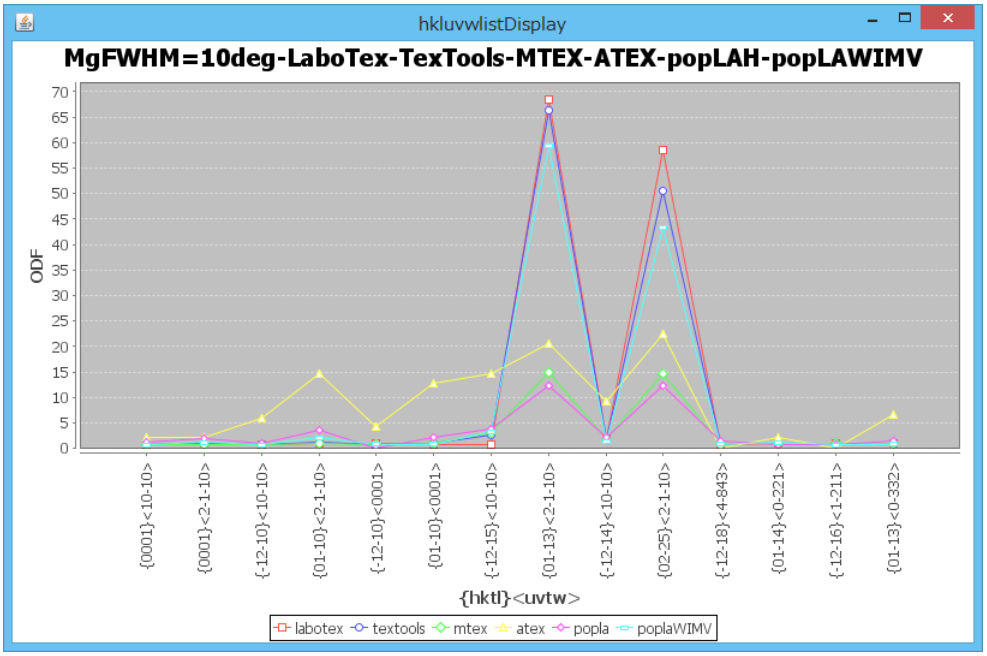
Mg-TD-split による

ＬａｂｏＴｅｘ－ＴｅｘＴｏｏｌｓ－ＭＴＥＸＯＤＦ解析比較

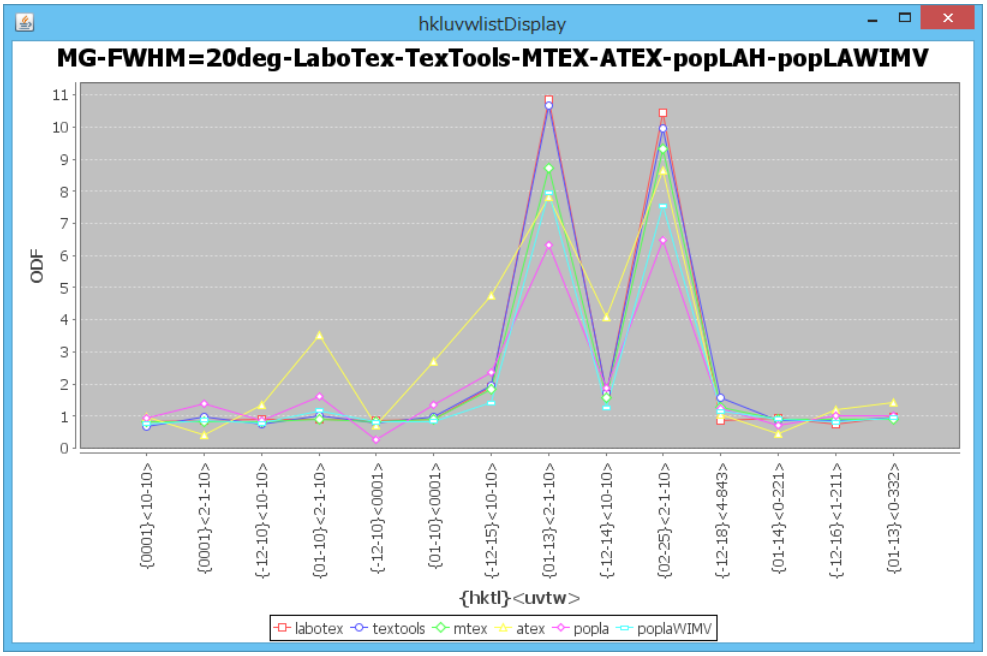
＋ＡＴＥＸ＋ｐｏｐＬＡ比較

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

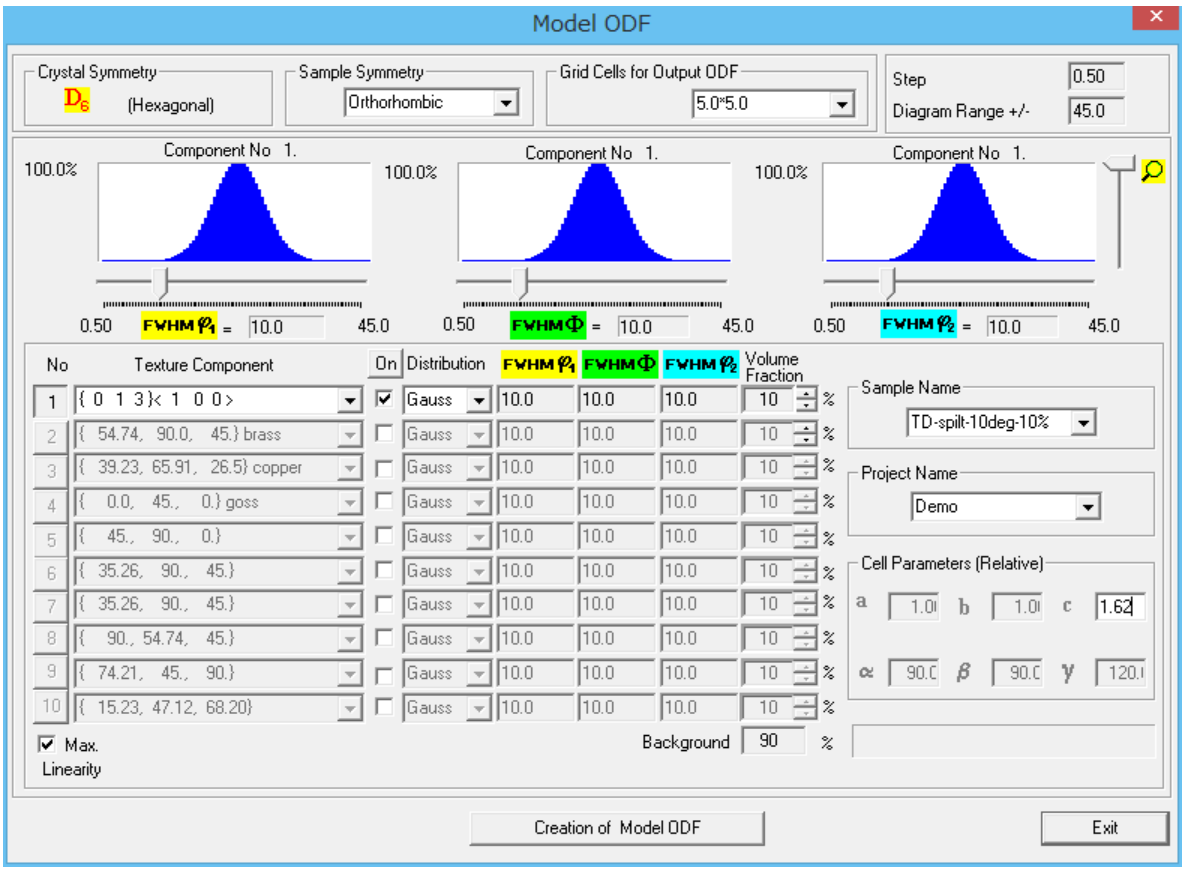
ＨｅｌｐｅｒＴｅｘ　Ｏｆｆｉｃｅ

概要

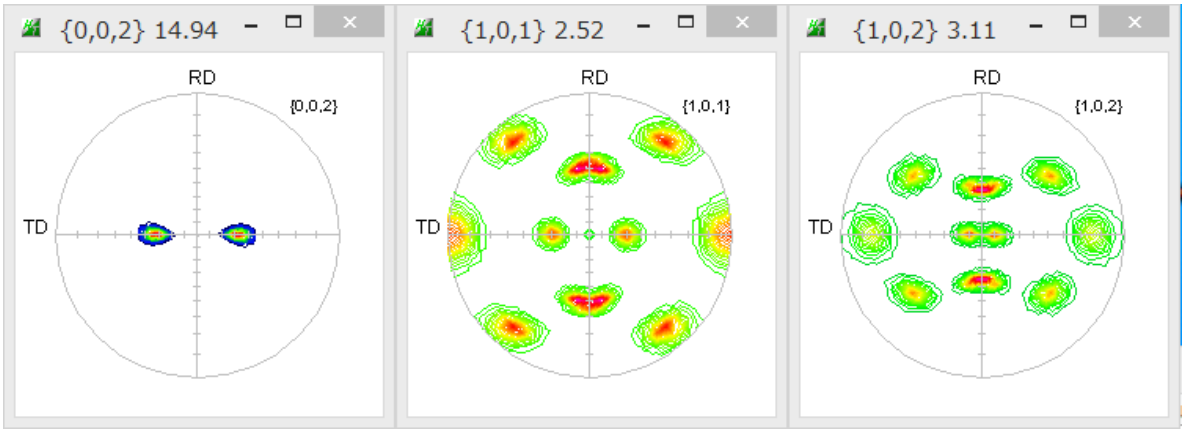
ＴＤ－ｓｐｌｉｔに関し、ＯＤＦの半価幅が 10deg の場合、LaboTex と MTEX の解析結果が異なり半価幅が 20deg の場合、一致する事が確認されている。又、ODF 解析結果の結晶方位位置がずれる事が確認されている。

