ポリエチレンなどのＯｒｔｈｏｒｈｏｍｂｉｃＯＤＦ解析比較

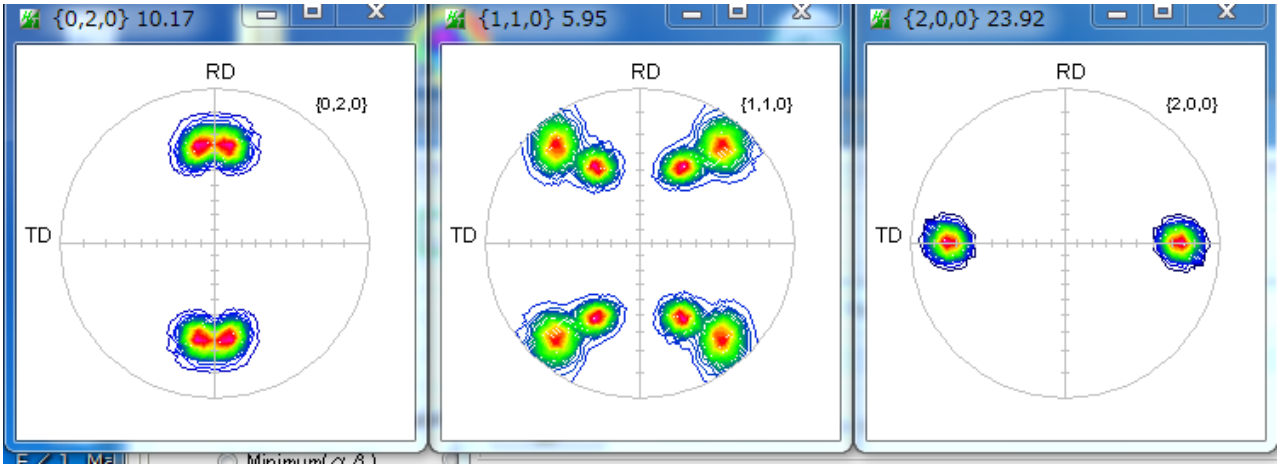
０１９年１０月２４日

ＨｅｌｐｅｒＴｅｘ　Ｏｆｆｉｃｅ

概要

Ｃｕｂｉｃ、Ｈｅｘａｇｏｎａｌまでは、各種ＯＤＦ解析結果表現に大きな違いがないが、Ｏｒｔｈｏｒｈｏｍｂｉｃ以降は極点図、ＯＤＦ図、逆極点図に大きな違いがあります。
ポリエチレンを例に説明します。

