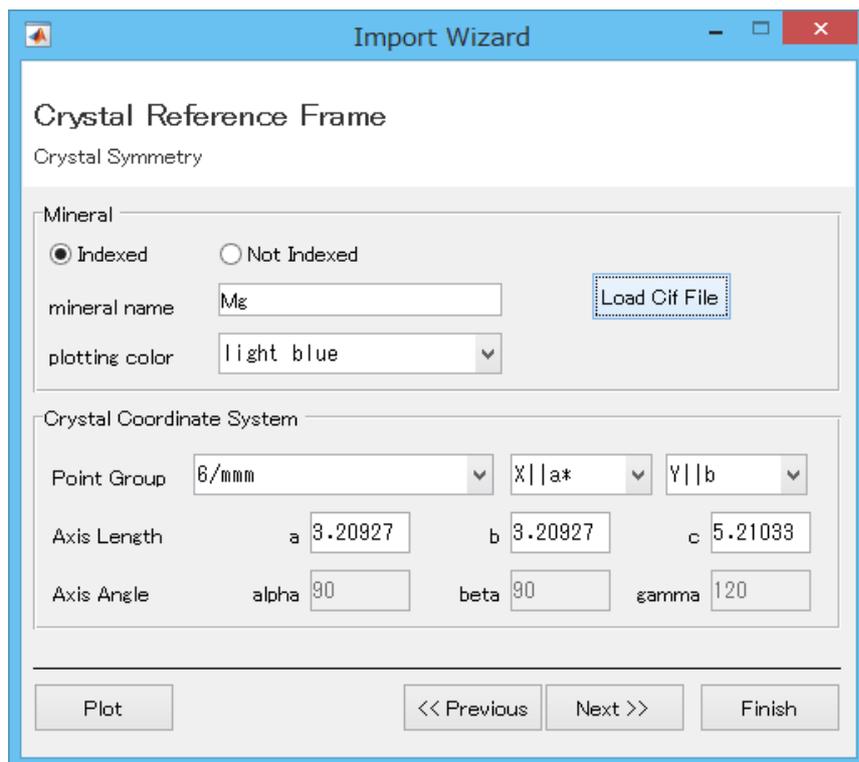
(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=14.98



LaboTex, TexToolsに比べ、バタバタしている

MTEXの解析結果結晶方位位置に関して

cifファイルから入力



LaboTexはTexToolsに合わせ格子定数修正

```
% crystal symmetry  
CS = crystalSymmetry('6/mmm', [3.2093 3.2093 5.2103], 'X||a*', 'Y||b', 'Z||c*', 'mineral', 'Mg', 'color', 'light blue');
```

から

```
CS = crystalSymmetry('6/mmm', [3.2061 3.2061 5.2091], 'X||a*', 'Y||b', 'Z||c*', 'mineral', 'Mg', 'color', 'light blue');
```

に修正

取り込まれる値は

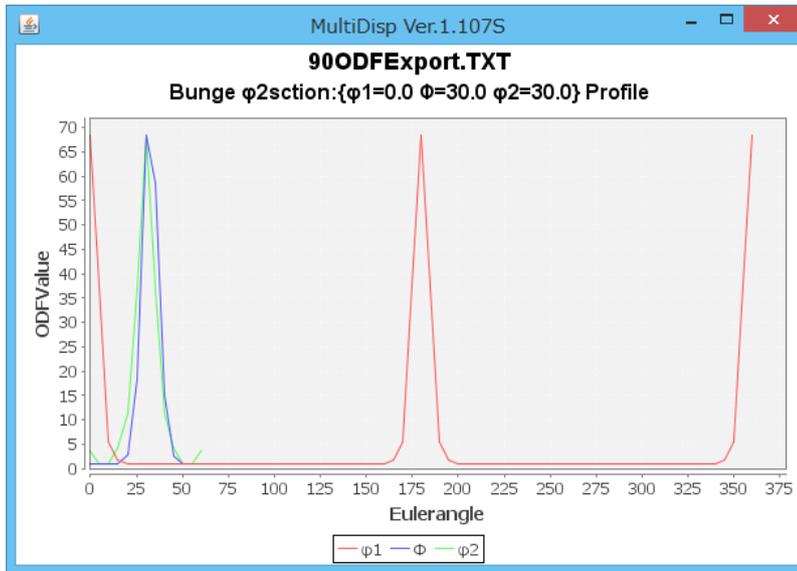
```
>> CS
```

```
CS = crystalSymmetry (show methods, plot)
```

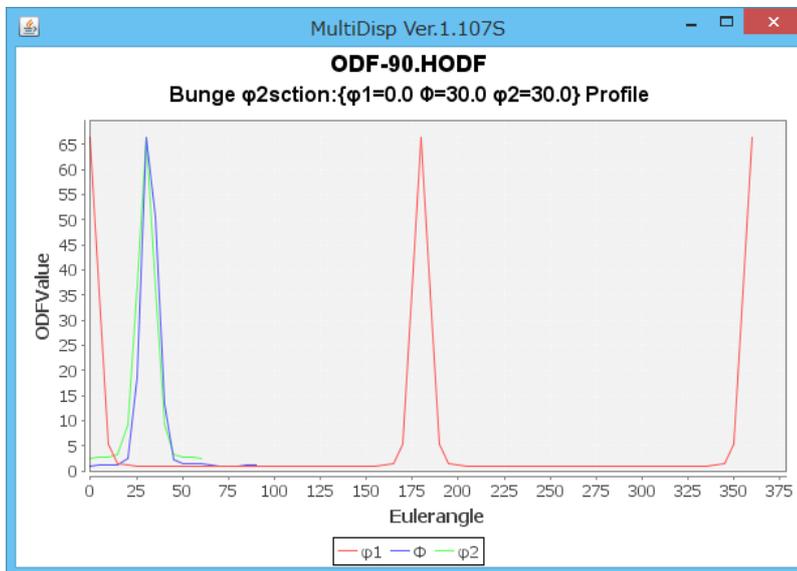
```
mineral      : Mg  
color        : light blue  
symmetry     : 6/mmm  
a, b, c     : 3.2, 3.2, 5.2  
reference frame: X||a*, Y||b, Z||c
```