今回、TexTools も比較してみました。

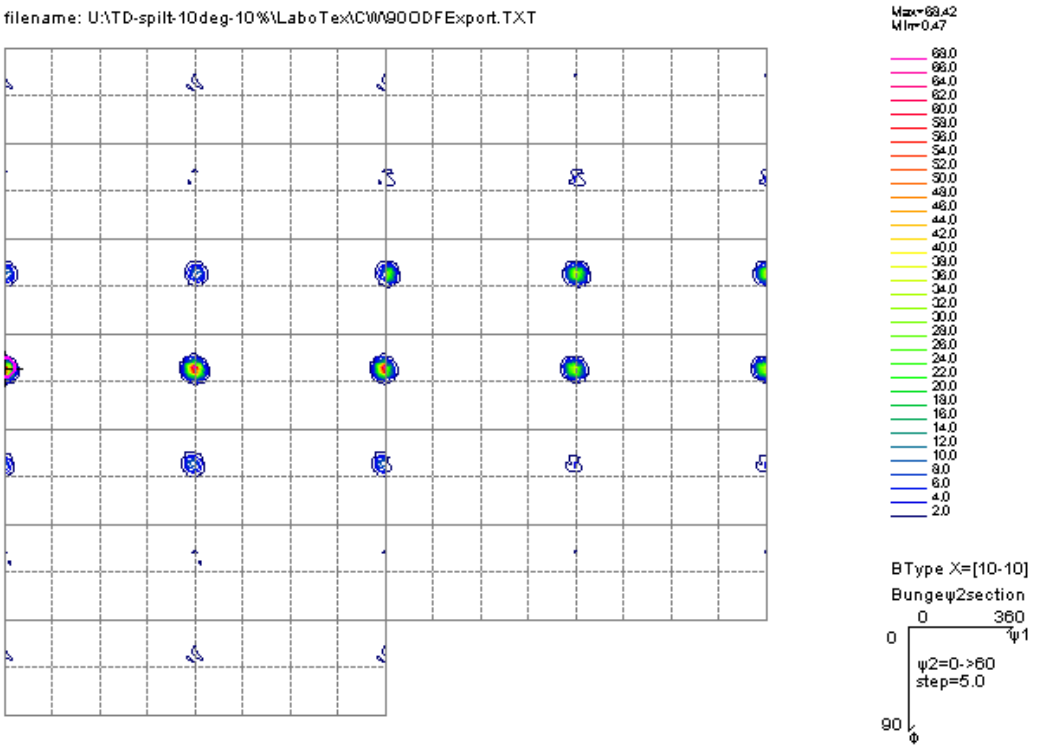
極点図作成

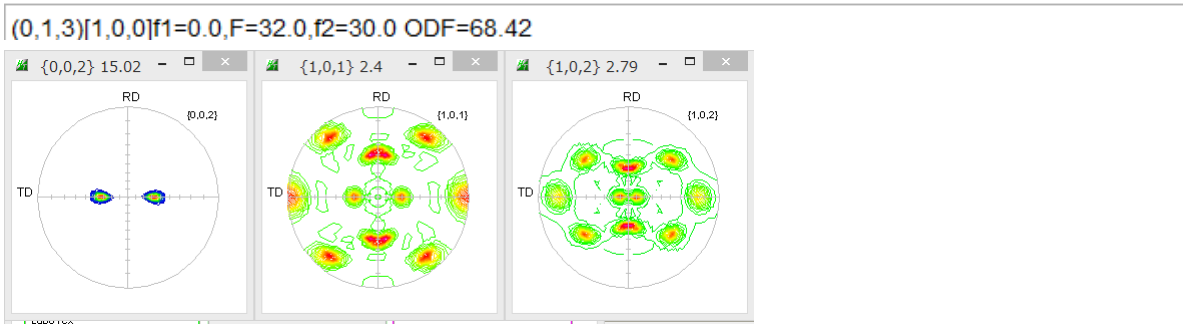


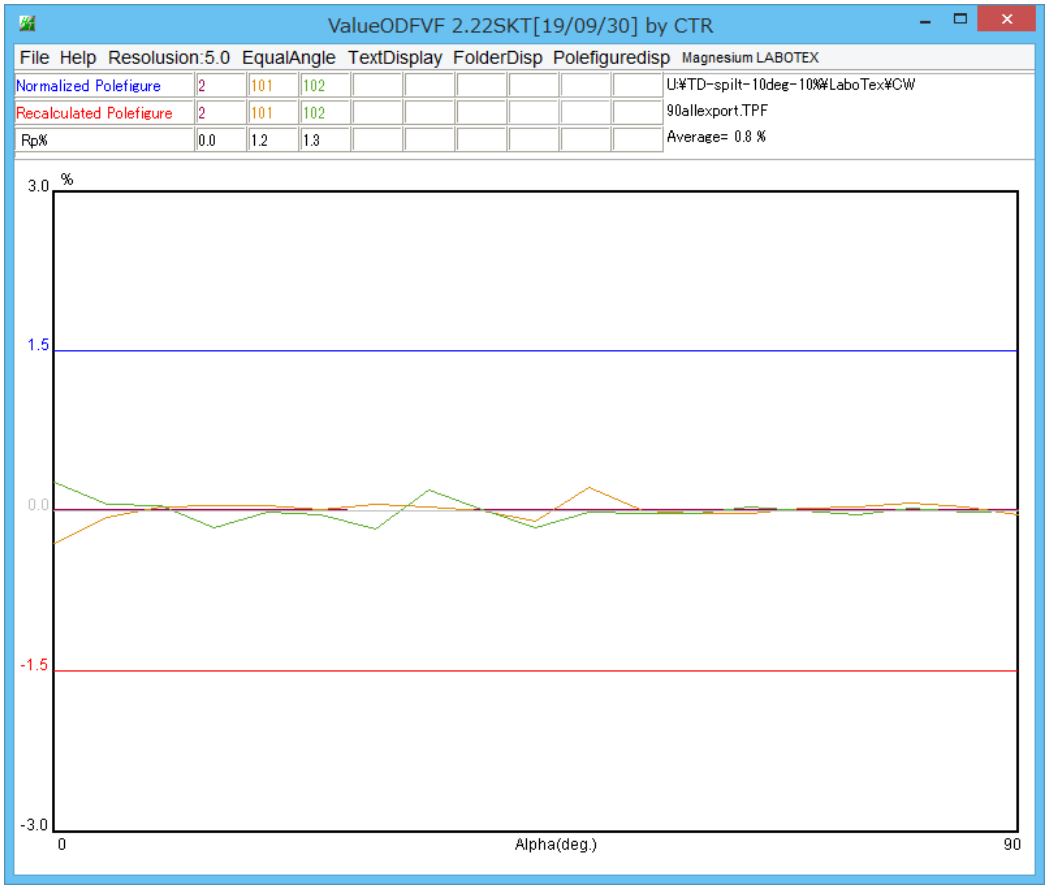
作成される極点図



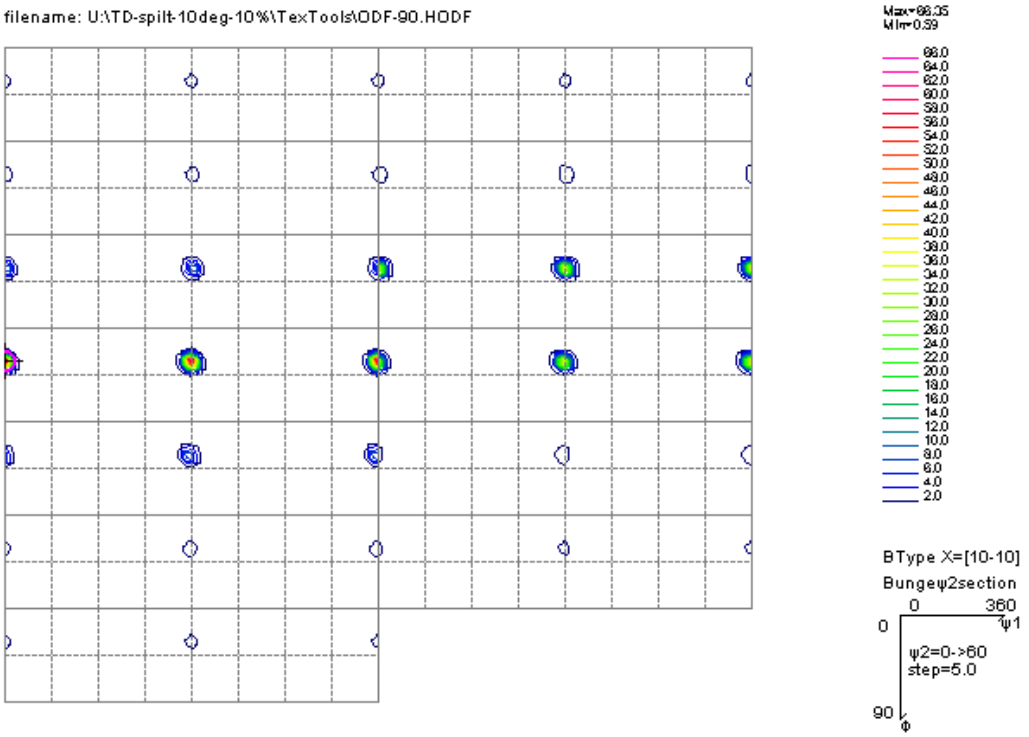
ＬａｂｏＴｅｘ解析結果



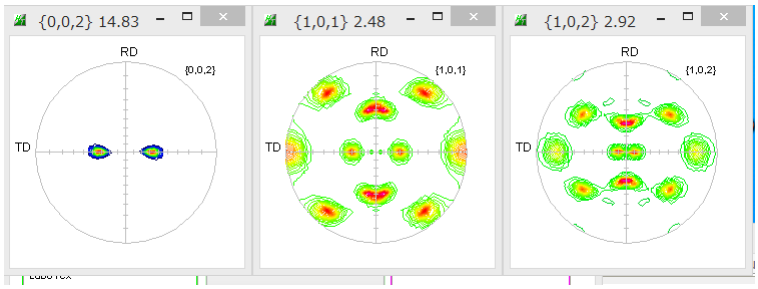


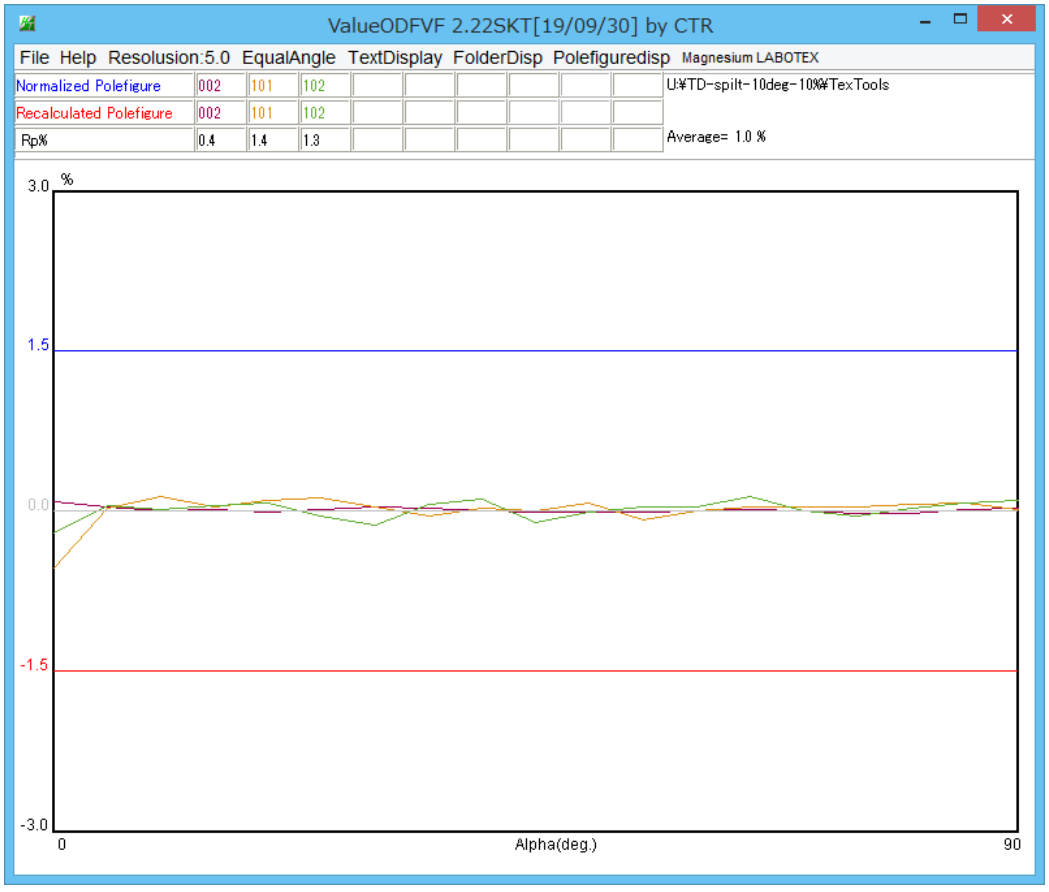


ＴｅｘＴｏｏｌｓ解析結果

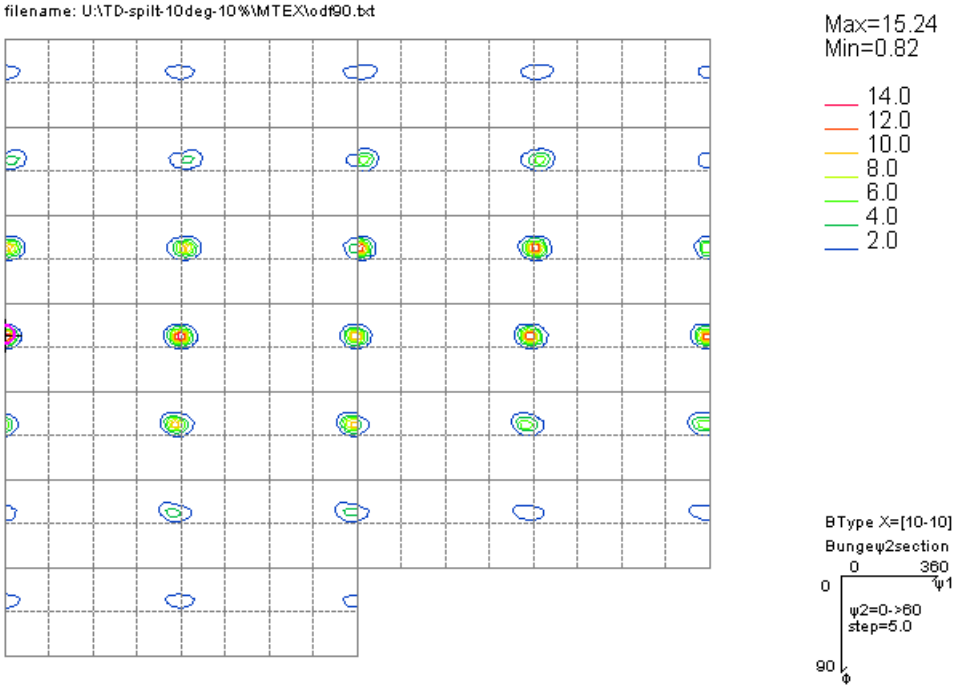


(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=66.35