入力極点図

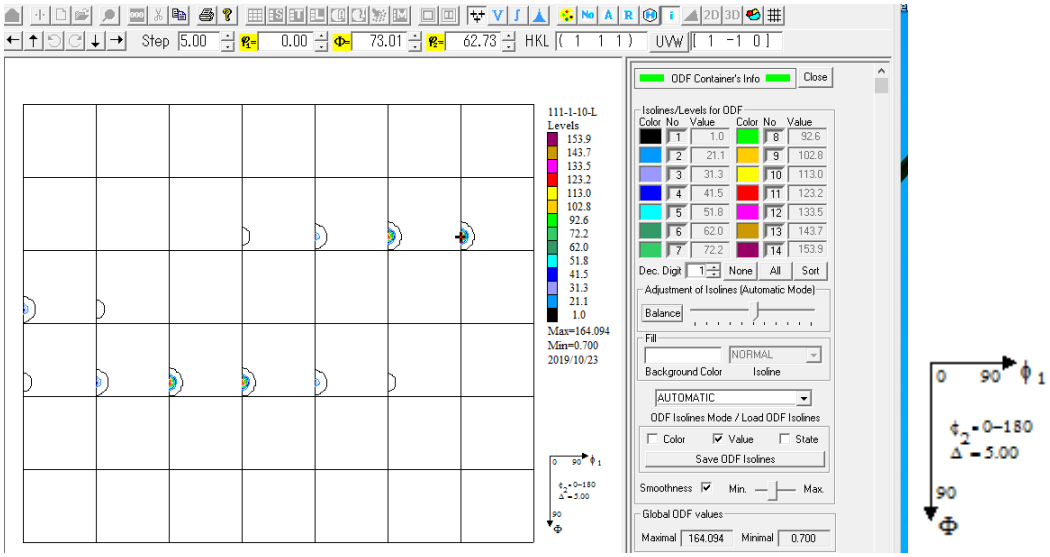


比較するＯＤＦソフトウエア

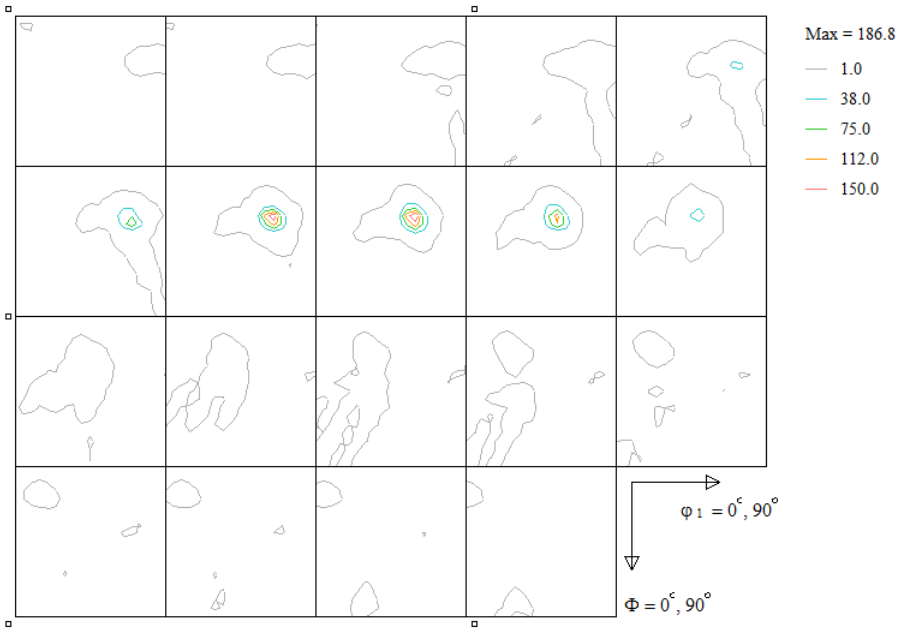
ＬａｂｏＴｅｘ
ＴｅｘＴｏｏｌｓ
ＭＴＥＸ

ＯＤＦ解析結果の比較

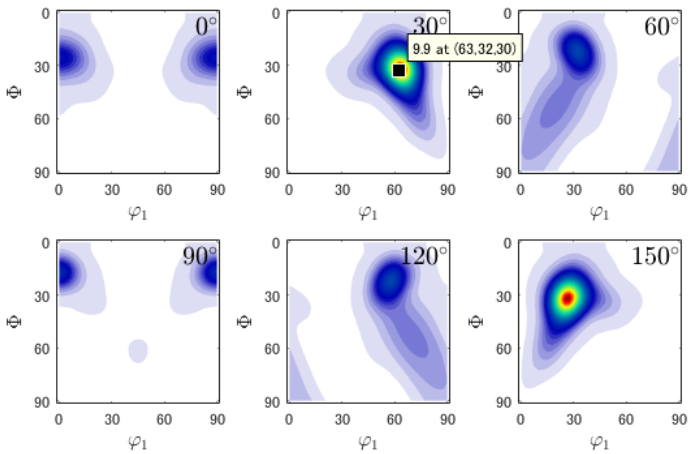
ＬａｂｏＴｅｘ（１／４対称）



ＴｅｘＴｏｏｌｓ（１／４対称）

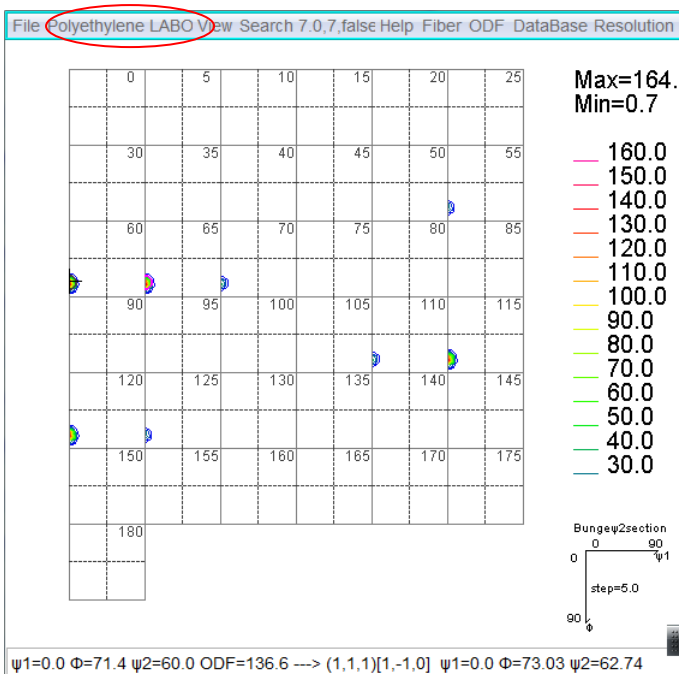


ＭＴＥＸ（`SS = specimenSymmetry('4');`で１／４計算）

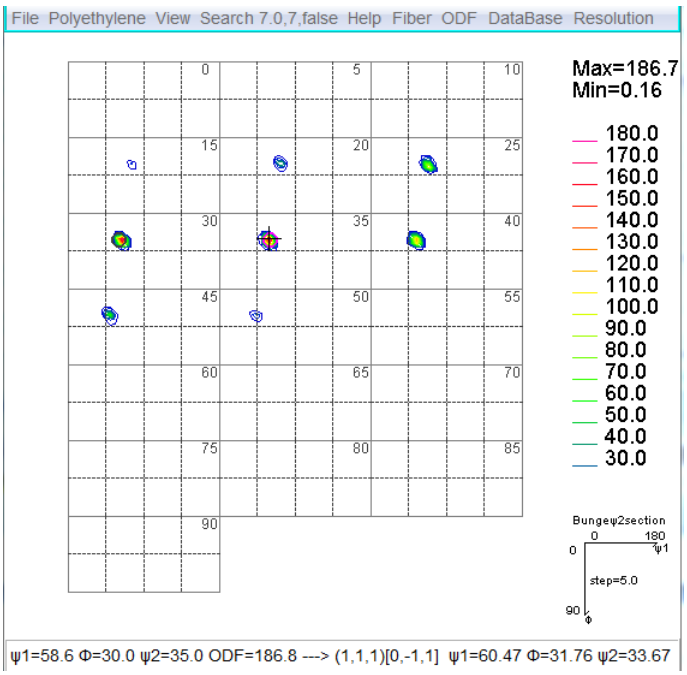


ＯＤＦ図を１／４対称で表示した場合をＣＴＲで表示

ＬａｂｏＴｅｘ



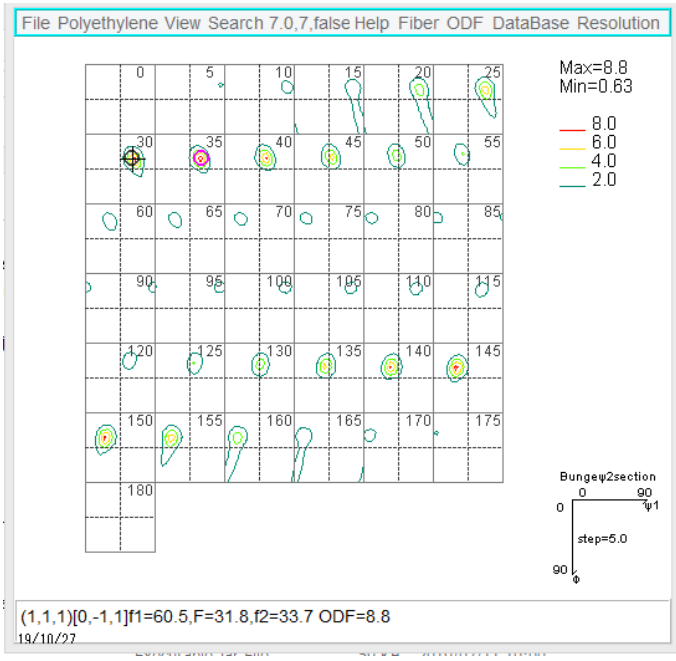
TexTools

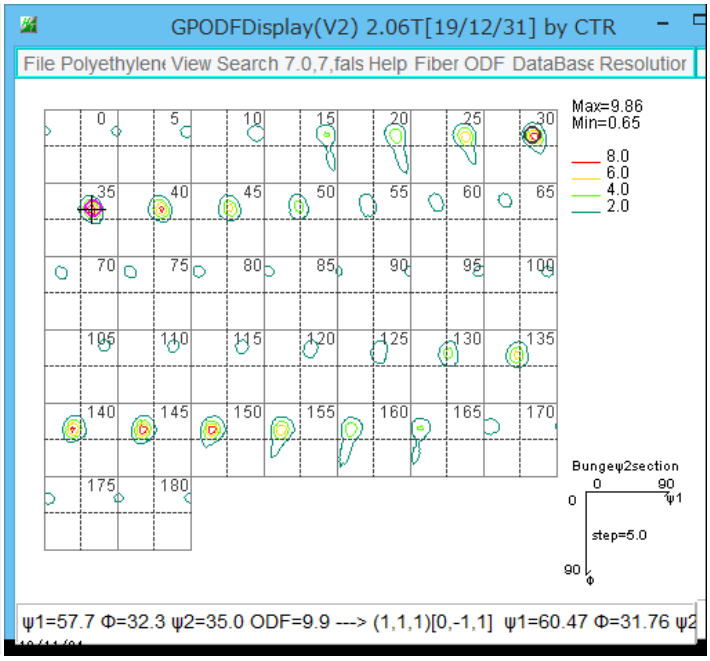


MTEX　Triclinic->Orthrhombic

```
% specimen symmetry
SS = specimenSymmetry('4');
```