c/aは一致している。

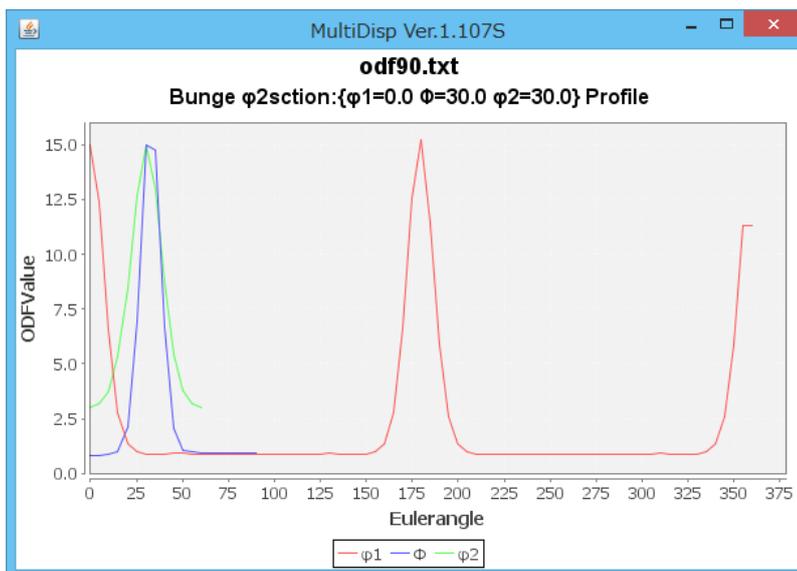
方位の広がり



LaboTex



TextTools



MTEX

結晶方位プロフィール比較

hkluvwlistDisplay 1.05T[19/09/30] by CTR

File DispODF Help

U:\TD-spilt-10deg-10%\LaboTex\CW\labotex.csv ● Dispselect DispODF labotex

U:\TD-spilt-10deg-10%\TexTools\textools.csv ● Dispselect DispODF textools

U:\TD-spilt-10deg-10%\MTEX\mtex.csv ● Dispselect DispODF mtex

Dispselect DispODF

Dispselect DispODF

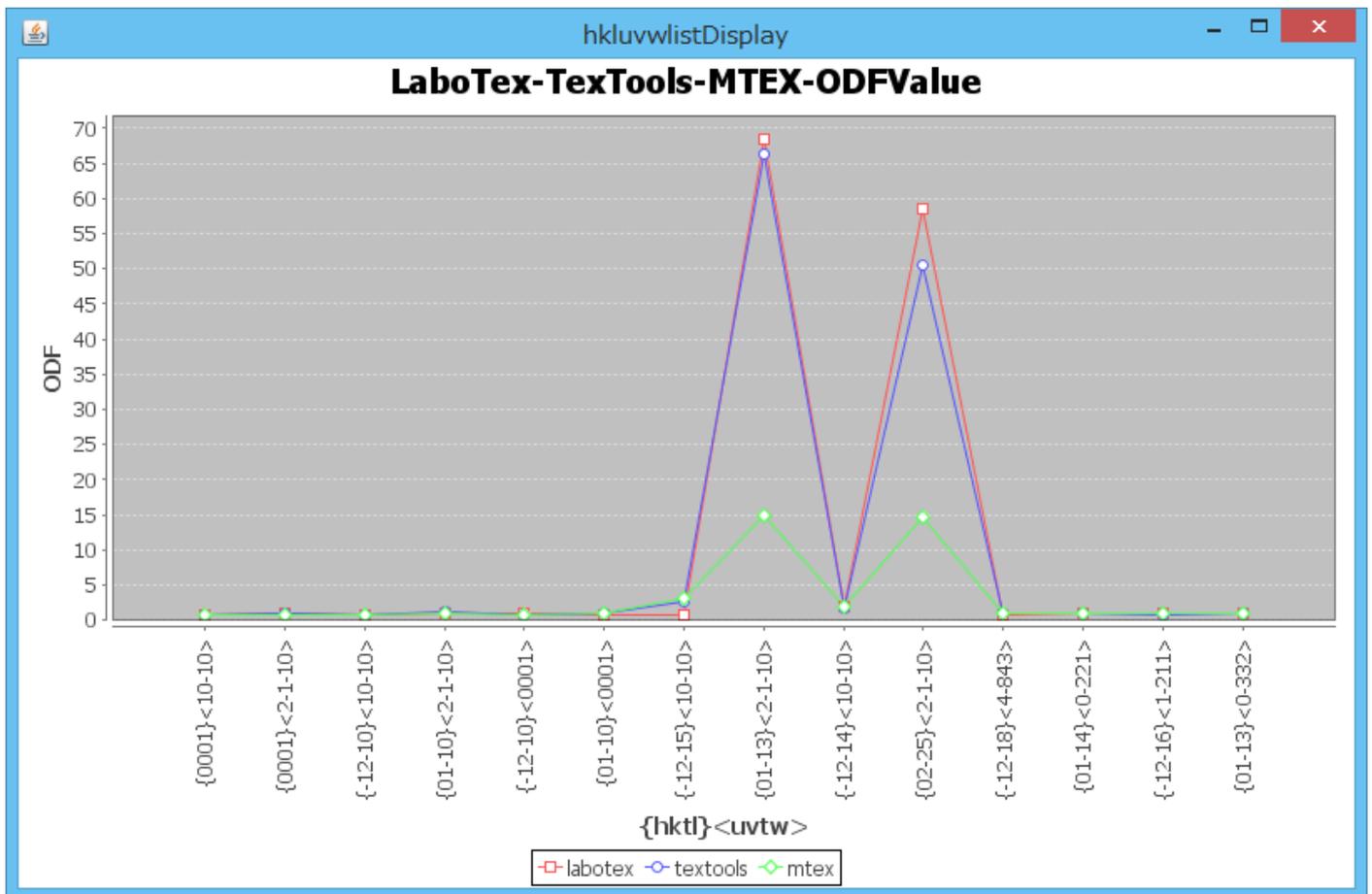
Dispselect DispODF

Dispselect DispODF

Dispselect DispODF

MakeCSVFile Load C:\CTR\work\hkluvwlistDisplay\hkluvwlist.csv V-Axis ODF hkluvwlistDisplayGraph

Comment LaboTex-Textools-MTEX-ODFValue



```

0 1 -1 3 2 -1 -1 0 0.0 32.02 30.0
-1 2 -1 4 1 0 -1 0 0.0 39.089 0.0
0 2 -2 5 2 -1 -1 0 0.0 36.885 30.0
    
```

半価幅 20 deg の場合

Model ODF

Crystal Symmetry: D_6 (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% | Component No. 1. 100.0% | Component No. 1. 100.0%

0.50 FWHM ϕ_1 = 20.00 45.0 | 0.50 FWHM Φ = 20.00 45.0 | 0.50 FWHM ϕ_2 = 20.00 45.0

No	Texture Component	On	Distribution	FWHM ϕ_1	FWHM Φ	FWHM ϕ_2	Volume Fraction
1	{ 0 1 3 } < 1 0 0 >	<input checked="" type="checkbox"/>	Gauss	20.00	20.00	20.00	10 %
2	{ 54.74, 90.0, 45. } brass	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
3	{ 39.23, 65.91, 26.5 } copper	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
4	{ 0.0, 45., 0. } goss	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
5	{ 45., 90., 0. }	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
6	{ 35.26, 90., 45. }	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
7	{ 35.26, 90., 45. }	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
8	{ 90., 54.74, 45. }	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
9	{ 74.21, 45., 90. }	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
10	{ 15.23, 47.12, 68.20 }	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %

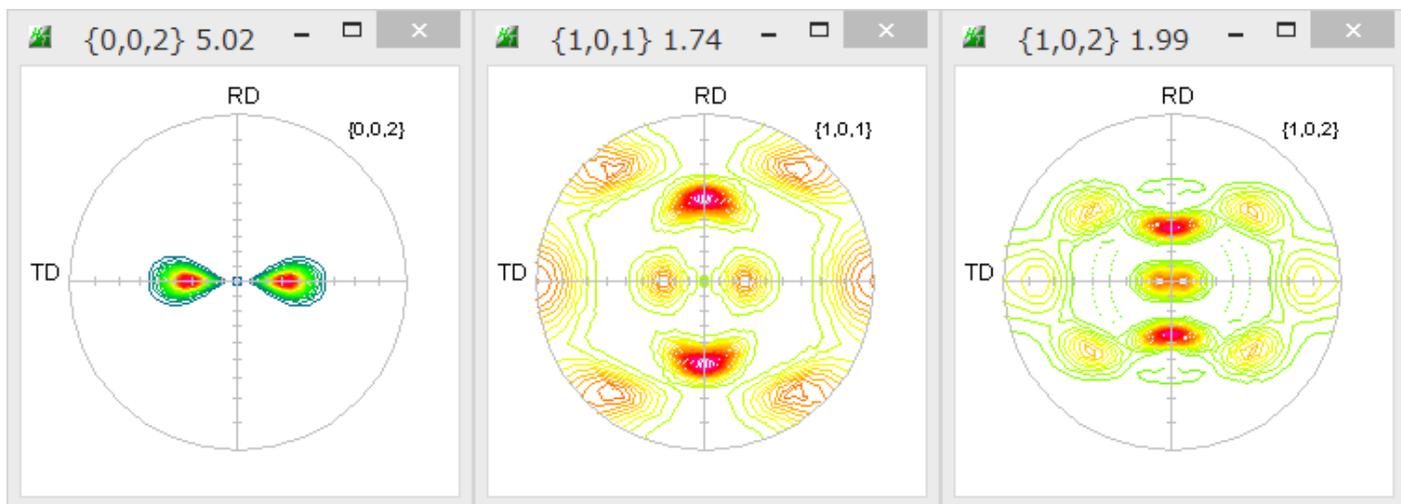
Sample Name: TD-split-20deg-10% | Project Name: Demo

Cell Parameters (Relative): a: 1.0 | b: 1.0 | c: 1.62 | α : 90.0 | β : 90.0 | γ : 120.0