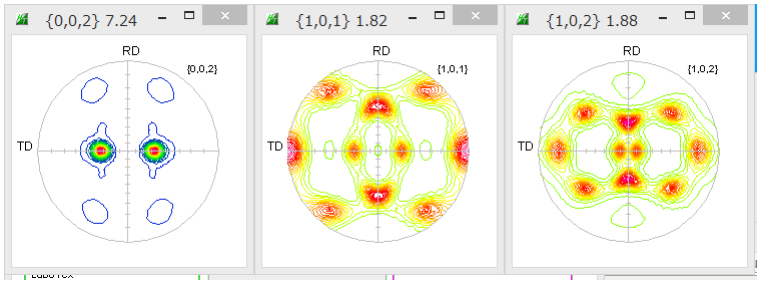


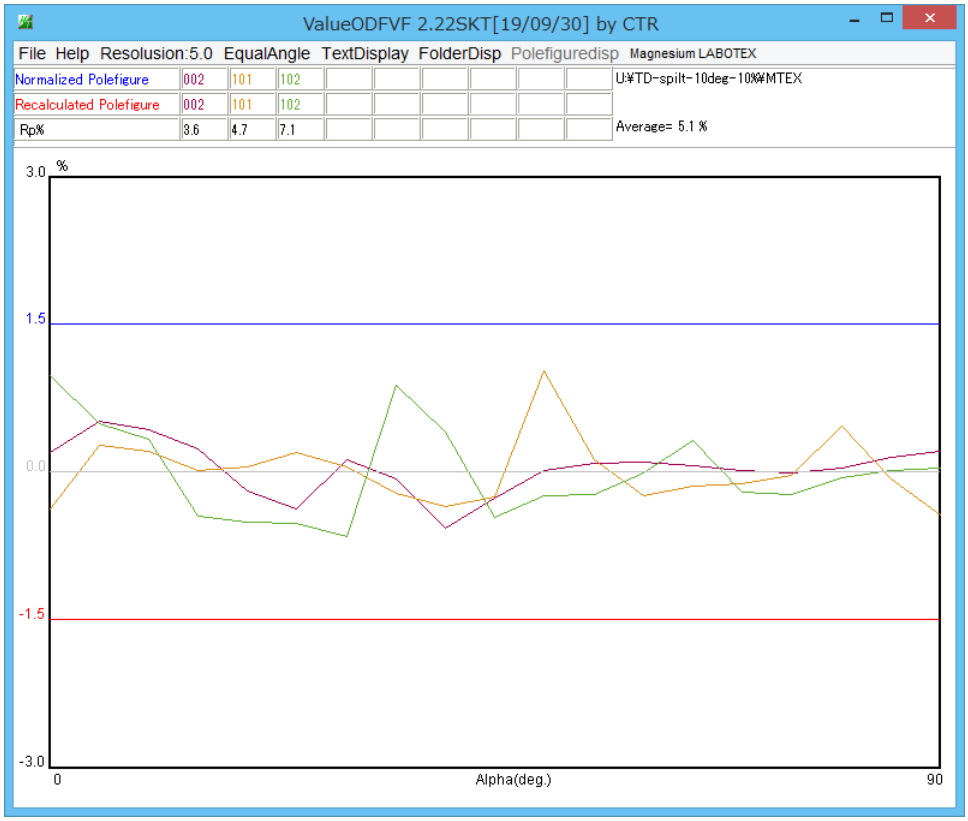


ＭＴＥＸの解析結果



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

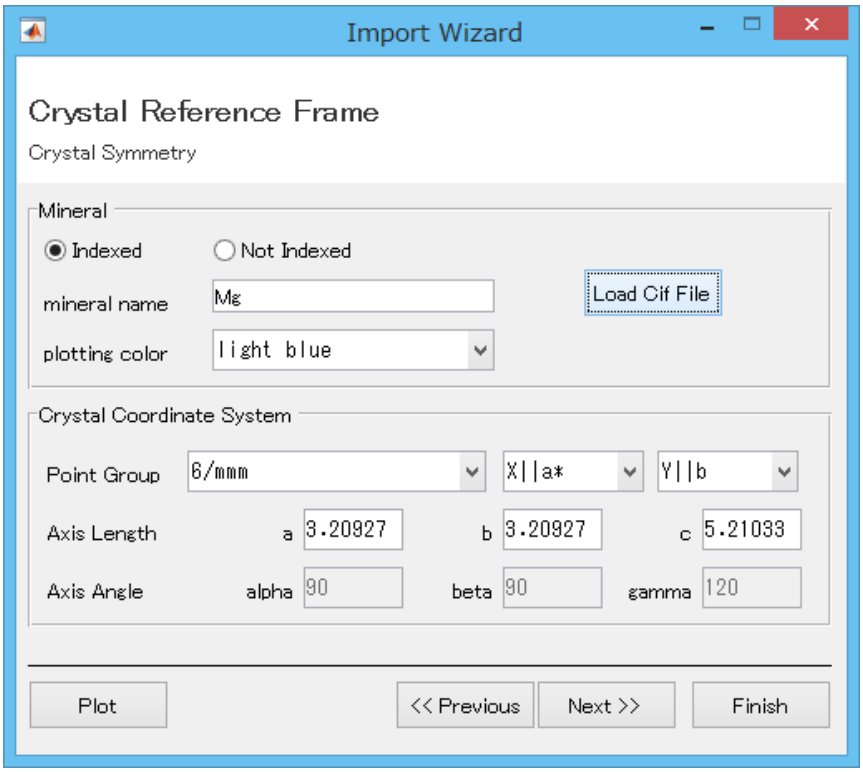




ＬａｂｏＴｅｘ，ＴｅｘＴｏｏｌｓに比べ、バタバタしている

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

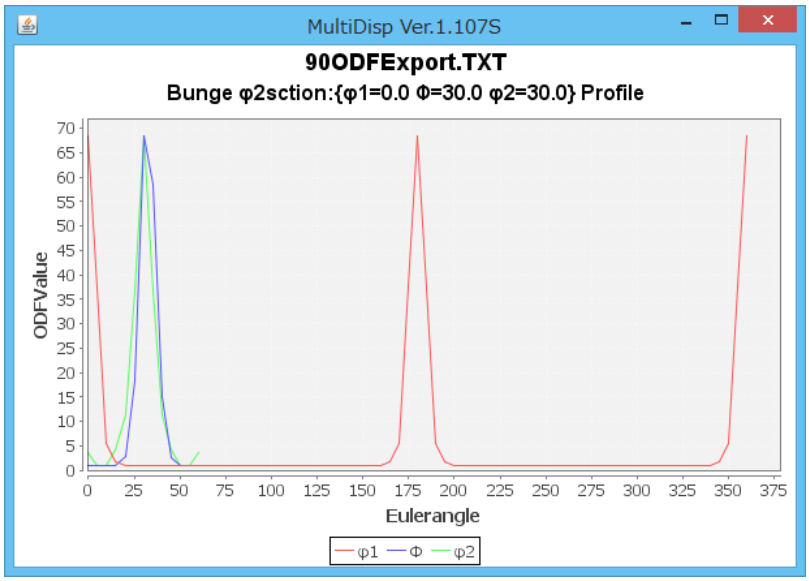
取り込まれる値は

```
>> 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
```