1/4 直接計算





表示範囲（φ１，Φ、φ２）と求められた結晶方位

ＬａｂｏＴｅｘ

（９０，９０，１８０）　｛１１１｝＜１－１０＞

ＴｅｘＴｏｏｌｓ

（９０，１８０，９０）　｛１１１｝＜０－１１＞

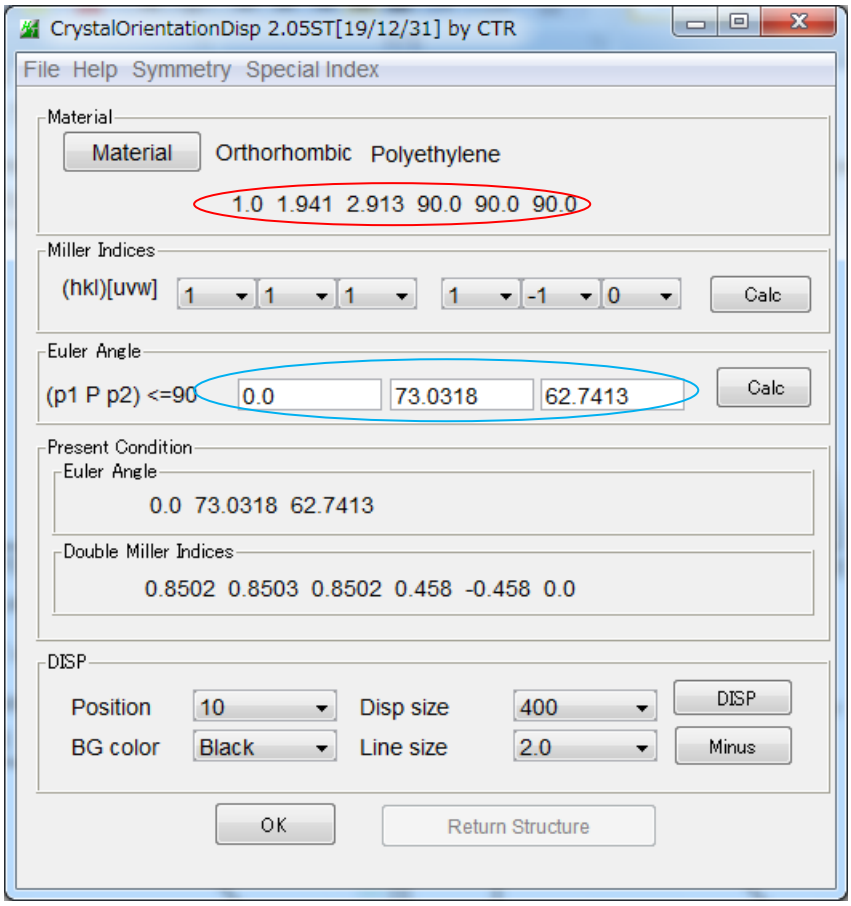
ＭＴＥＸ

｛９０，９０，１８０｝　｛１１１｝＜０－１１＞

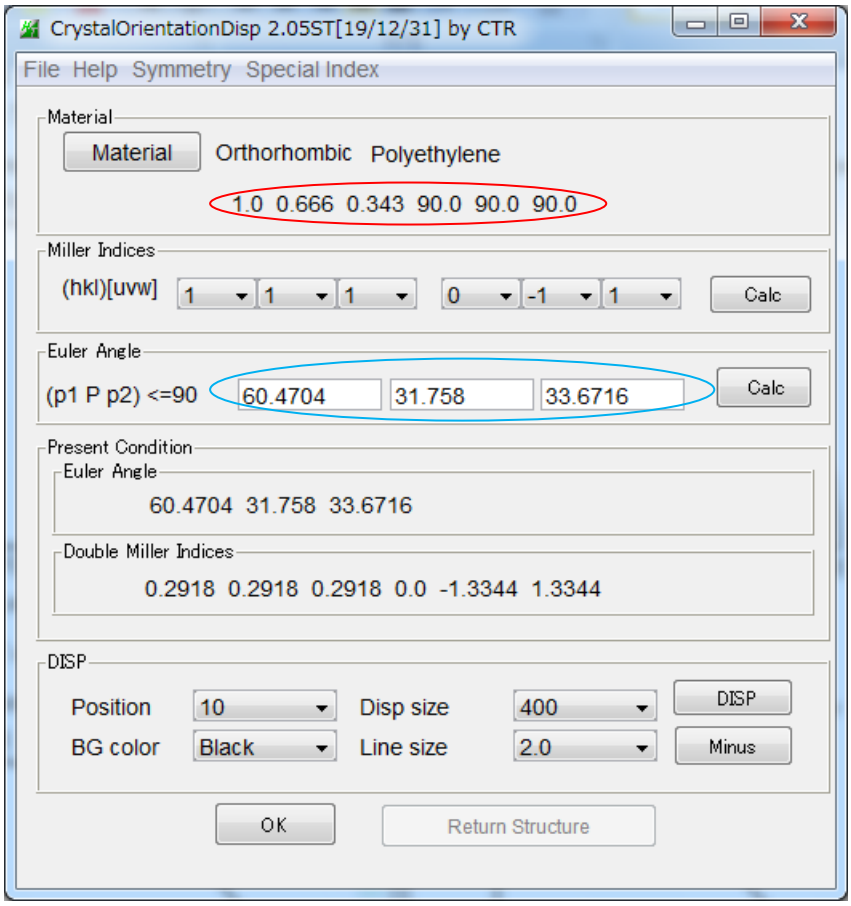
ＬａｂｏＴｅｘは格子定数の取り方が異なります。

格子定数と結晶方位計算

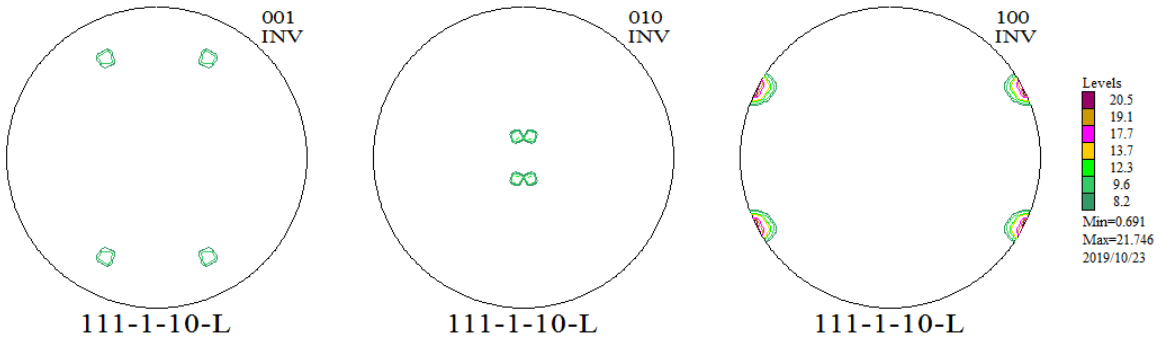