Max. Linearity | Background: 90 %

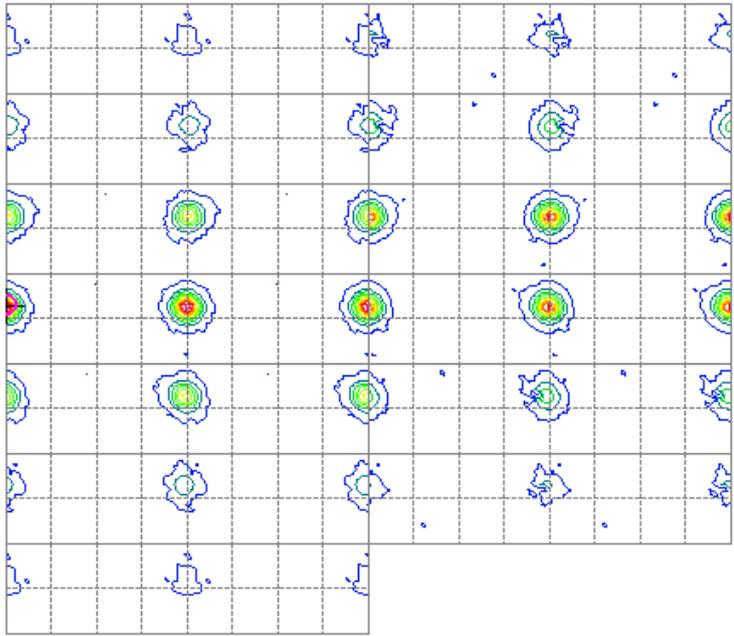
Creation of Model ODF | Exit

作成される極点図



FWHM 20 degをLaboTex解析結果

filename: U:\TD-split-20deg-10%\LaboTex\CW\20deg.TXT

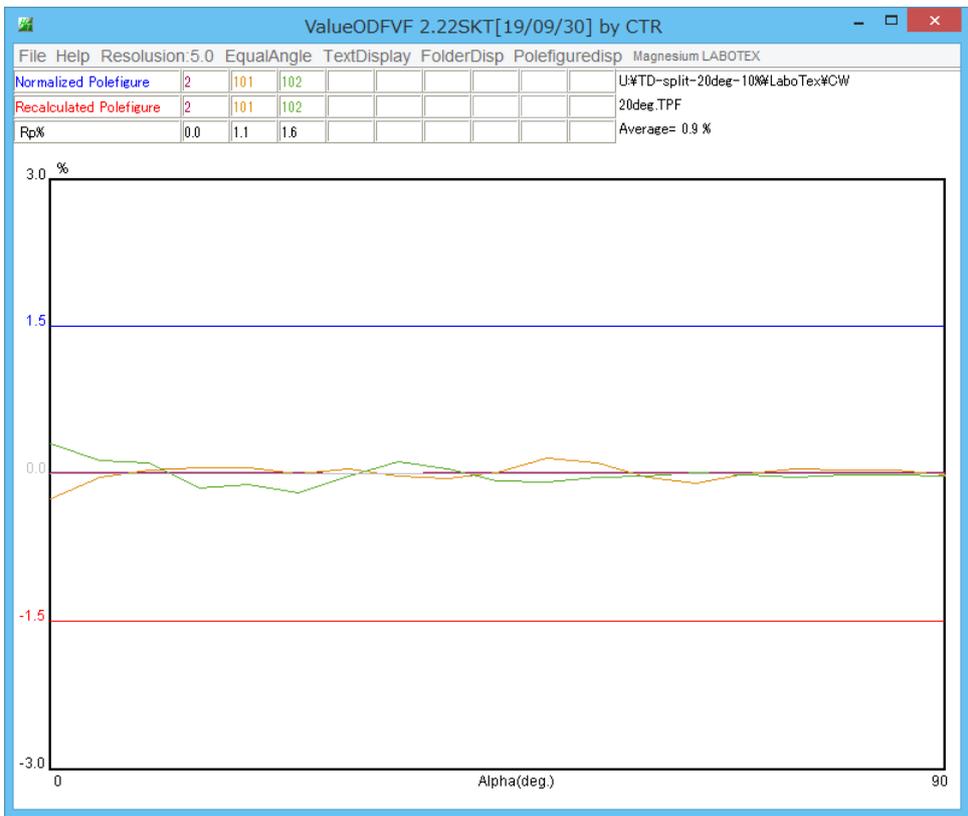
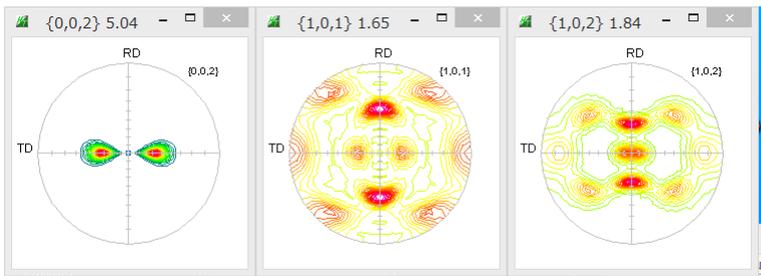


Max=10.85
Min=0.46



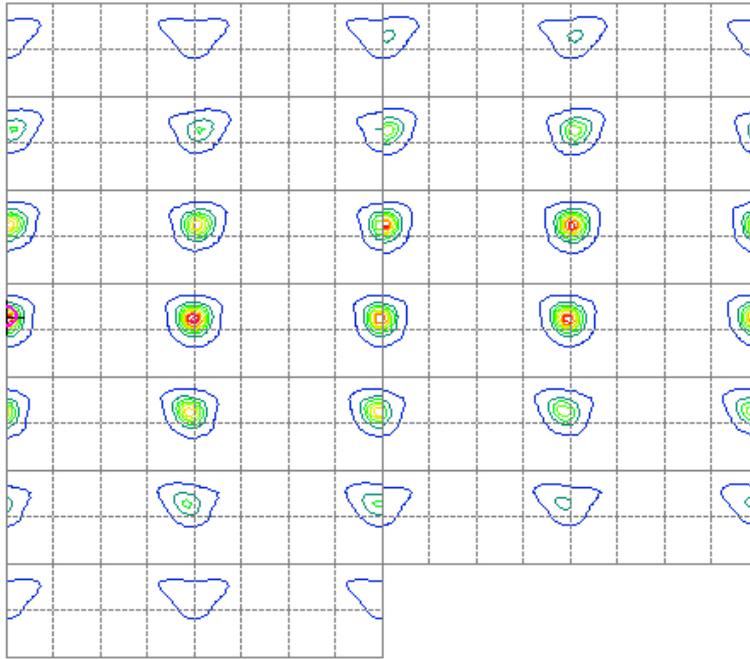
BType X=[10-10]
Bungeψ2section
0 360
ψ1
ψ2=0->80
step=5.0
90
φ