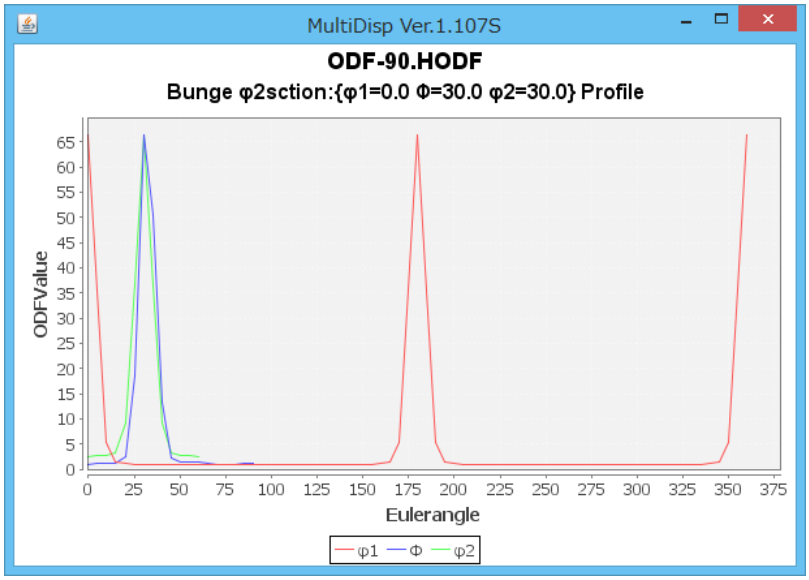
ｃ／ａは一致している。

方位の広がり

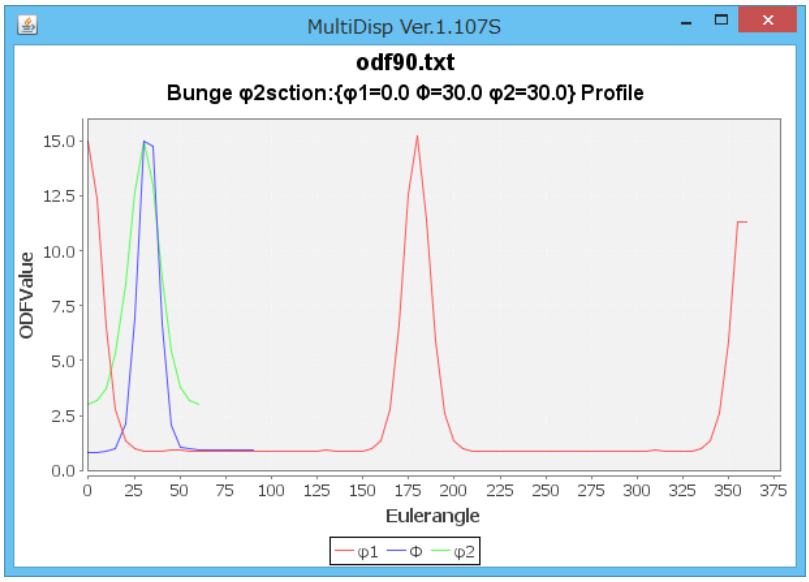
ＬａｂｏＴｅｘ



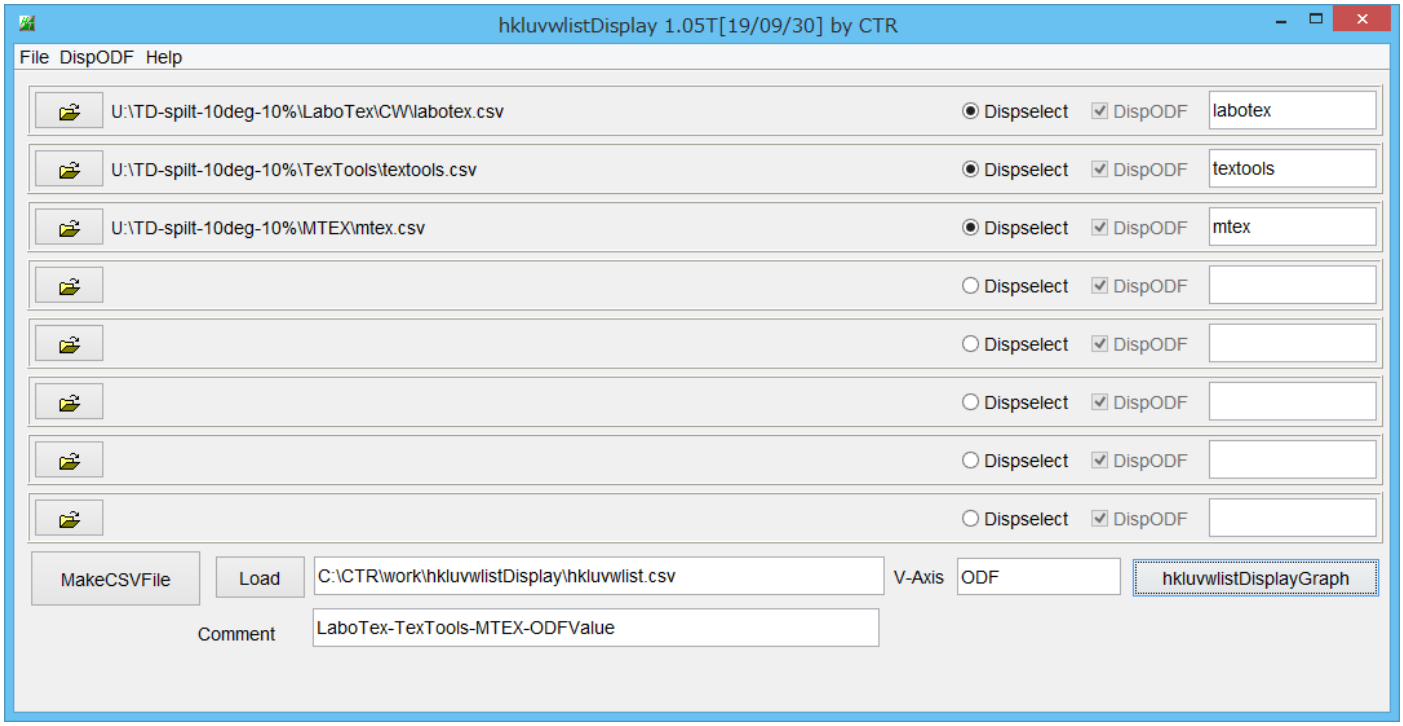
ＴｅｘＴｏｏｌｓ

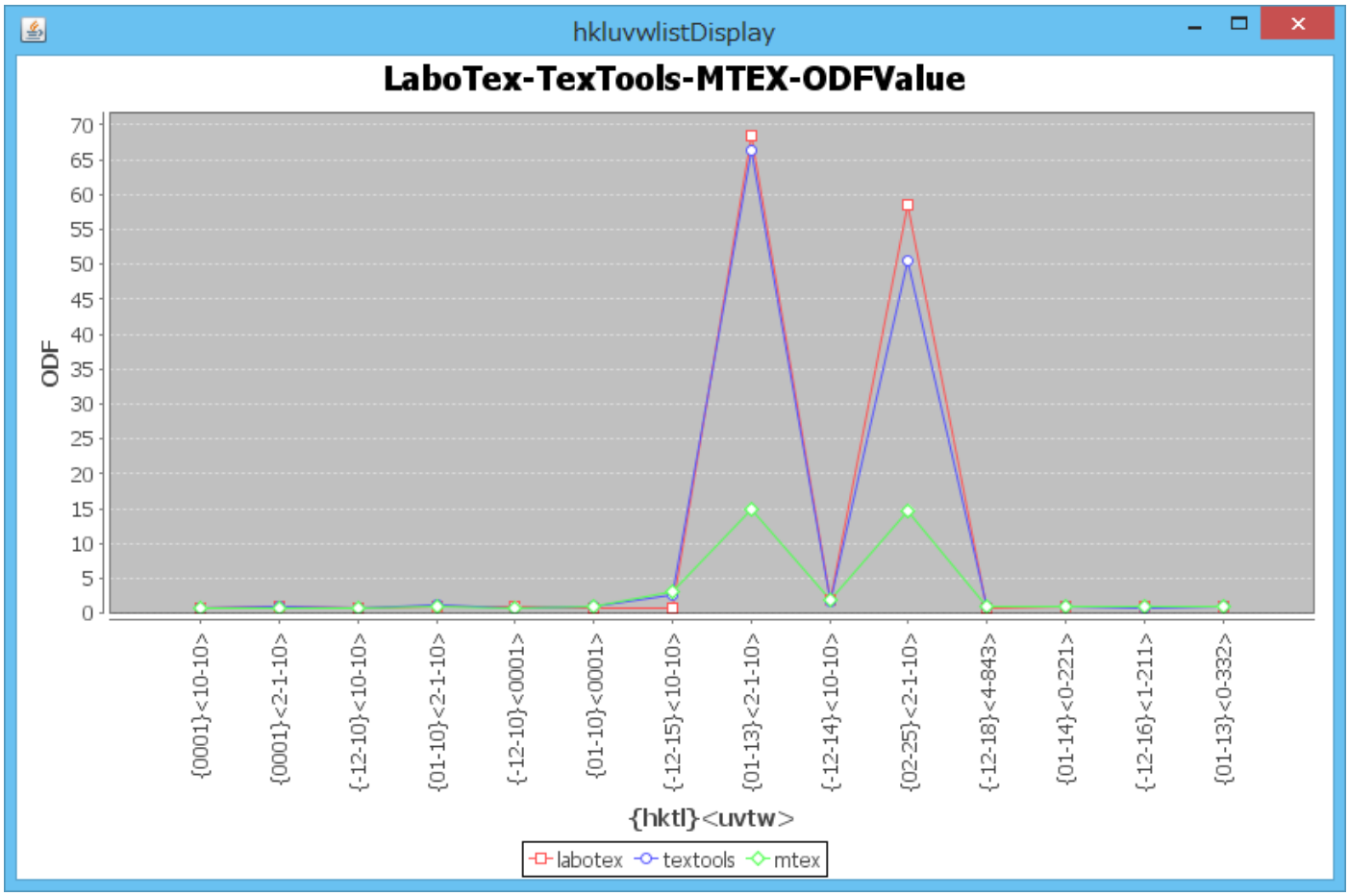


ＭＴＥＸ



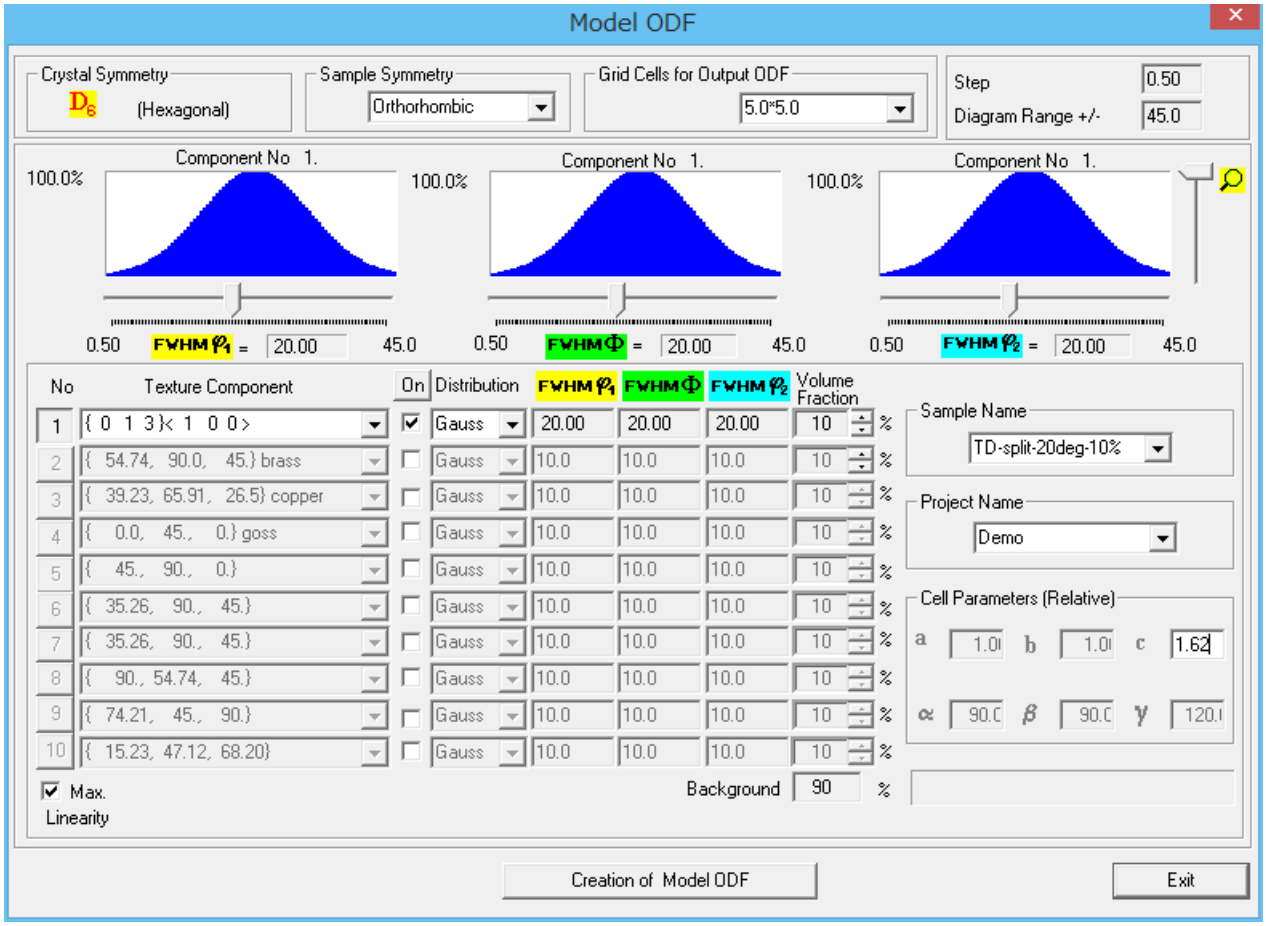
結晶方位プロファイル比較



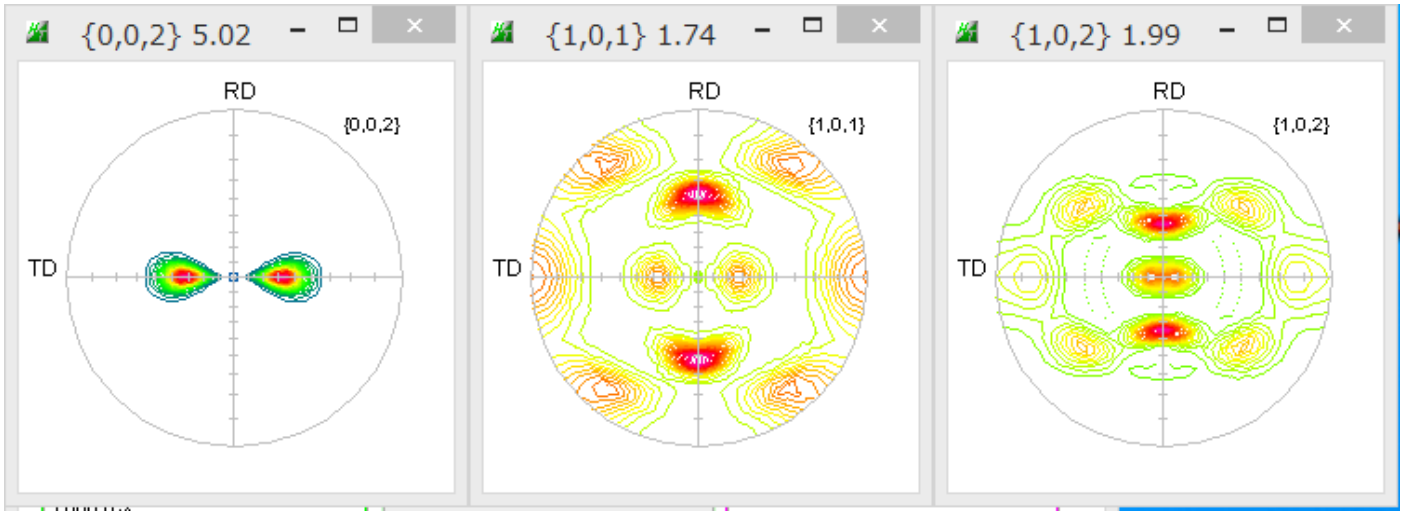



```
0 1 -1 3 2 -1  -1 0 0.0 32.02 30.0
-1 2 -1 4 1 0  -1 0 0.0 39.089 0.0
0 2 -2 5 2 -1  -1 0 0.0 36.885 30.0
```