ＬａｂｏＴｅｘ



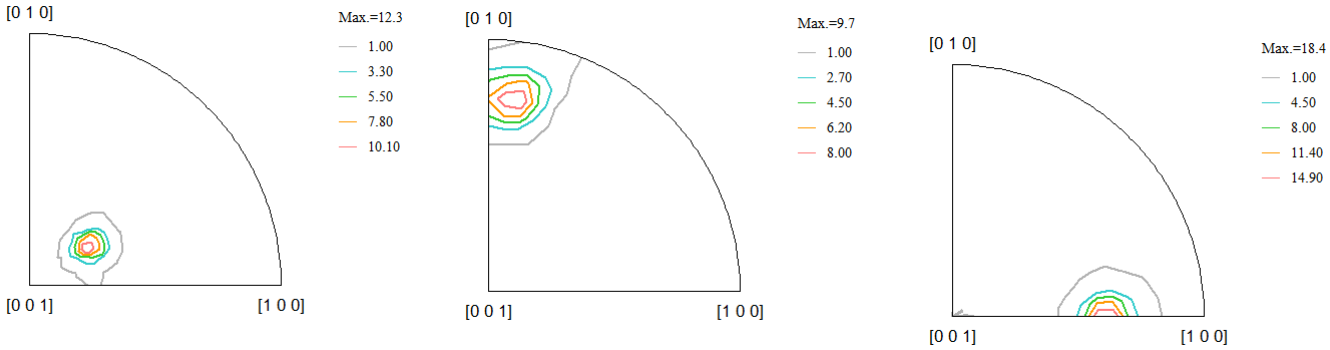
ＭＴＥＸ



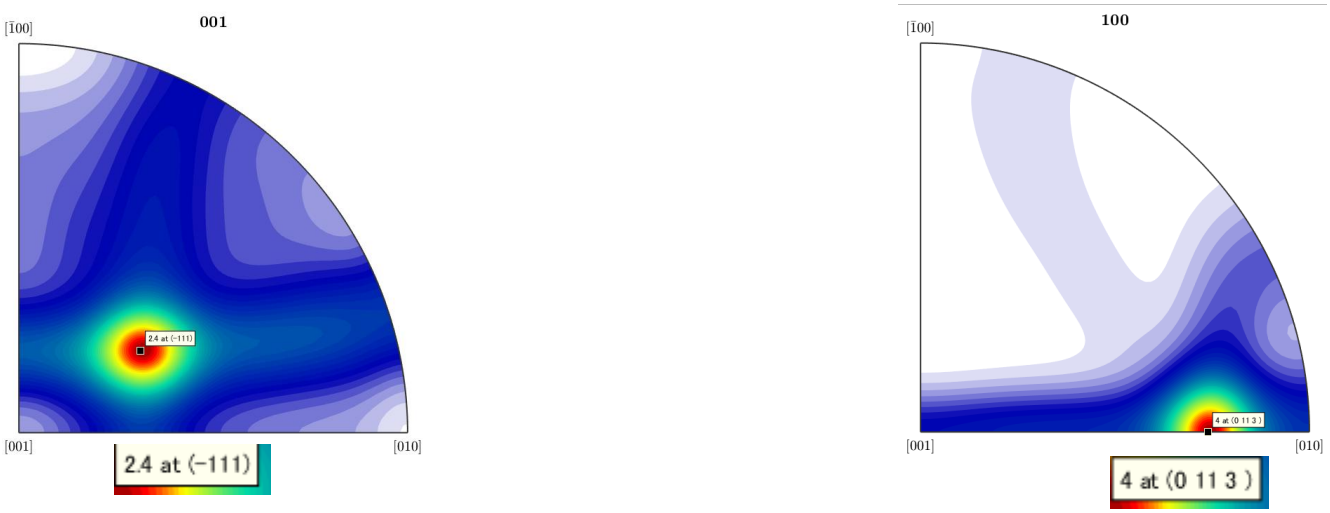
逆極点図（等面積表示）



ＴｅｘＴｏｏｌｓ（等面積表示）



ＭＴＥＸ（等角度表示）



基本方位

ＬａｂｏＴｅｘ

［００１］－［１００］－［０１０］－Ｐｌａｎｅ表示

ＴｅｘＴｏｏｌｓ

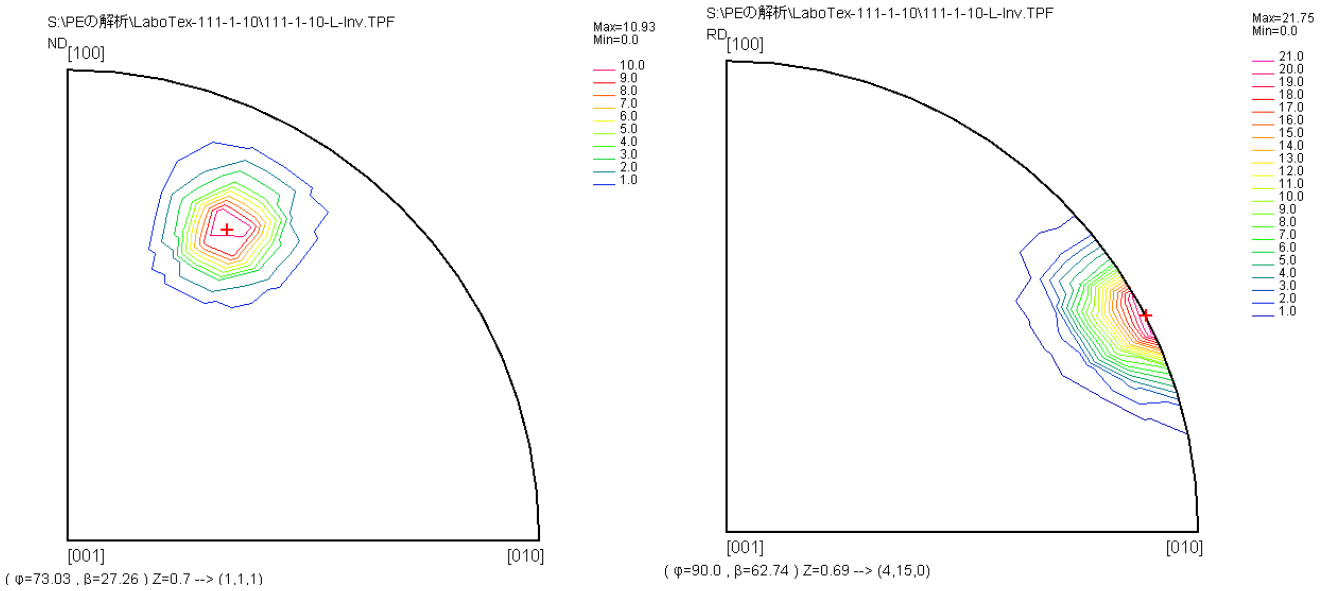
［００１］－［１００］－［０１０］

ＭＴＥＸ

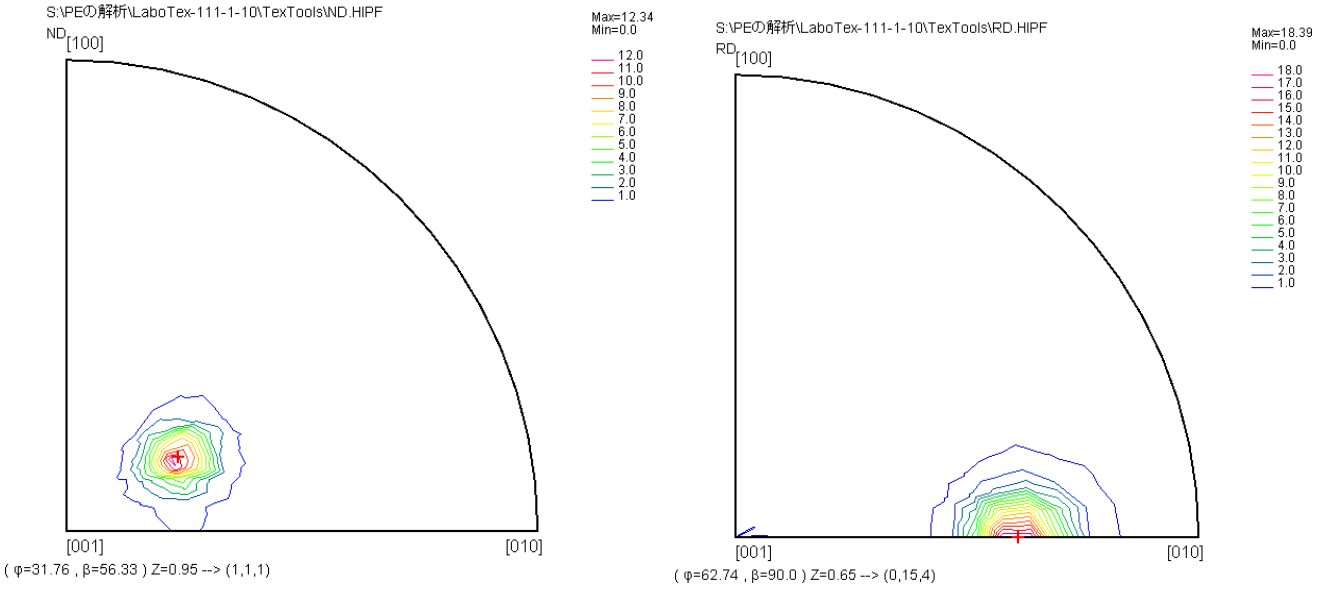