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=10.85



20degをMTEX解析結果

filename: U:\TD-split-20deg-10%\MTEX\odf.bt

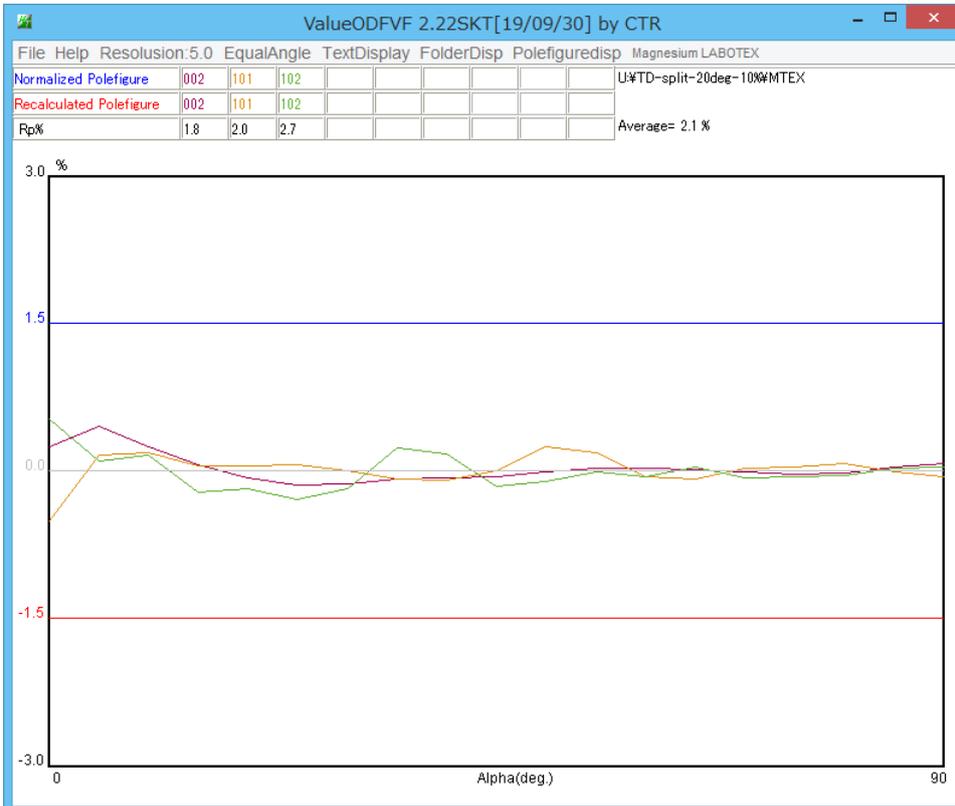
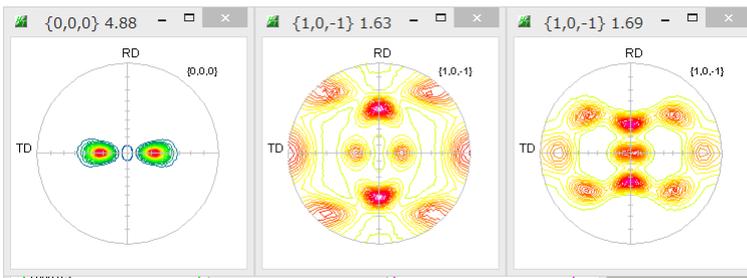


Max=9.55
Min=0.82

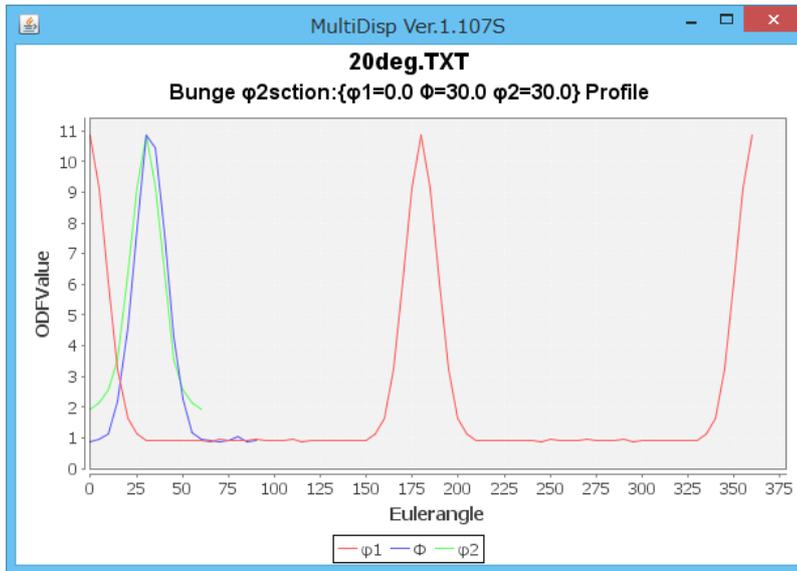


BType X=[10-10]
Bungeψ2section
0 360
ψ1
ψ2=0->80
step=5.0
90 φ

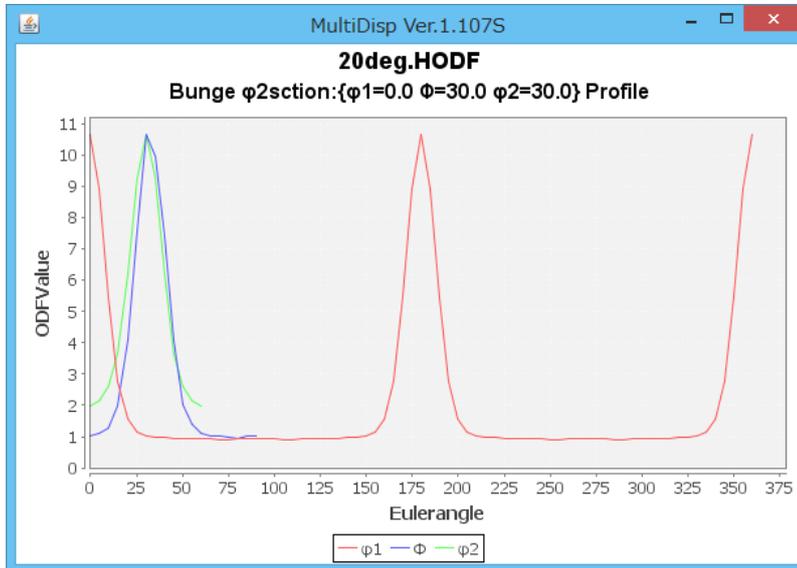
(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=8.74