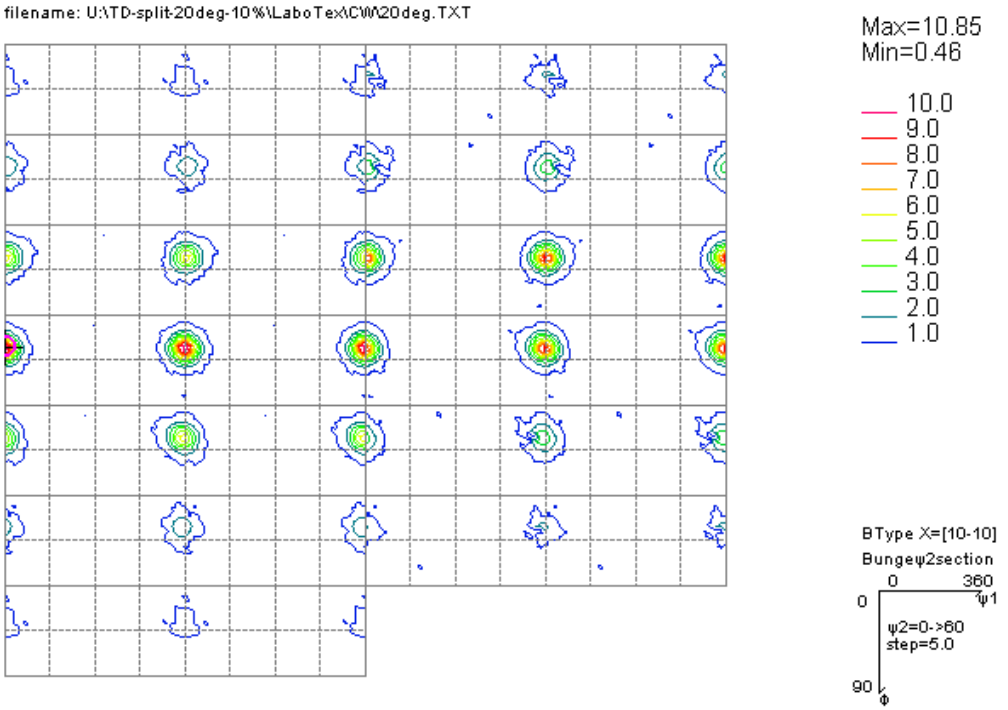
半価幅２０ｄｅｇの場合



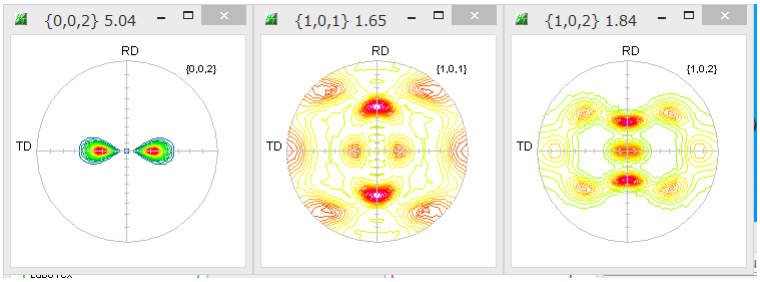
作成される極点図

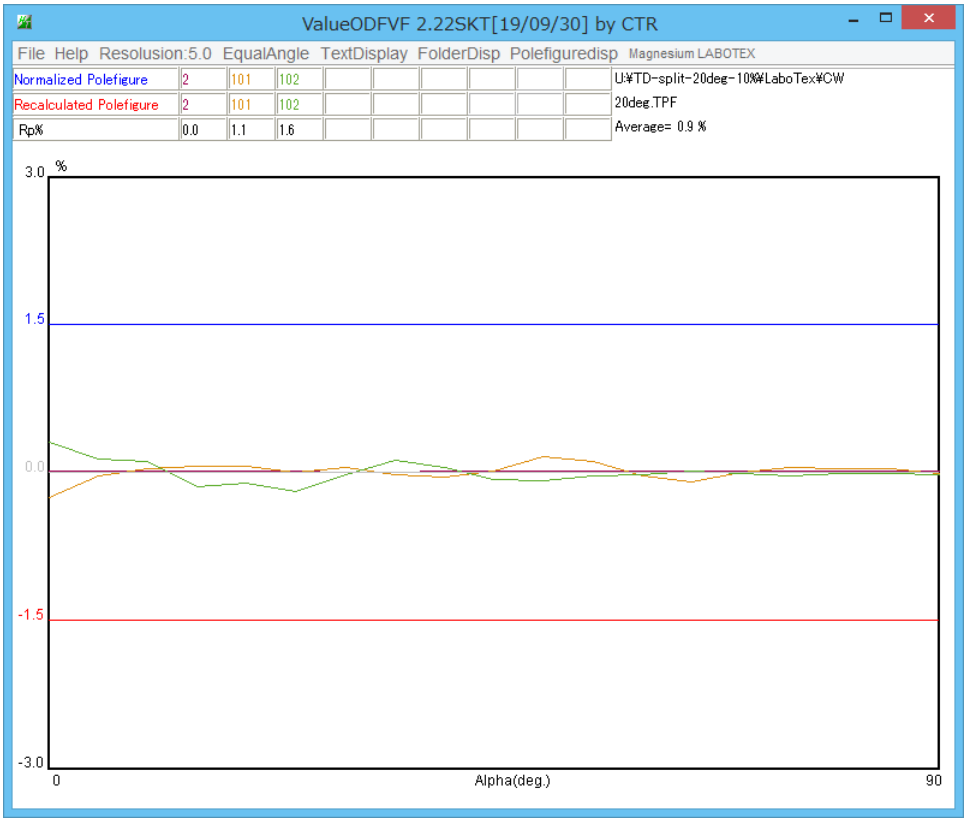


ＦＷＨＭ２０ｄｅｇをＬａｂｏＴｅｘ解析結果

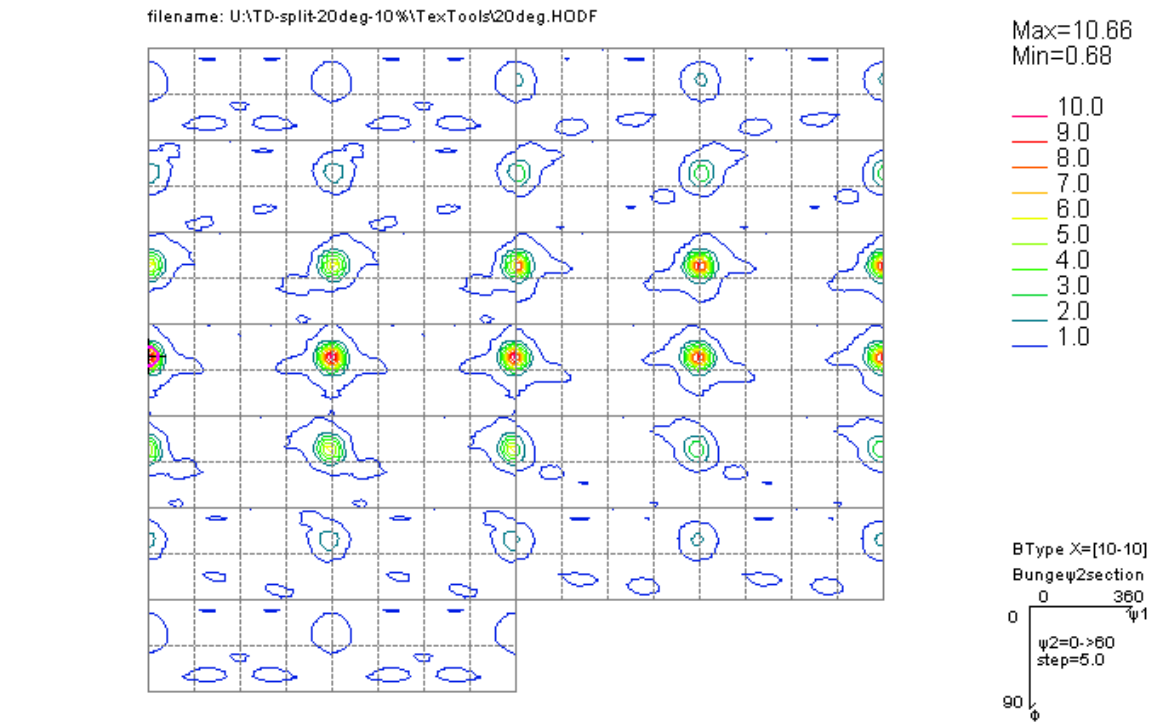


(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=10.85

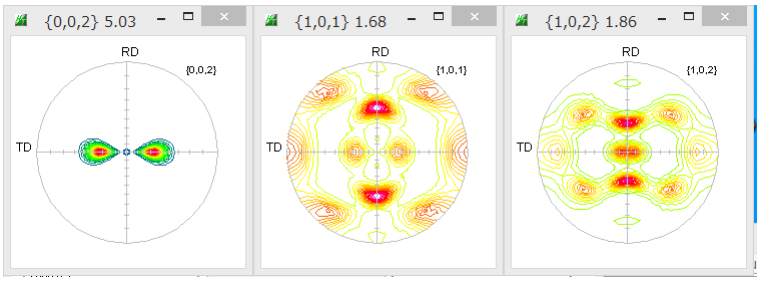


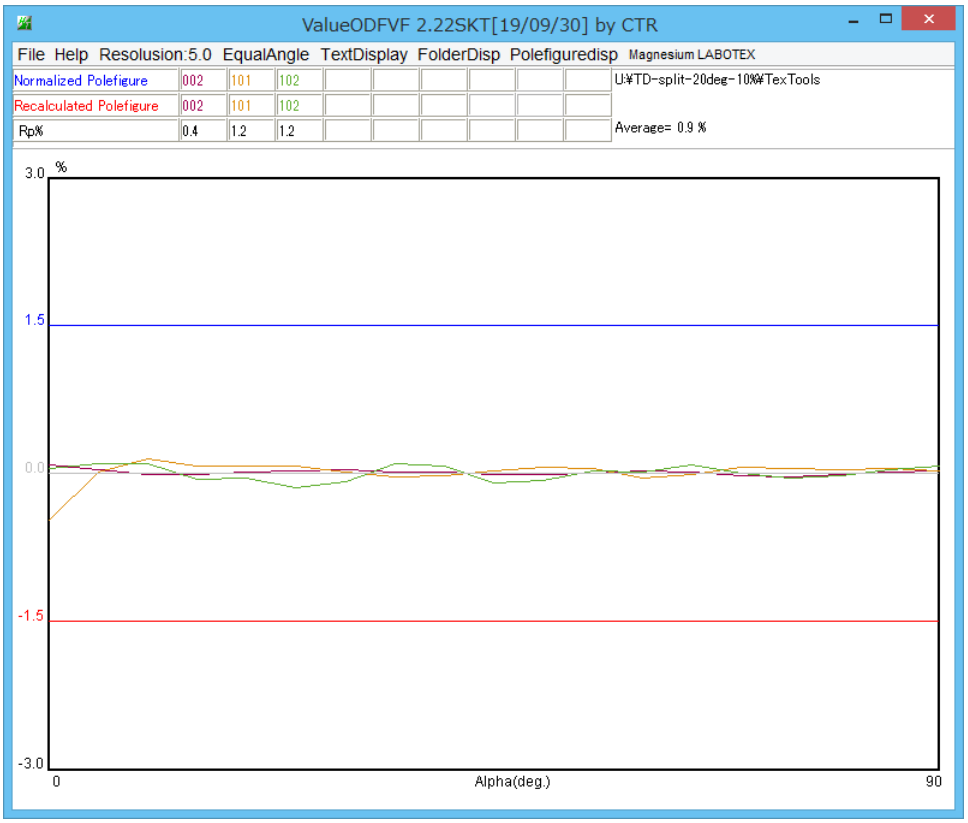


２０ｄｅｇをＴｅｘＴｏｏｌｓ解析結果

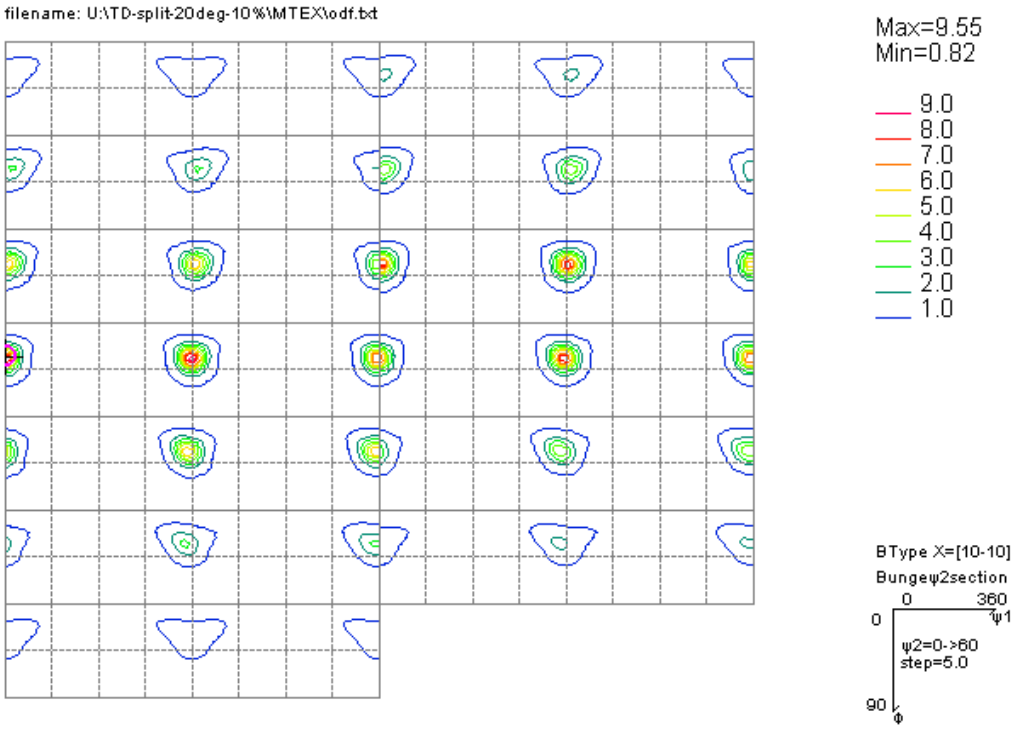


(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=10.66

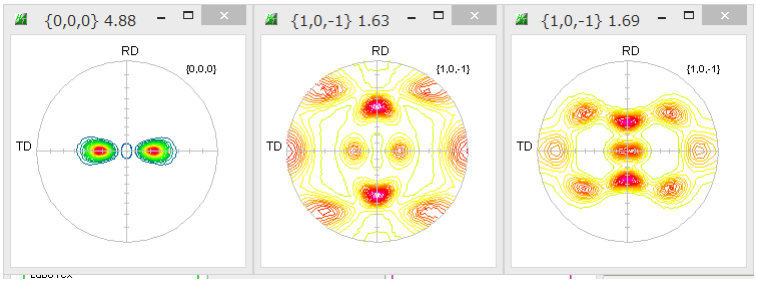


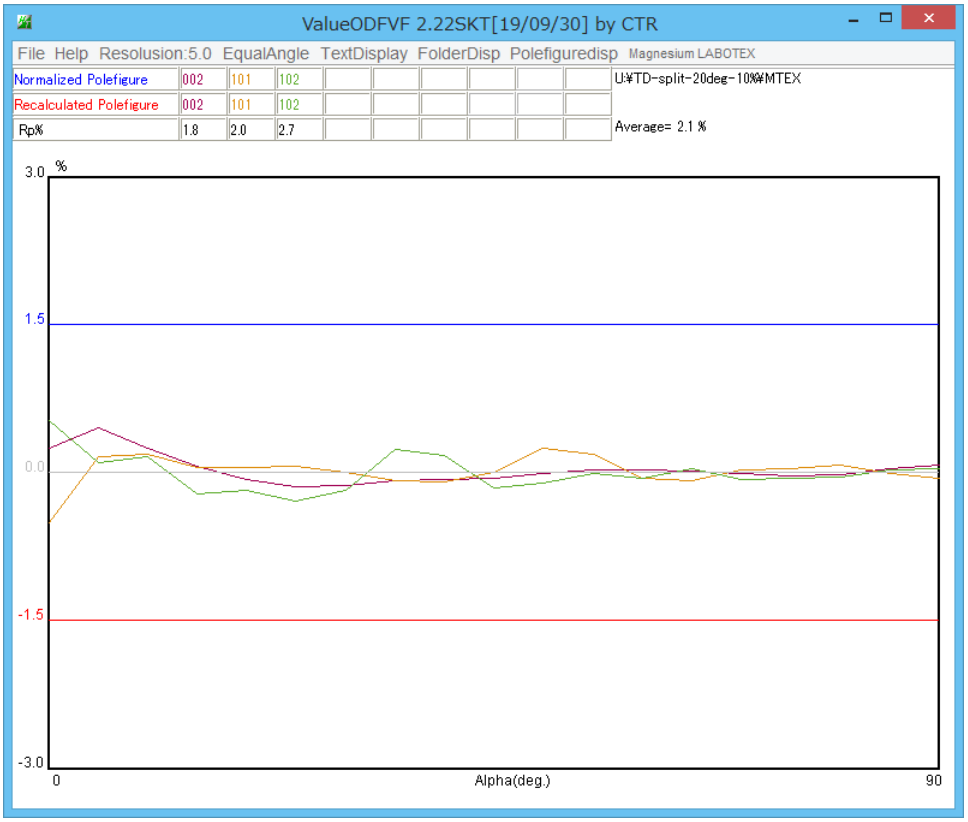


２０ｄｅｇをＭＴＥＸ解析結果



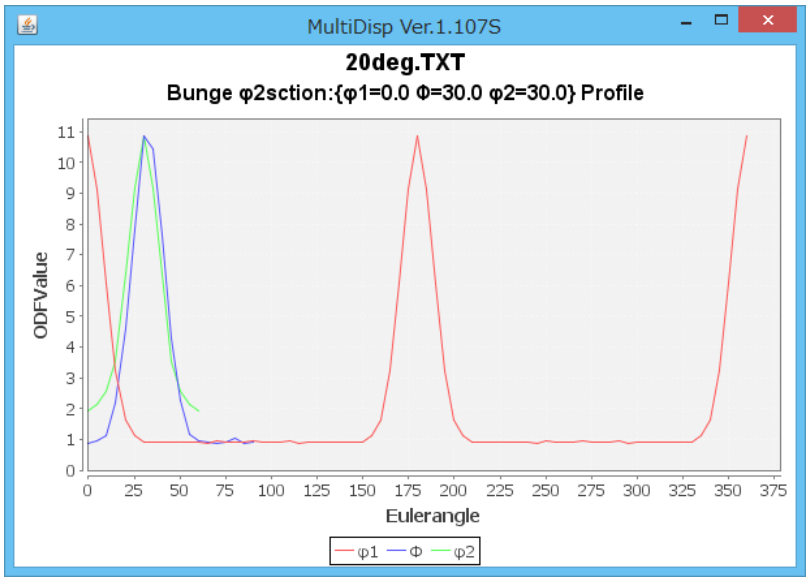
(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=8.74