［００１］－［０１０］－［－１００］－Ｐｌａｎｅ表示

逆極点図をＣＴＲで表示（Ｐｌａｎｅ等面積表示）

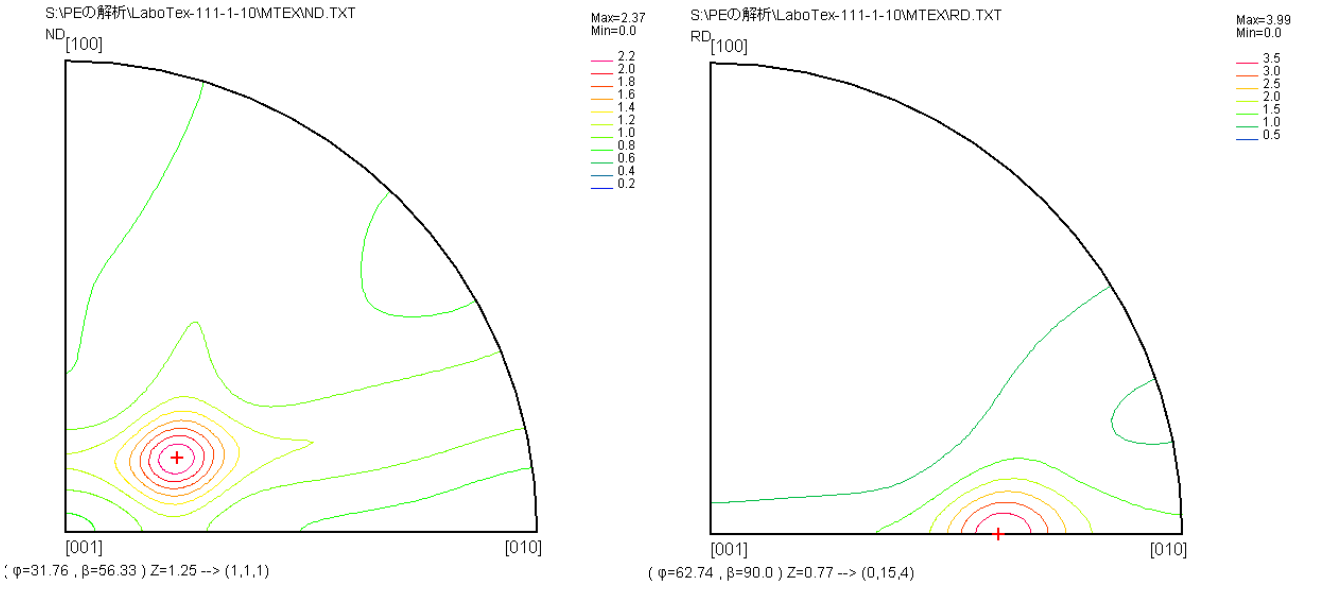
ＬａｂｏＴｅｘ



ＴｅｘＴｏｏｌｓ

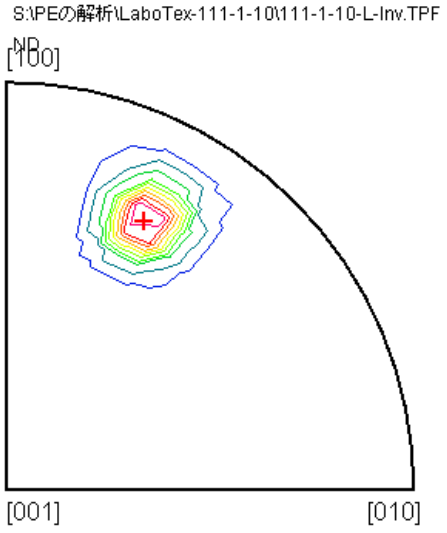


ＭＴＥＸ

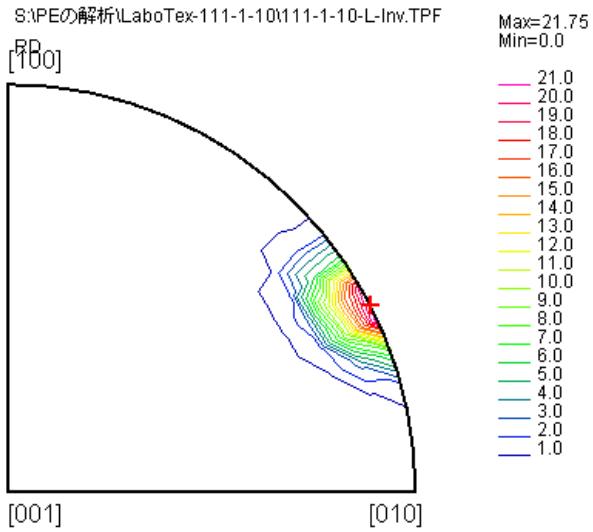


逆極点図（Ｄｉｒｅｃｔｉｏｎ等面積表示）

ＬａｂｏＴｅｘ

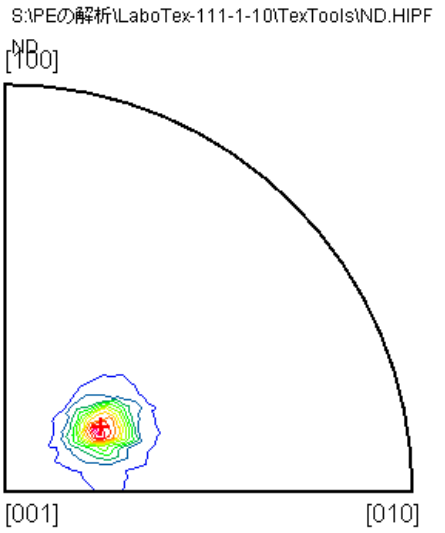