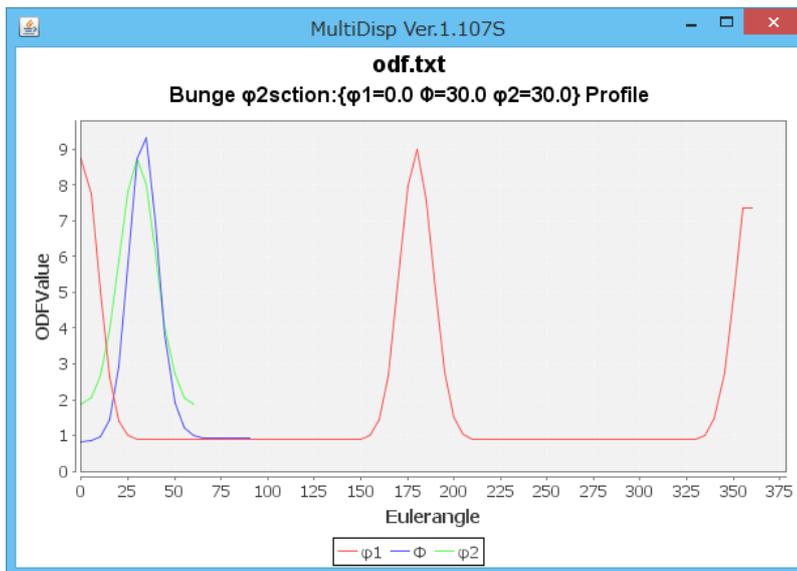
方位の広がり



LaboTex



TextTools



MTEX

結晶方位プロフィール比較

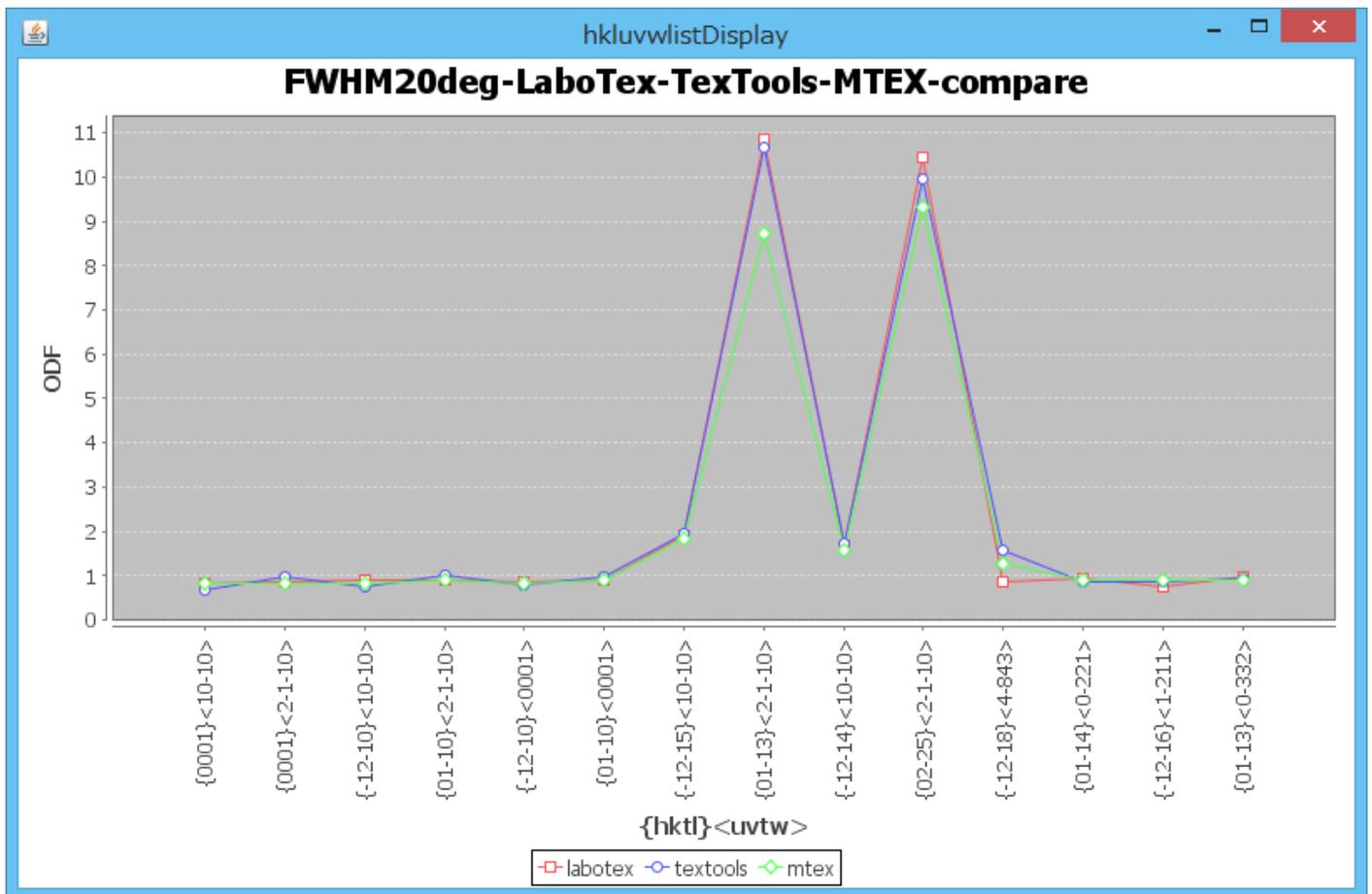
hkluvwlistDisplay 1.05T[19/09/30] by CTR

File DispODF Help

U:\TD-split-20deg-10%\LaboTex\CW\labotex.csv	<input checked="" type="radio"/> Dispselect	<input checked="" type="checkbox"/> DispODF	labotex
U:\TD-split-20deg-10%\TexTools\textools.csv	<input checked="" type="radio"/> Dispselect	<input checked="" type="checkbox"/> DispODF	textools
U:\TD-split-20deg-10%\MTEX\mtex.csv	<input checked="" type="radio"/> Dispselect	<input checked="" type="checkbox"/> DispODF	mtex
	<input type="radio"/> Dispselect	<input checked="" type="checkbox"/> DispODF	
	<input type="radio"/> Dispselect	<input checked="" type="checkbox"/> DispODF	
	<input type="radio"/> Dispselect	<input checked="" type="checkbox"/> DispODF	
	<input type="radio"/> Dispselect	<input checked="" type="checkbox"/> DispODF	
	<input type="radio"/> Dispselect	<input checked="" type="checkbox"/> DispODF	

MakeCSVFile Load C:\CTR\work\hkluvwlistDisplay\hkluvwlist.csv V-Axis ODF hkluvwlistDisplayGraph