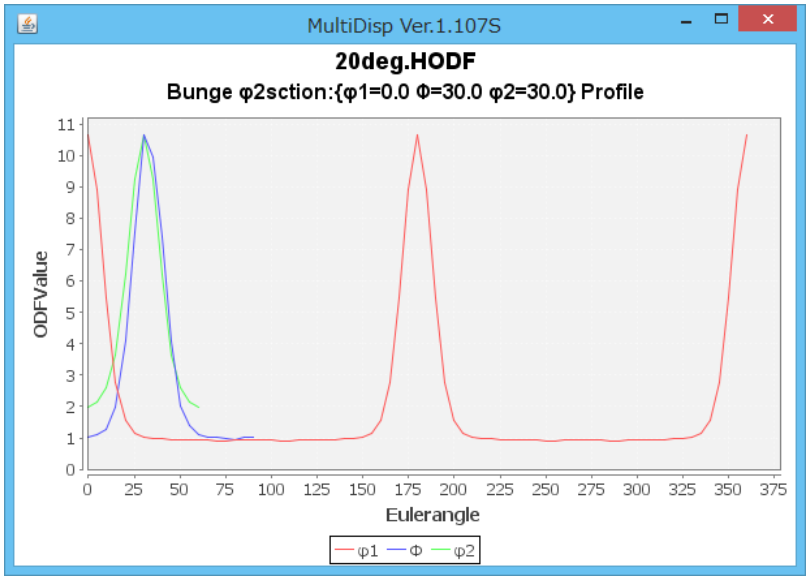


方位の広がり

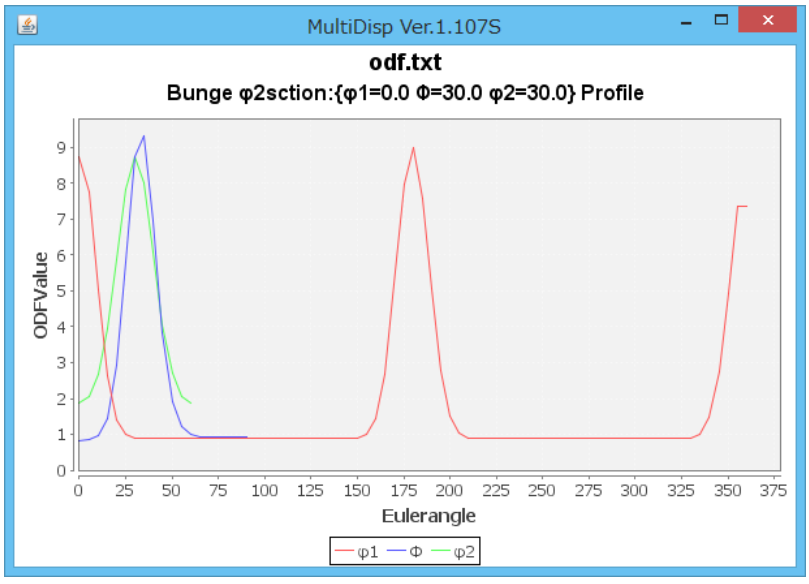
ＬａｂｏＴｅｘ



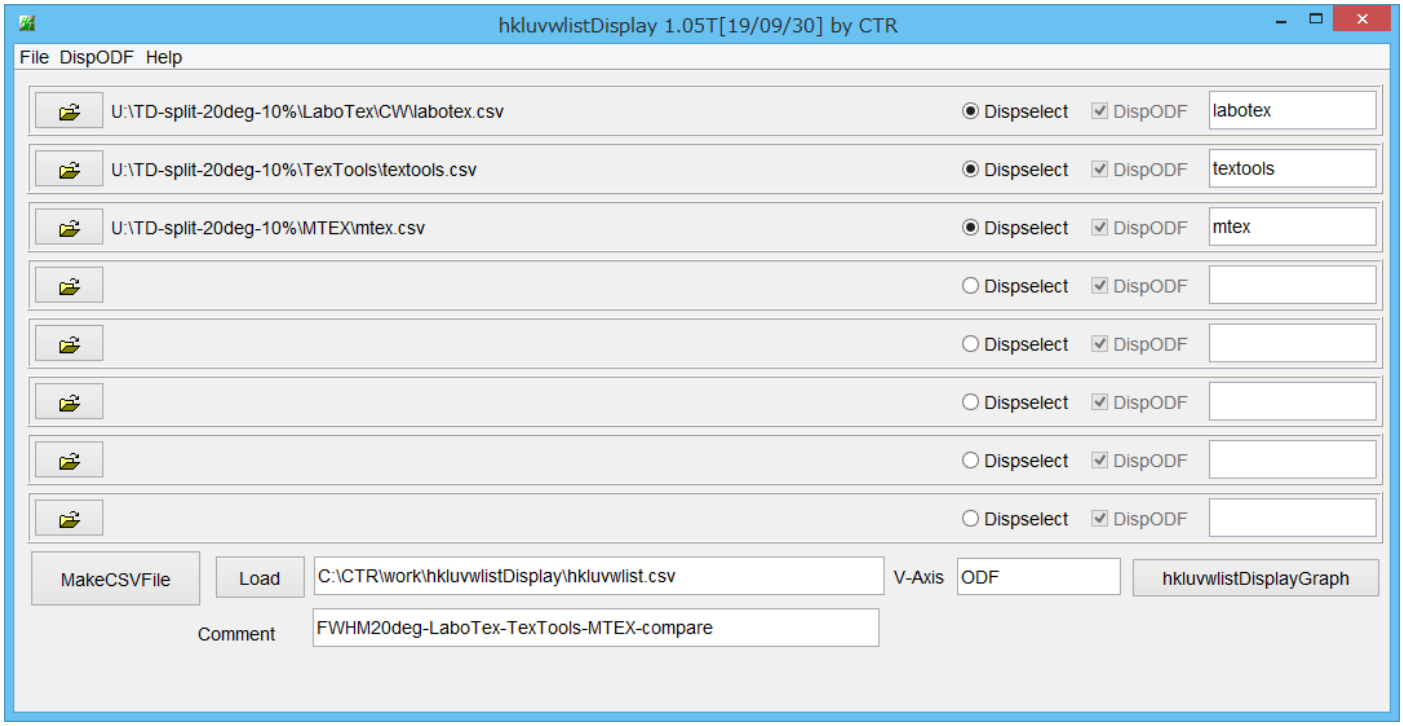
ＴｅｘＴｏｏｌｓ

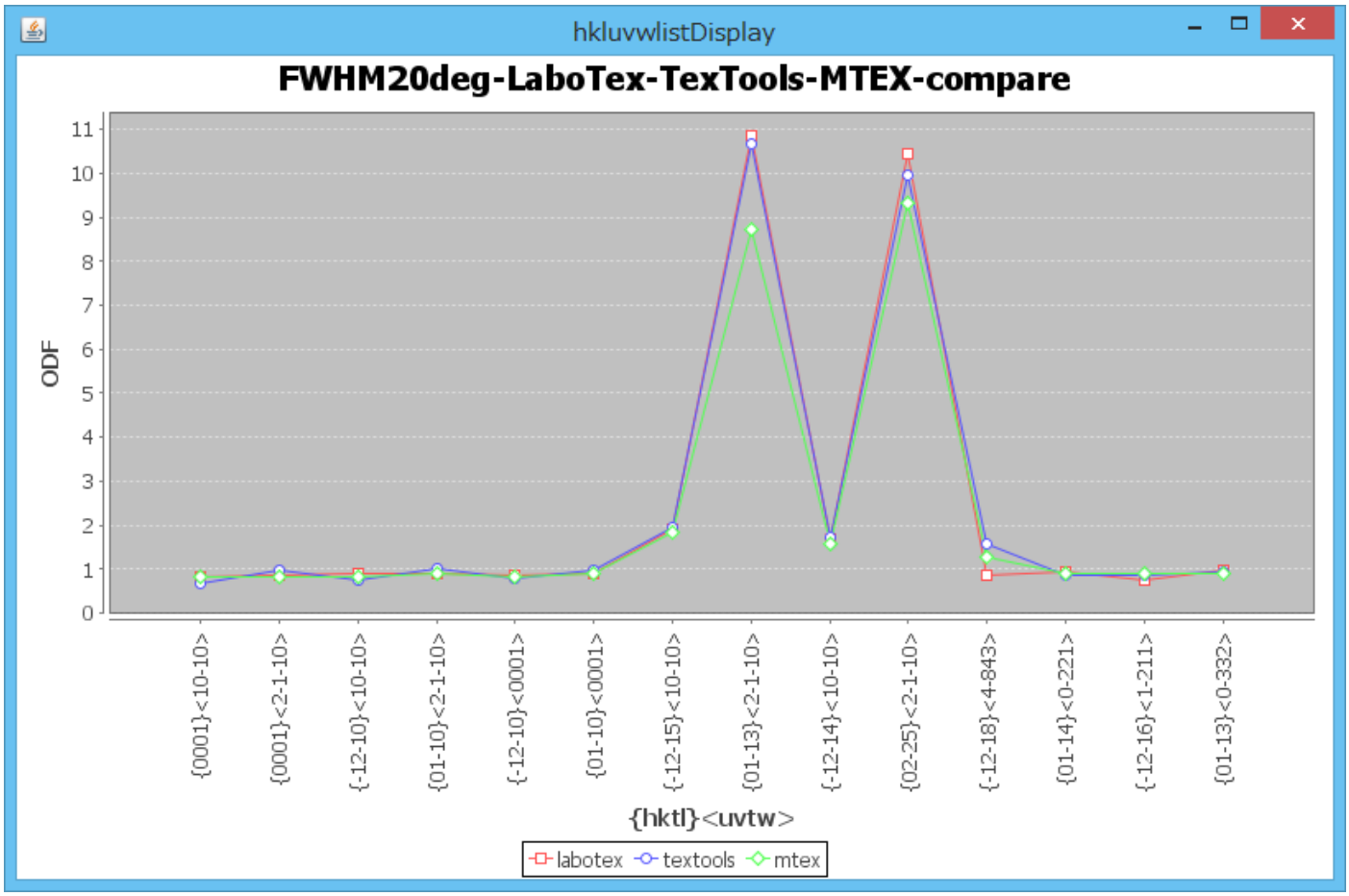


ＭＴＥＸ

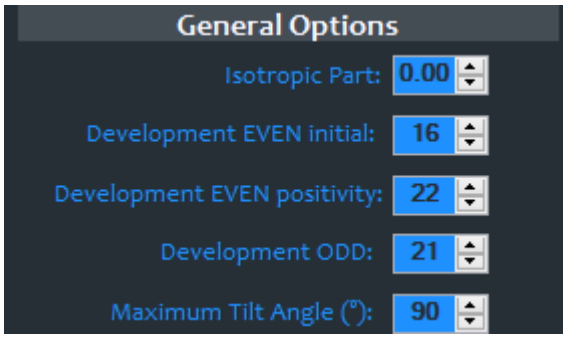


結晶方位プロファイル比較

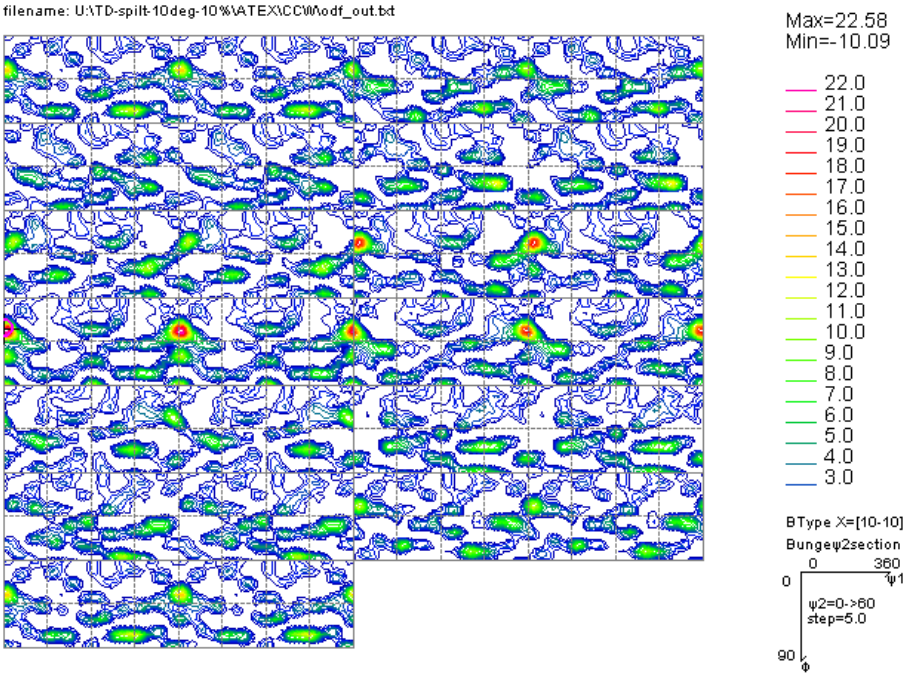




ＡＴＥＸによる解析

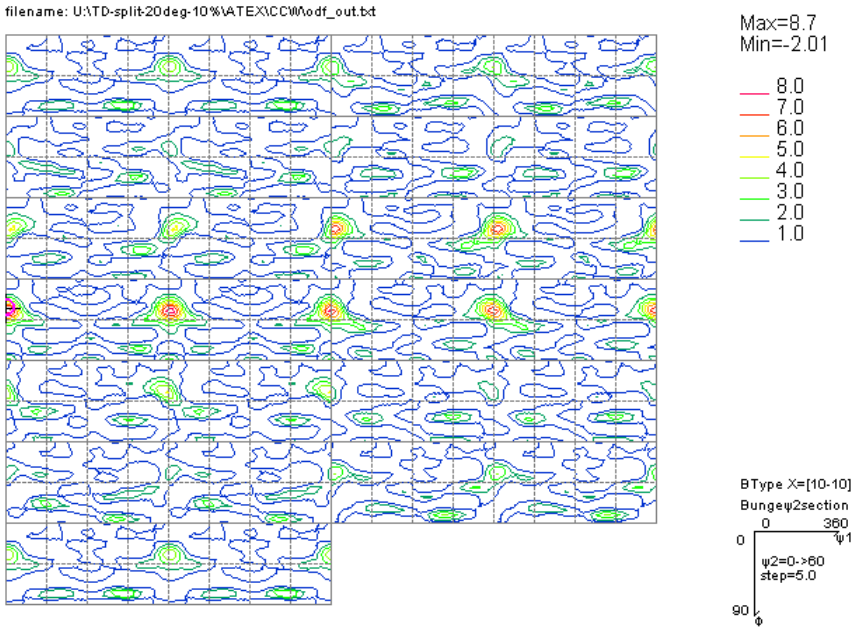


FWHM=10deg

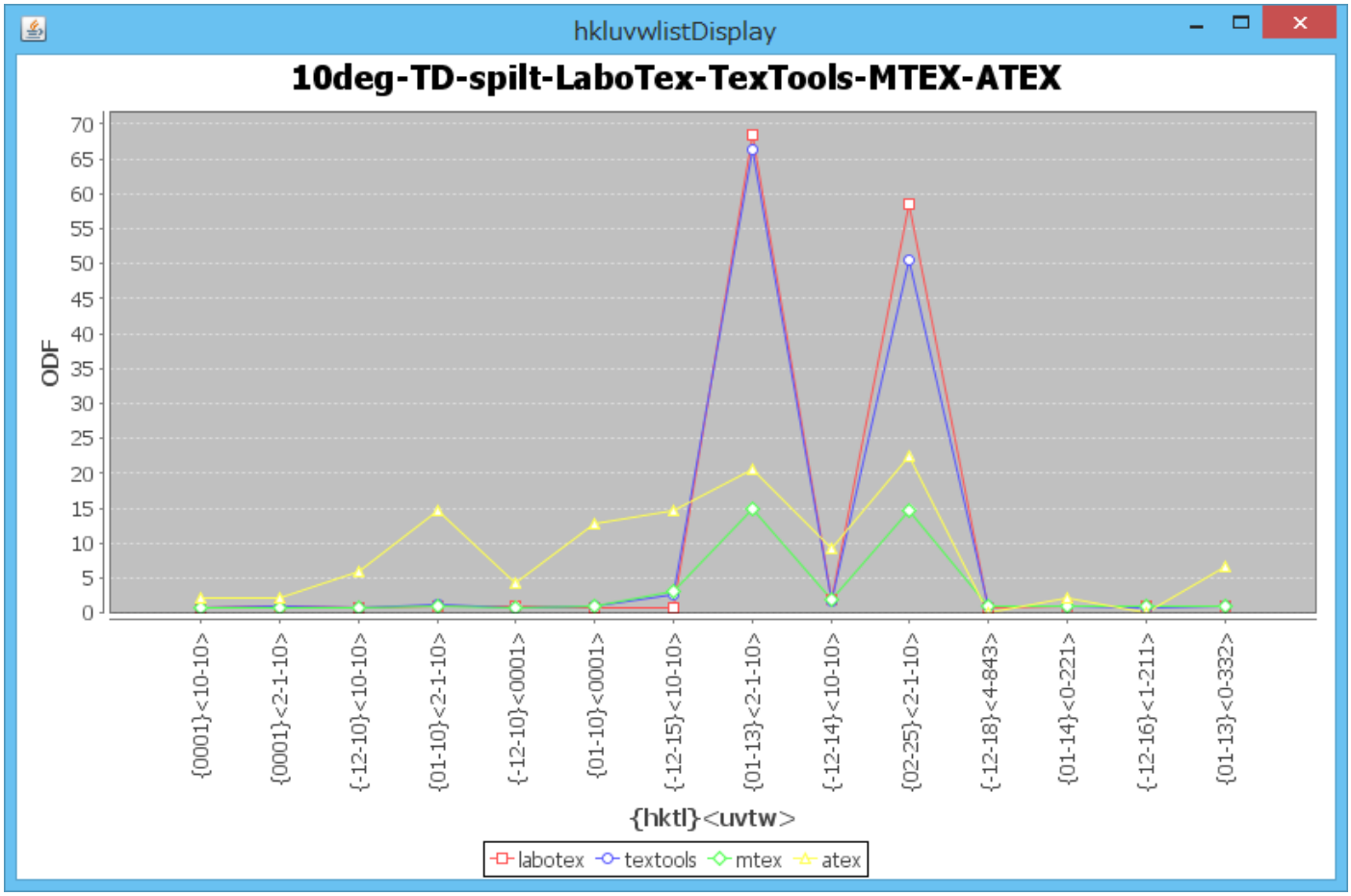


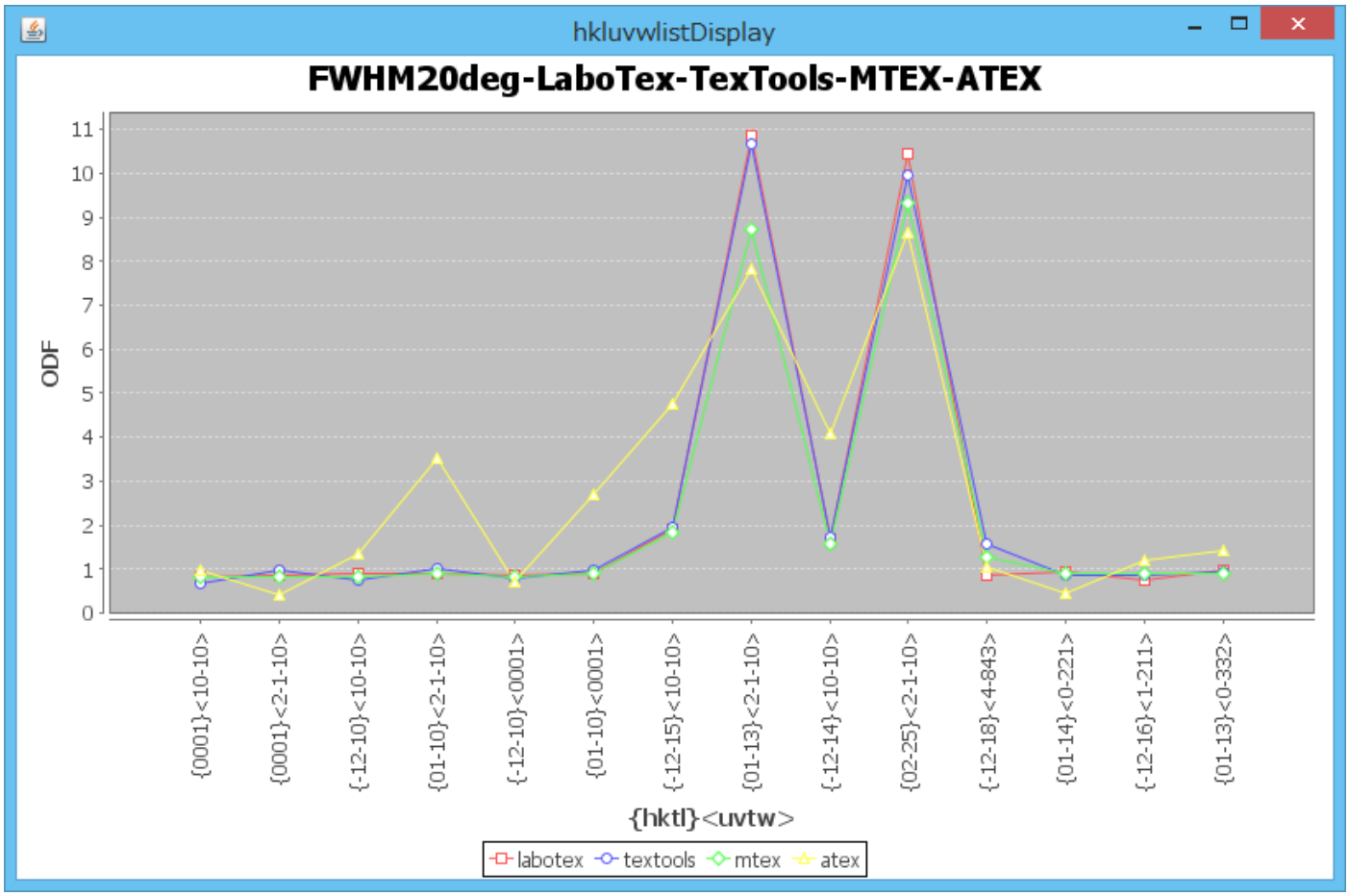
(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=20.56

FWHM=20deg



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


hkluvwlistDisplay
10deg-TD-spilt-LaboTex-TexTools-MTEX-ATEX
ODF