(φ=73.03 , β=27.26) Z=0.7 --> [8,2,1]

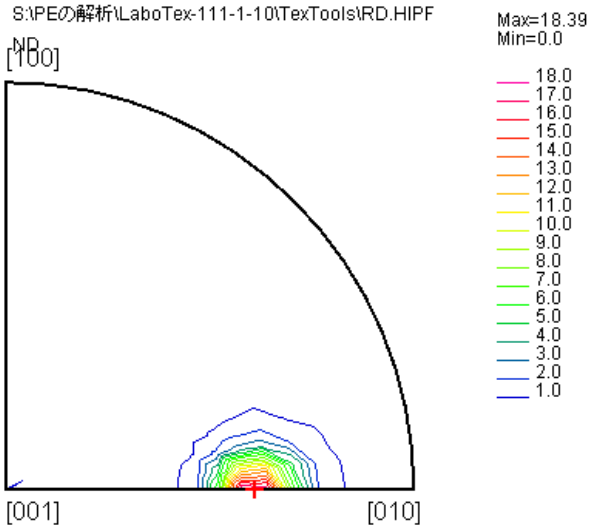


(φ=90.0 , β=62.74) Z=0.69 --> [1,1,0]

ＴｅｘＴｏｏｌｓ

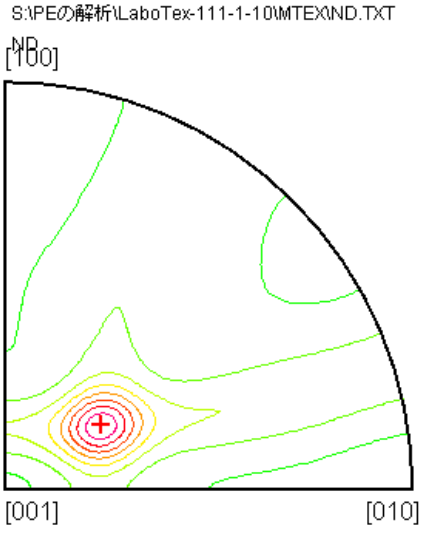


(φ=31.76 , β=56.33) Z=0.95 --> [1,2,8]

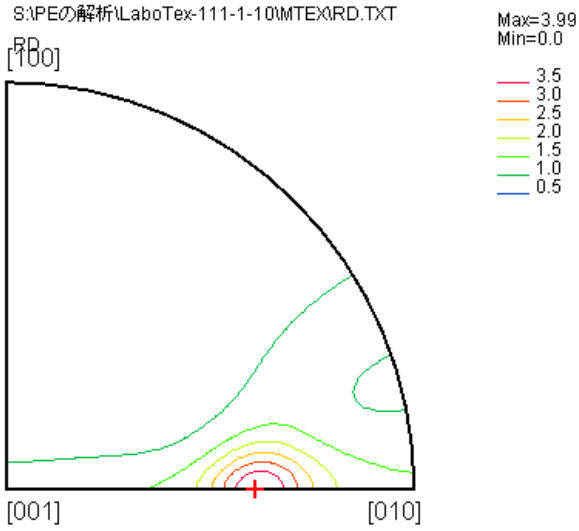


(φ=62.74 , β=90.0) Z=0.65 --> [0,-1,1]