Comment FWHM20deg-LaboTex-Textools-MTEX-compare



A T E Xによる解析

General Options

Isotropic Part: 0.00

Development EVEN initial: 16

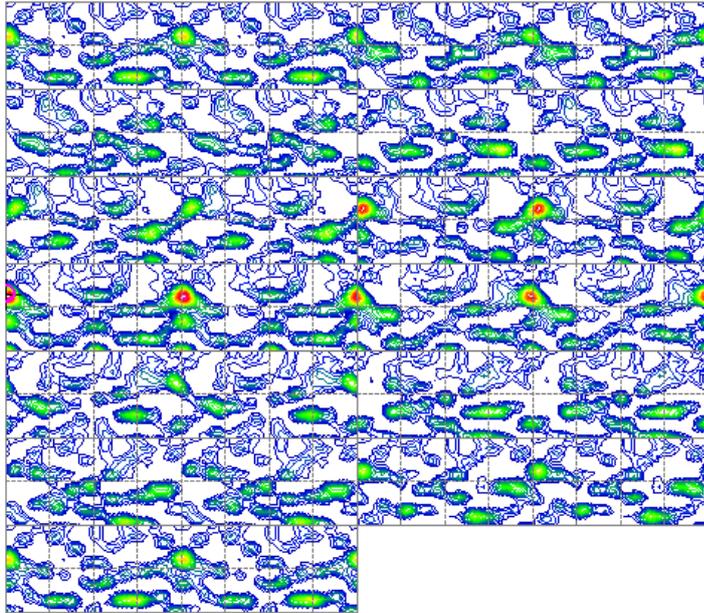
Development EVEN positivity: 22

Development ODD: 21

Maximum Tilt Angle (°): 90

FWHM=10deg

filename: U:\TD-split-10deg-10%\ATEX\ICWmodf_out.bt



Max=22.58
Min=-10.09

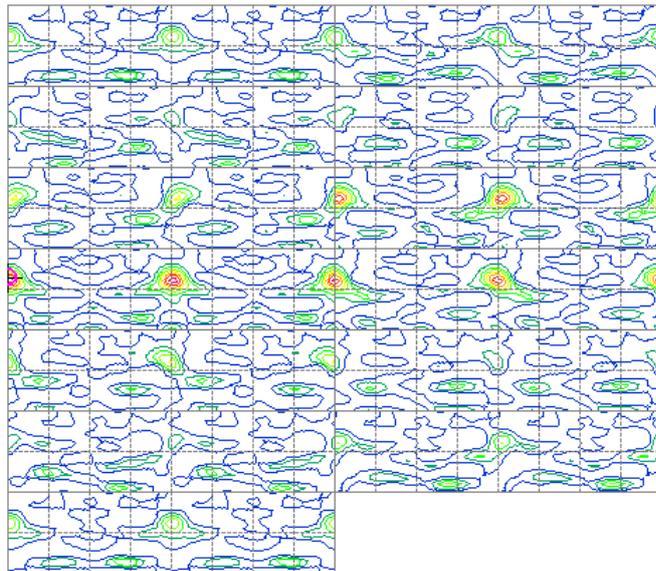


BType X=[10-10]
Bungeψ2section
0 360
ψ1
ψ2=0->60
step=5.0
90
ψ

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=20.56

FWHM=20deg

filename: U:\TD-split-20deg-10%\ATEX\ICWmodf_out.bt

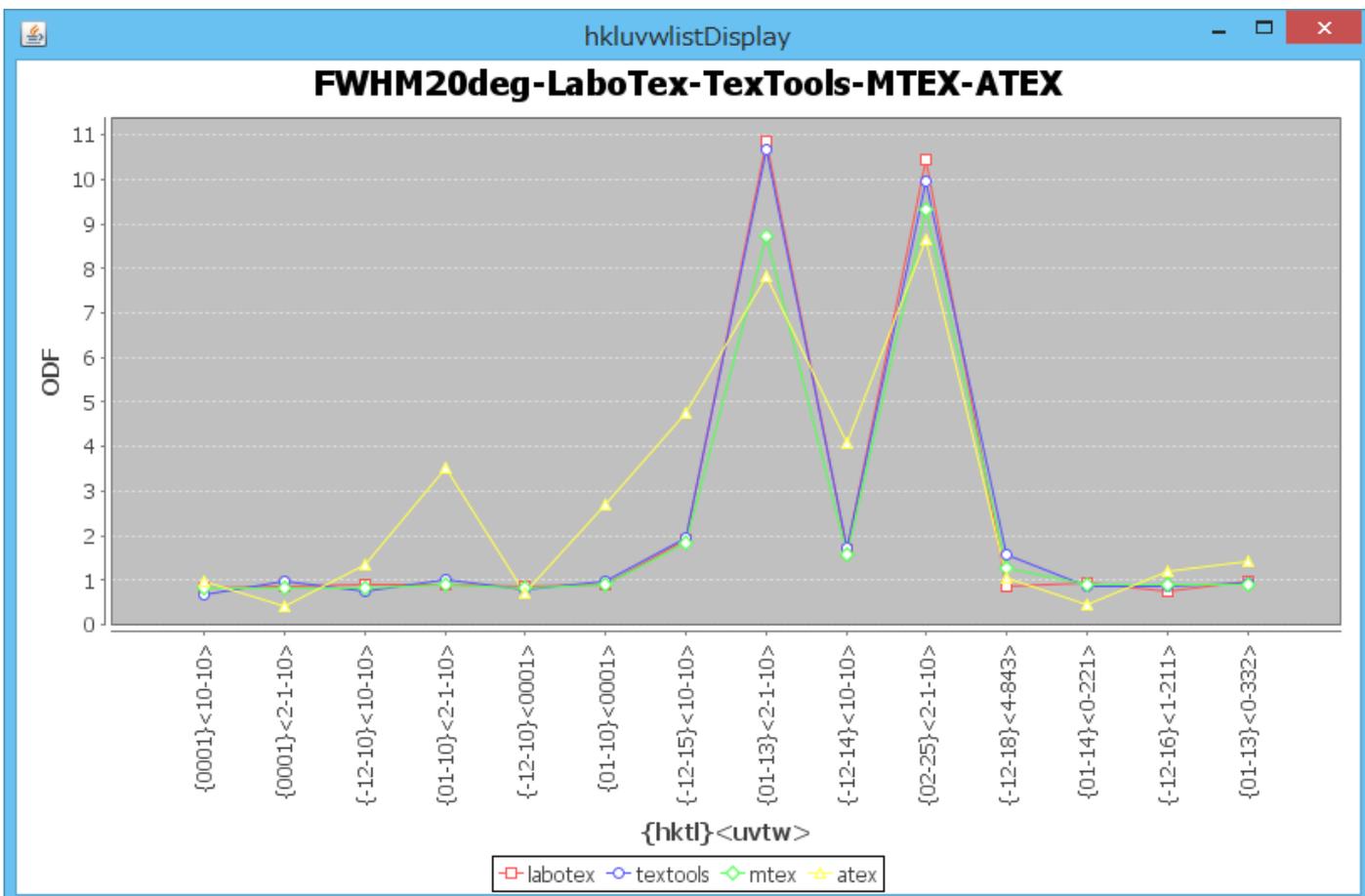
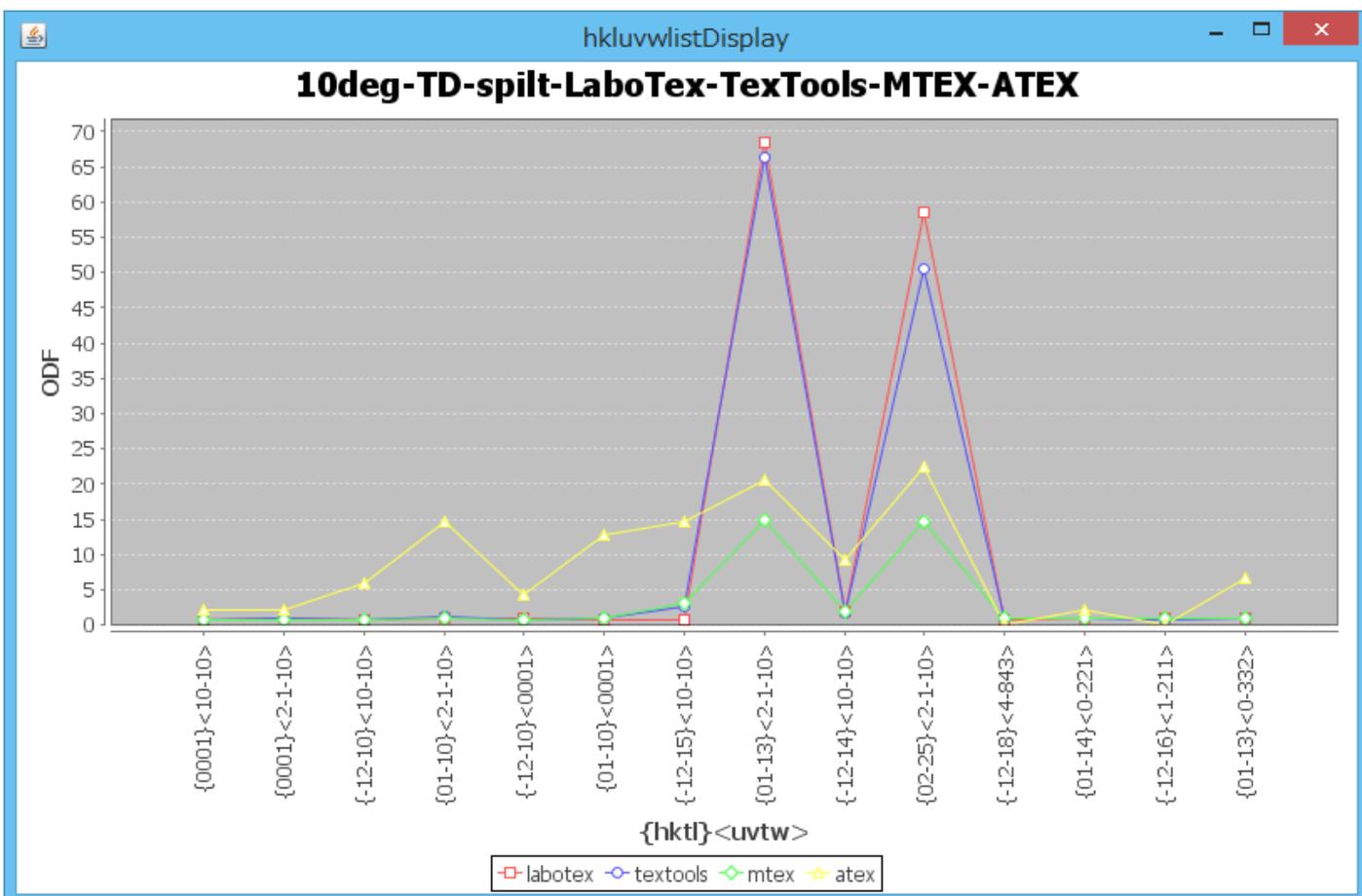


Max=8.7
Min=-2.01



BType X=[10-10]
Bungeψ2section
0 360
ψ1
ψ2=0->60
step=5.0
90
ψ

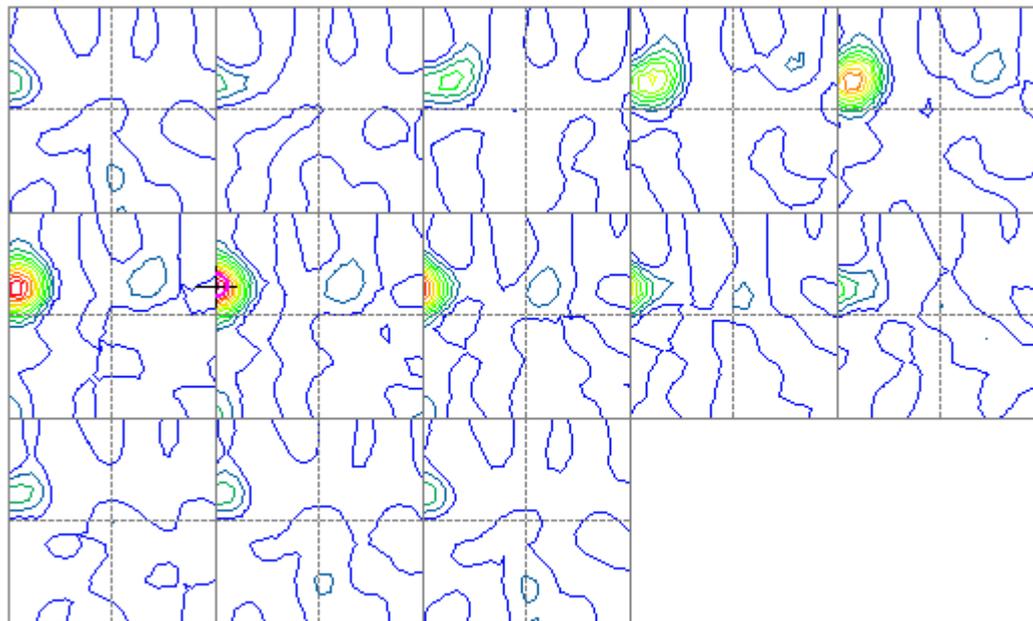
(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=7.81