{hktl}<uvtw>
{0001}<10-10>
{0001}<2-1-10>
{-12-10}<10-10>
{01-10}<2-1-10>
{-12-10}<0001>
{01-10}<0001>
{-12-15}<10-10>
{01-13}<2-1-10>
{-12-14}<10-10>
{02-25}<2-1-10>
{-12-18}<4-843>
{01-14}<0-221>
{-12-16}<1-211>
{01-13}<0-332>
labotex
textools
mtex
atex


hkluvwlistDisplay
FWHM20deg-LaboTex-TexTools-MTEX-ATEX
ODF
{hktl}<uvtw>
{0001}<10-10>
{0001}<2-1-10>
{-12-10}<10-10>
{01-10}<2-1-10>
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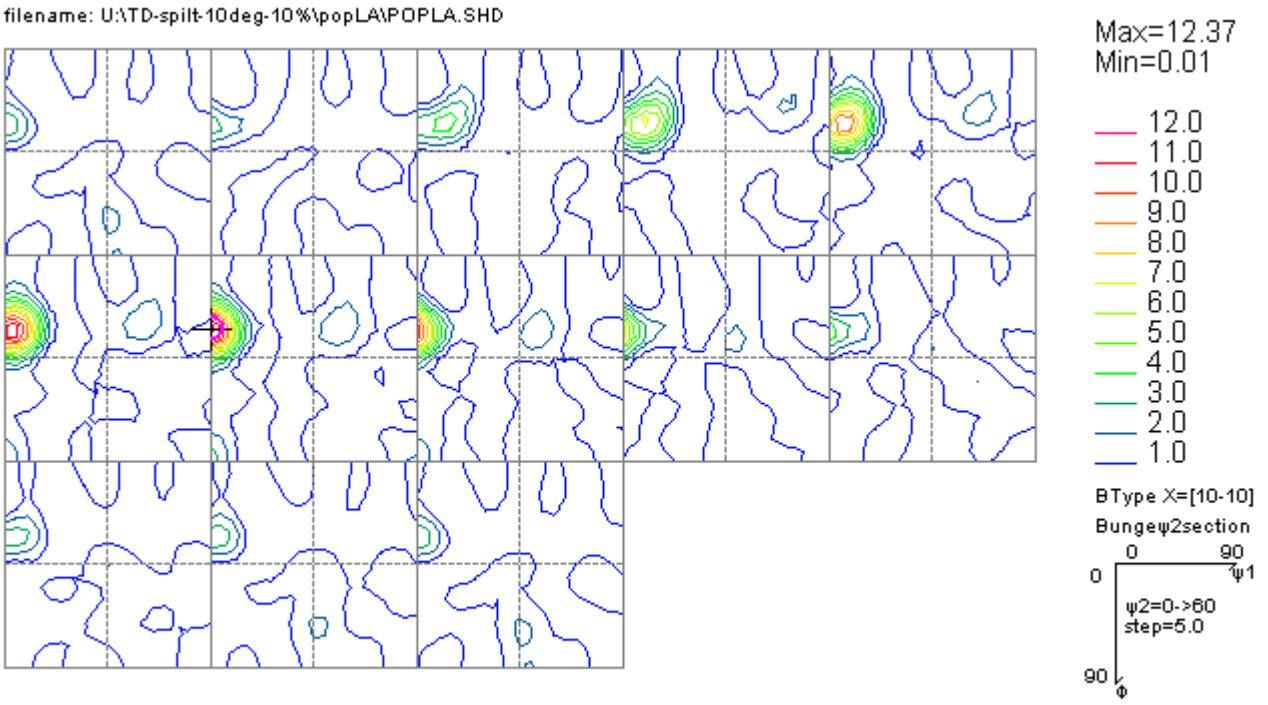
{01-10}<0001>
{-12-15}<10-10>
{01-13}<2-1-10>
{-12-14}<10-10>
{02-25}<2-1-10>
{-12-18}<4-843>
{01-14}<0-221>
{-12-16}<1-211>
{01-13}<0-332>
labotex
textools
mtex
atex