ＭＴＥＸ



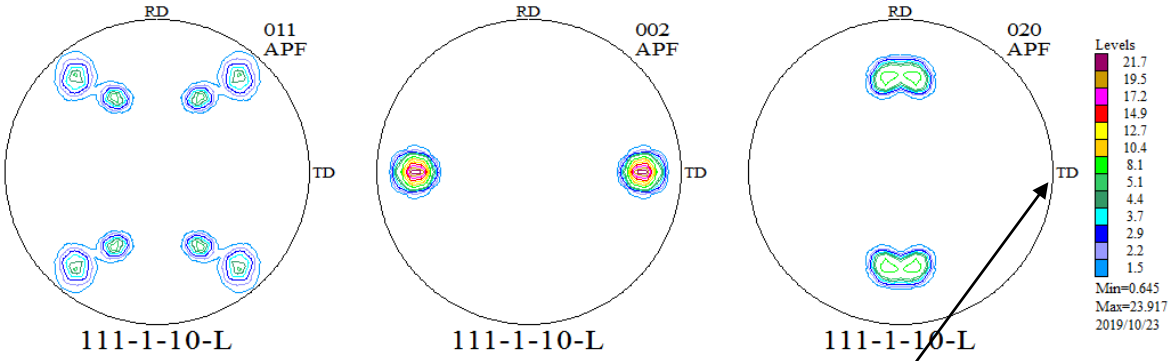
(φ=31.76 , β=56.33) Z=1.25 --> [1,2,8]



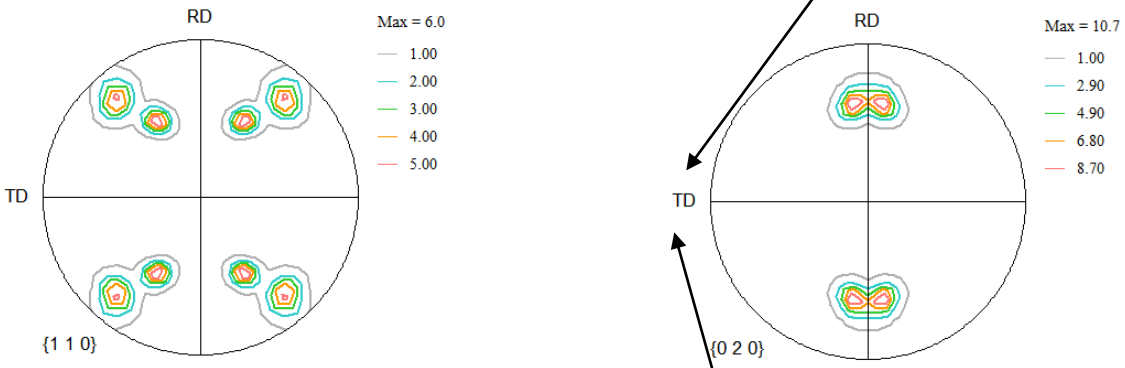
(φ=62.74 , β=90.0) Z=0.77 --> [0,1,1]

極点図

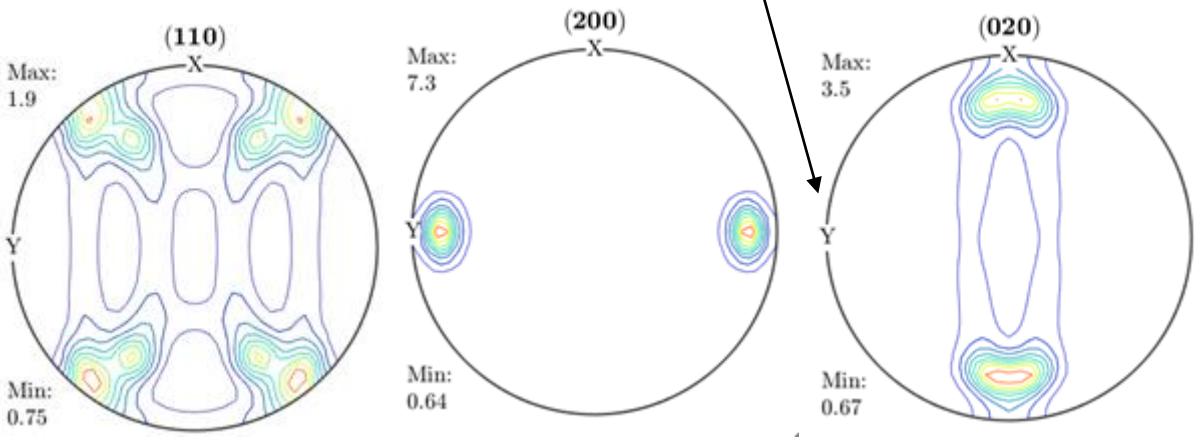
ＬａｂｏＴｅｘ



ＴｅｘＴｏｏｌｓ



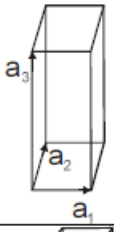
ＭＴＥＸ



ＬａｂｏＴｅｘ	｛０１１｝、｛２００｝、｛０２０｝等面積表記	ＴＤ右側
ＴｅｘＴｏｏｌｓ	｛１１０｝、｛２００｝、｛００２｝等面積表記	ＴＤ左側
ＭＴＥＸ	｛１１０｝、｛２００｝、｛００２｝等角度表記	ＴＤ左側

ＬａｂｏＴｅｘとＴｅｘＴｏｏｌｓ，ＭＴＥＸの格子定数の取り方

ＬａｂｏＴｅｘ

Orthorhombic	D_2	D_{2h},D_2	a < b < c	90° 90° 90°	
	C_2	C_{2v}			

TextDisplay 1.13S C:¥CTR¥work¥MYICDD¥DISP¥disp.txt

File Help

```
PolyethyleneDISP
Orthorhombic
2.54        (1.0)
4.93        (1.9409)
7.4         (2.9134)
90.0
90.0
90.0
1.54056
9
0    1    1    100.0    4.1029    21.642
0    0    2    35.0     3.7       24.032
0    1    2    5.0      2.9593    30.175
0    2    0    20.0     2.465     36.418
1    1    0    25.0     2.2579    39.893
0    1    3    20.0     2.206     40.875
1    1    1    20.0     2.1596    41.792
0    2    2    15.0     2.0514    44.109
1    1    3    25.0     1.6655    55.095
00-053-1859          Polyethylene          Formula: ( C2 H4 )n
```

ＴｅｘＴｏｏｌｓ，ＭＴＥＸ

```
PolyethyleneDISP
Orthorhombic
7.4         (1.0)
4.93        (0.6662)
2.54        (0.3432)
90.0
90.0
90.0
1.54056
9
1    1    0    100.0    4.1029    21.642
2    0    0    35.0     3.7       24.032
2    1    0    5.0      2.9593    30.175
0    2    0    20.0     2.465     36.418
0    1    1    25.0     2.2579    39.893
3    1    0    20.0     2.206     40.875
1    1    1    20.0     2.1596    41.792
2    2    0    15.0     2.0514    44.109
3    1    1    25.0     1.6655    55.095
00-053-1859          Polyethylene
```