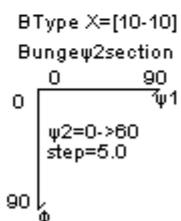
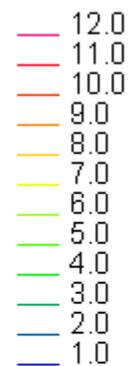
popLAHermonic

FWHM=10deg

filename: U:\TD-split-10deg-10%\popLA\POPLA.SHD



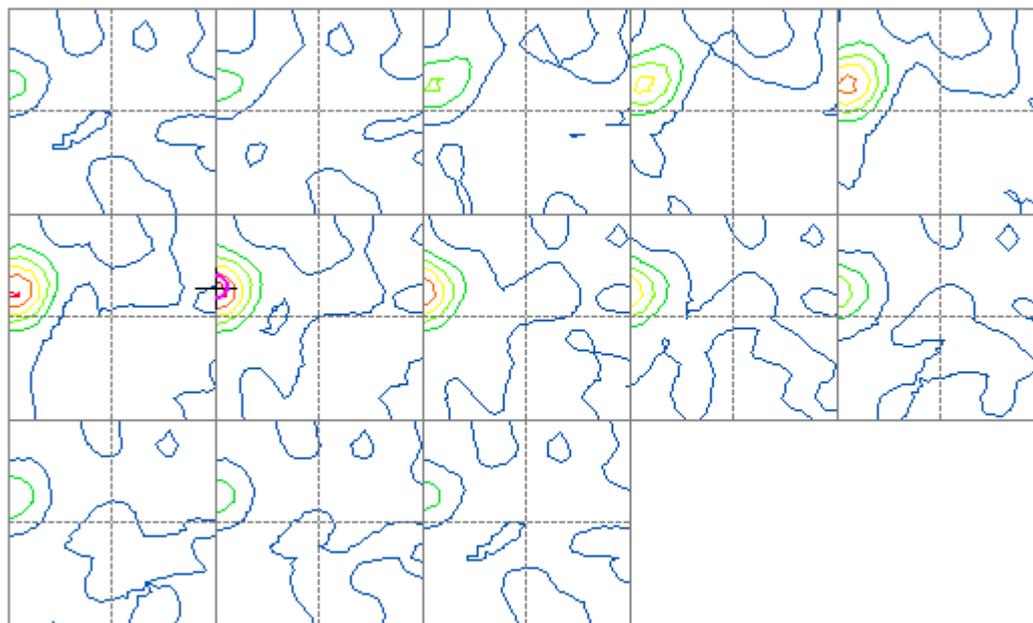
Max=12.37
Min=0.01



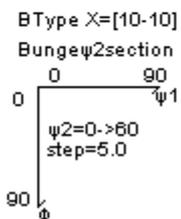
(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=12.37

FWHM=20deg

filename: U:\TD-split-20deg-10%\popLA\POPLA.SHD



Max=6.49
Min=0.2

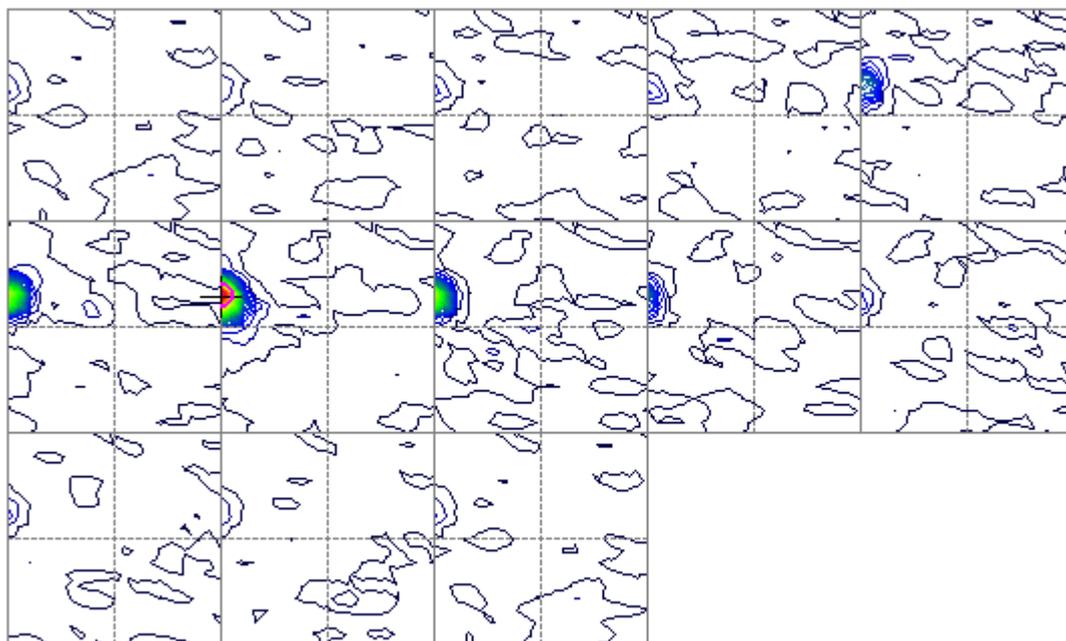


(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=6.31

popLAWIMV

FWHM=10deg

filename: U:\TD-spilt-10deg-10%\popLAWIMV\POPLAWI.SOD



Max=59.32
Min=0.46

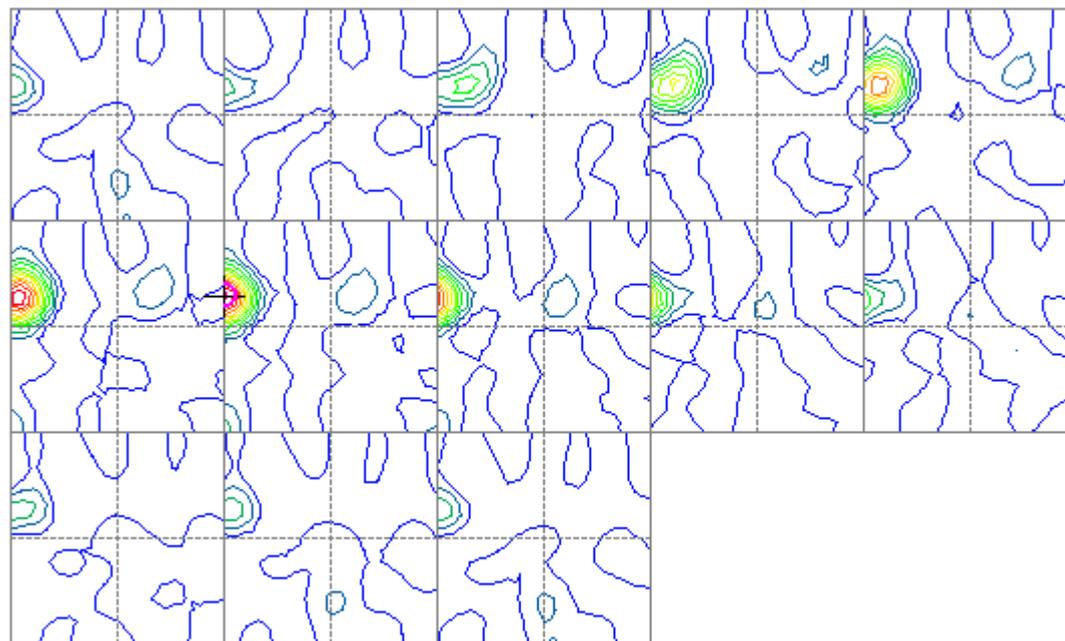


BType X=[10-10]
Bungeψ2section
0 90 ψ1
ψ2=0->60
step=5.0
90 φ

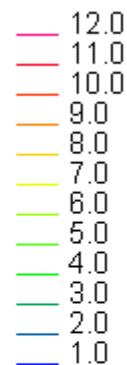
(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=59.32