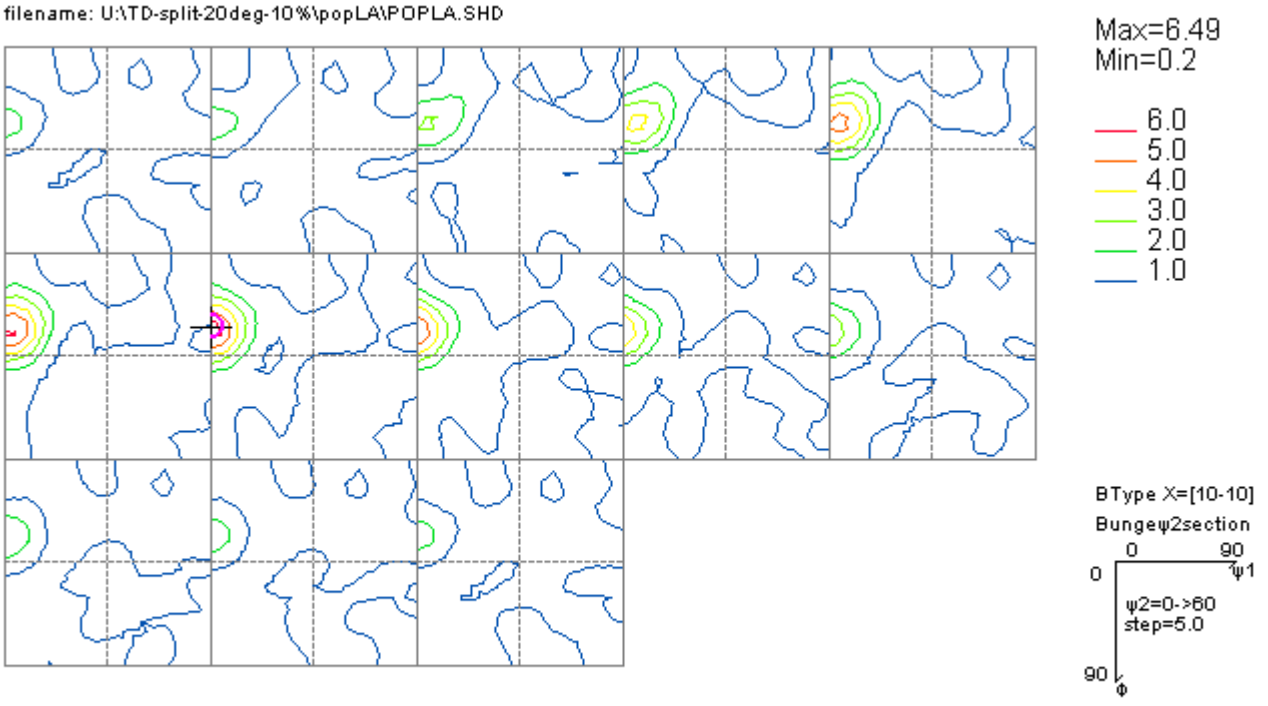
p o p L A H e r m o n i c

FWHM=10deg



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

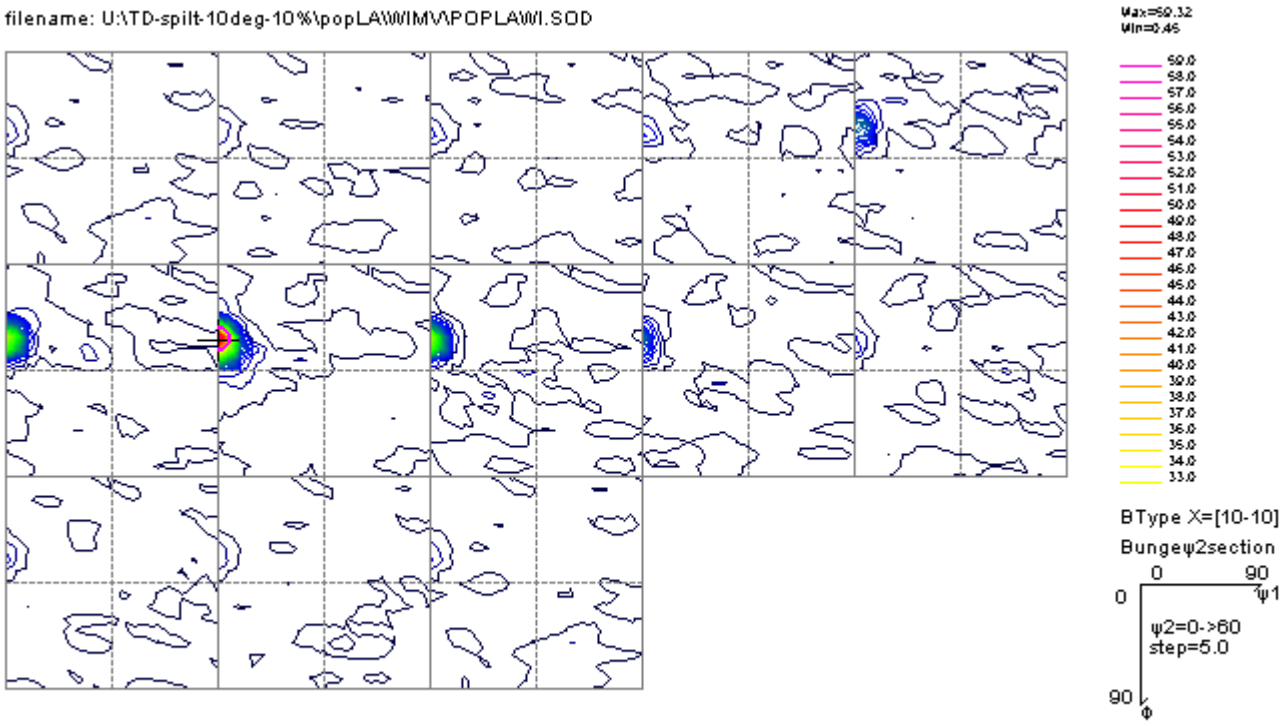
FWHM=20deg



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

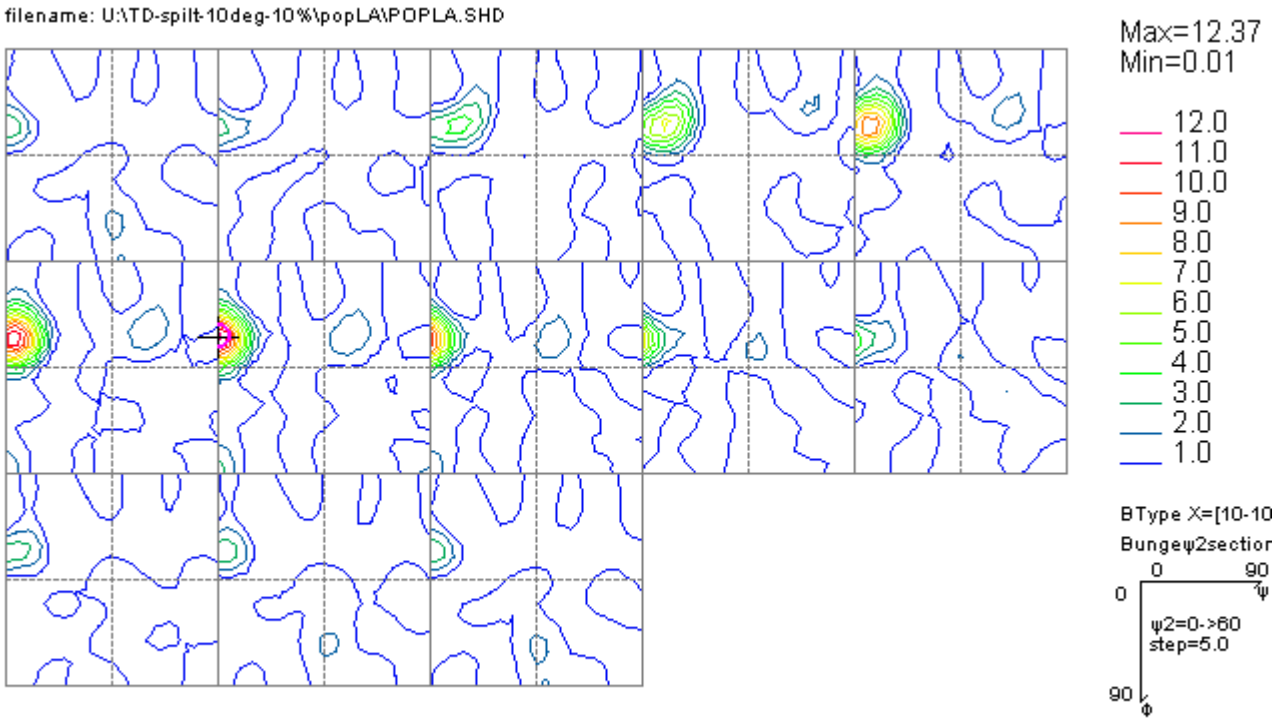
ｐｏｐＬＡＷＩＭＶ

FWHM=10deg

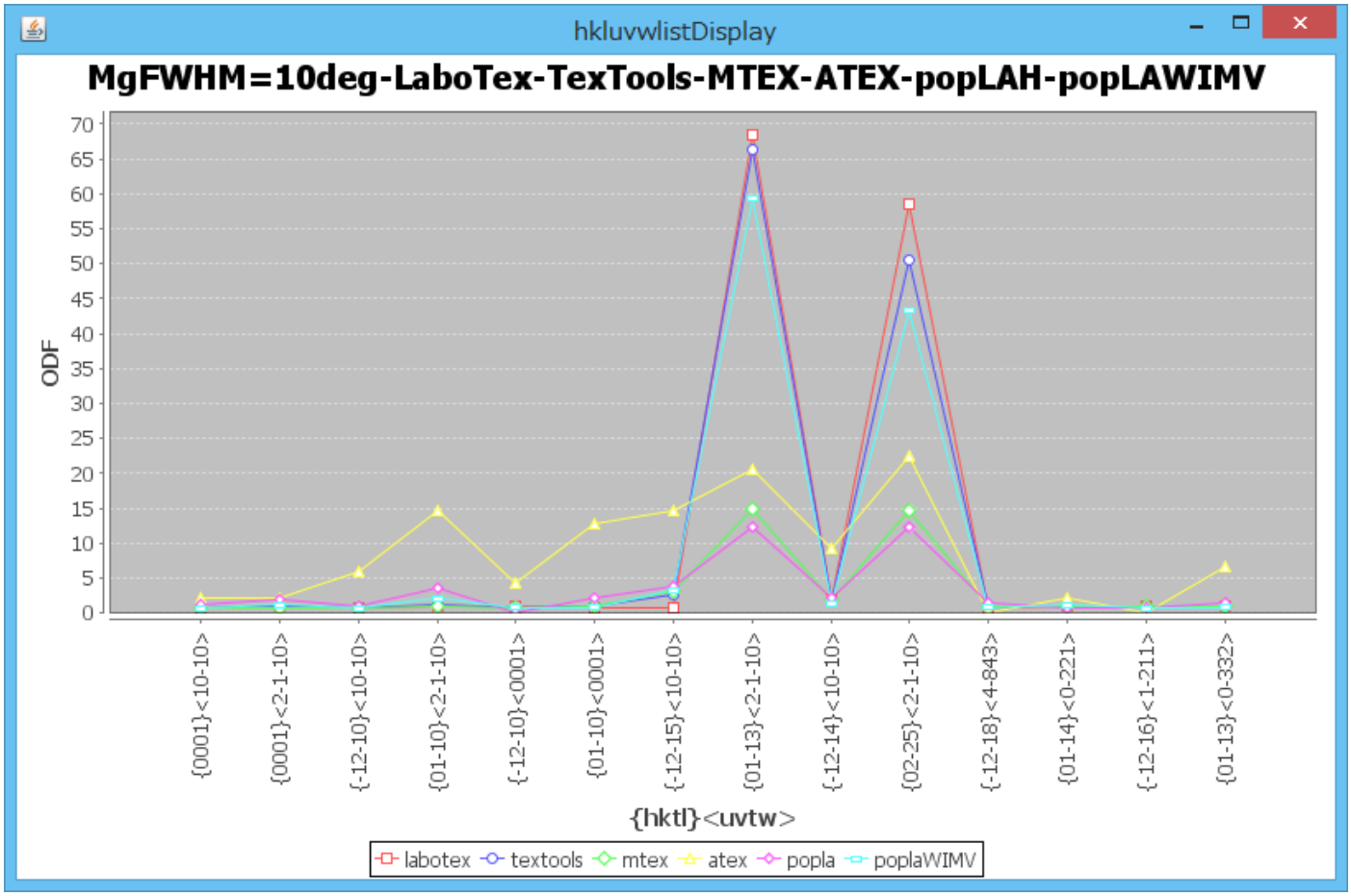


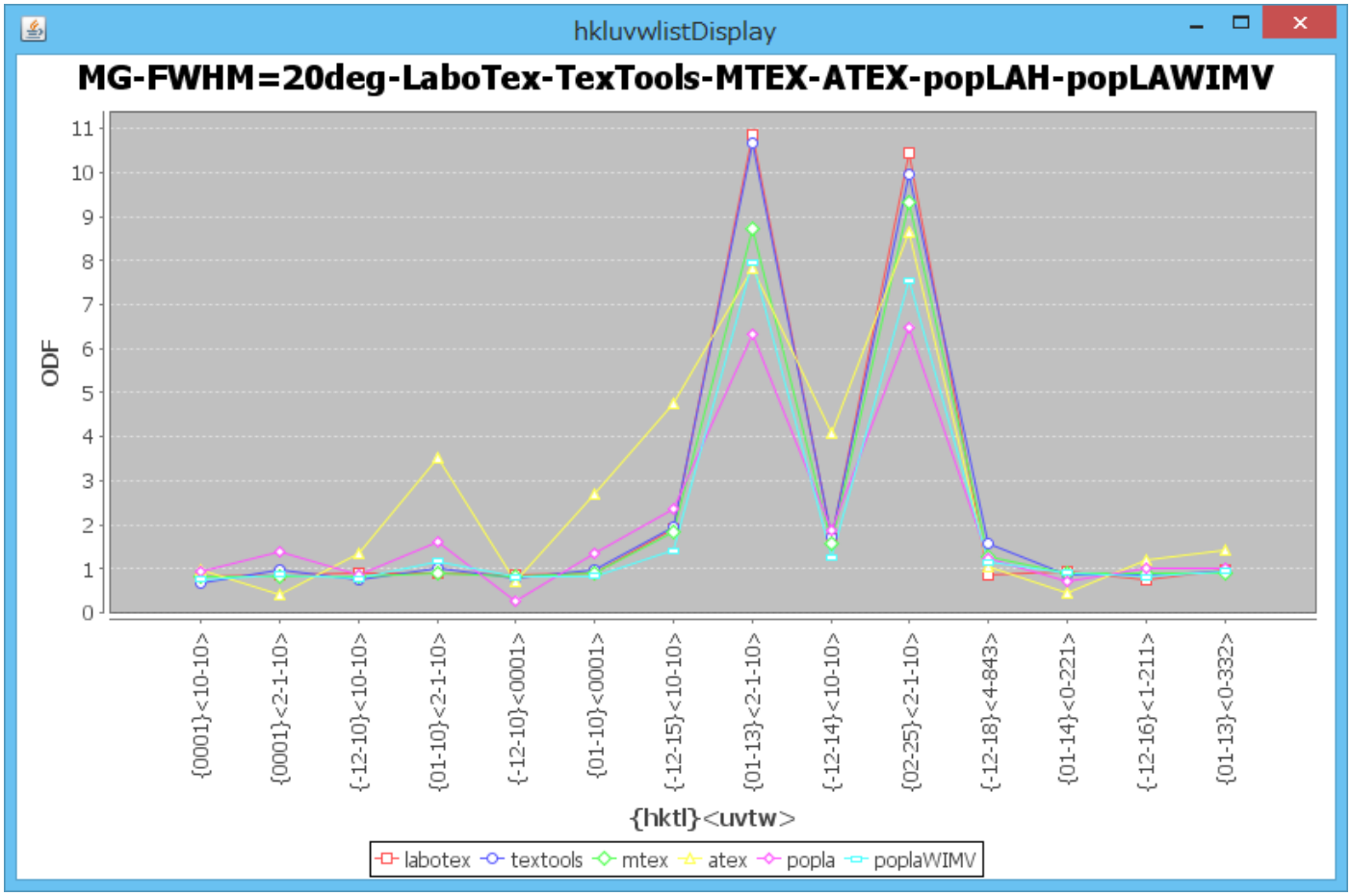
(0,1,3)[1,0,0]f1=0.0,F=32.0,f2=30.0 ODF=59.32

FWHM=20deg



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





半価幅が狭いと LaboTex-TexTools-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。