このため、

｛１１０｝　－＞　｛０１１｝

｛２００｝　－＞　｛００２｝

｛０２０｝　－＞　｛０２０｝

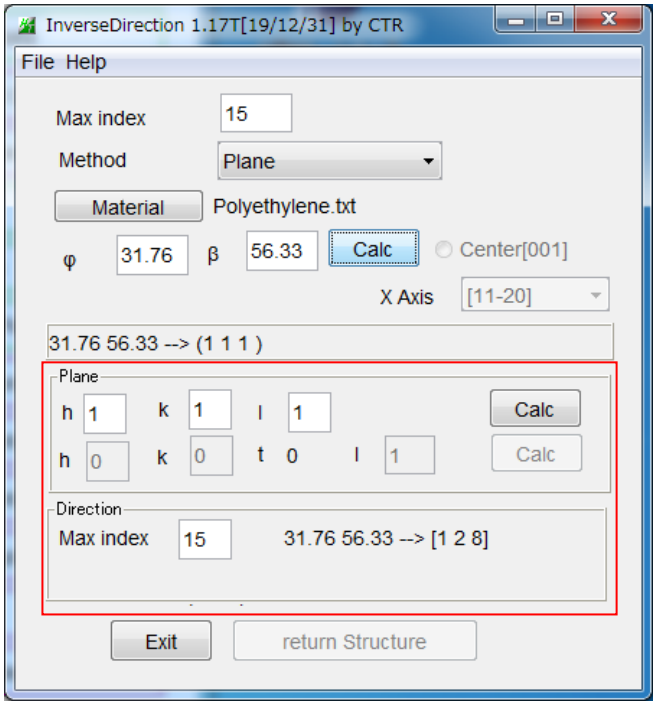
結晶方位

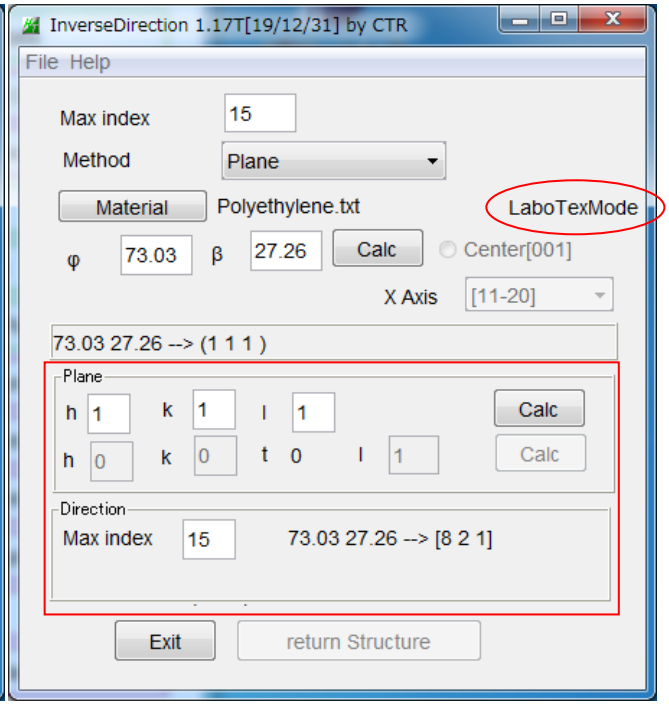
｛１１１｝＜１－１０＞　－＞｛１１１｝＜０－１１＞

逆極点図

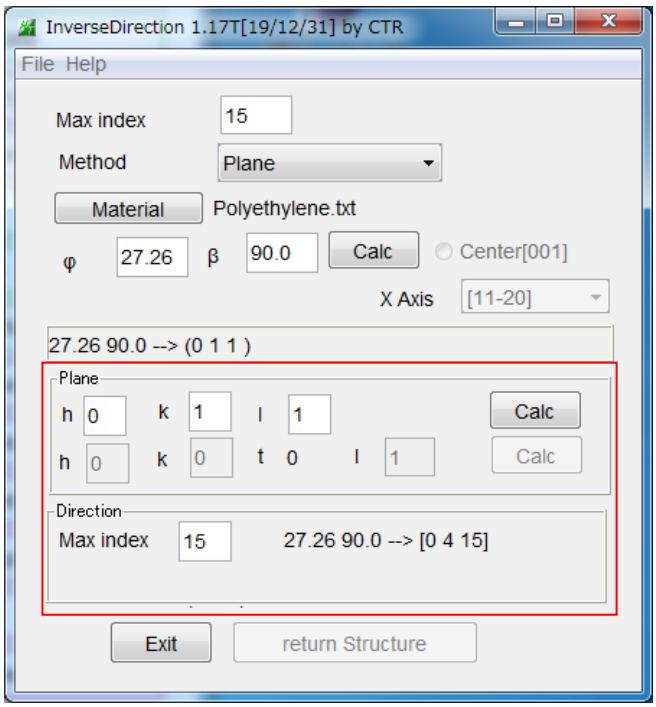
ＴｅｘＴｏｏｌｓ，ＭＴＥＸ　　ＬａｂｏＴｅｘ

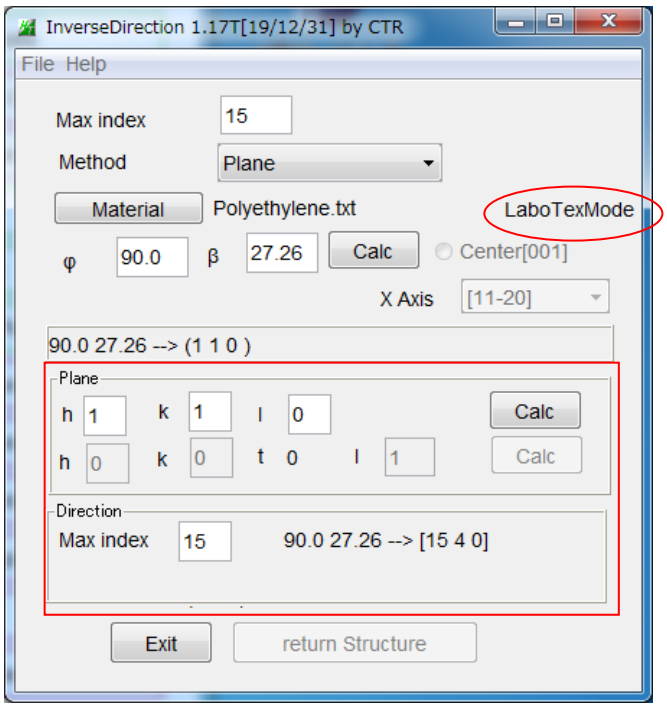
ＮＤ方向





ＲＤ方向





格子定数の取り方で図形が変わります。