FWHM=20deg

filename: U:\TD-spilt-10deg-10%\popLA\POPLA.SHD

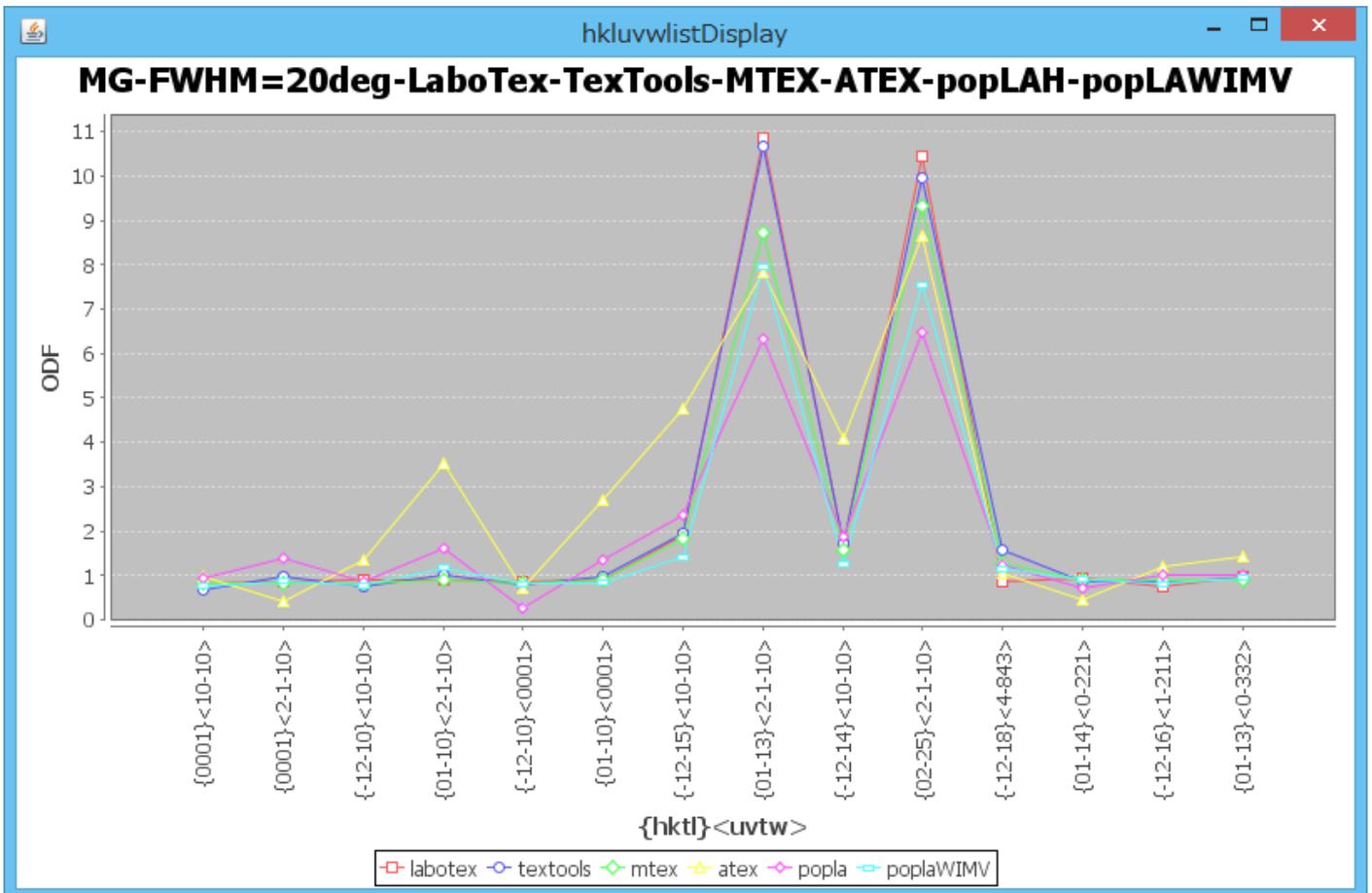
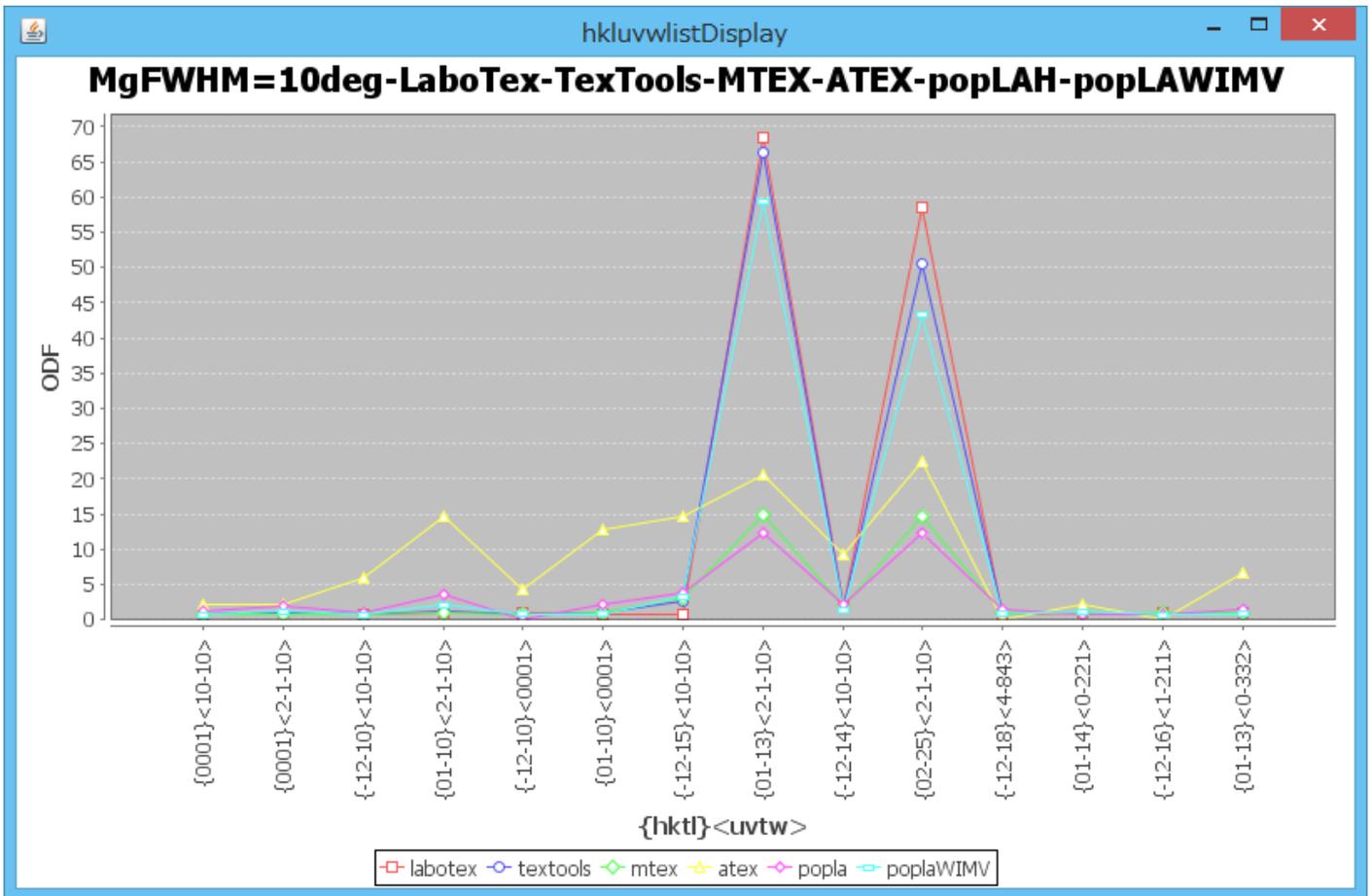


Max=12.37
Min=0.01



BType X=[10-10]
Bungeψ2section
0 90 ψ1
ψ2=0->60
step=5.0
90 φ

(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=12.37



半幅幅が狭いと LaboTex-TextTools-popLAWIMV と MTEX-ATEX-popLAHerminic に分かれる
この違いは直説法 (ADC,WIMV) と間接法 (Hermonic) の違いと思われる。