ＭｏｎｏｃｌｉｎｉｃにおけるＯＤＦ

２００９年０６月２３日

ＨｅｐｌｅｒＴｅｘ

DOC-資料¥LaboTex¥Monoclinic-LaboTex

ＬａｂｏＴｅｘでは格子定数 ａ　ｂ　ｃ　α　β　γに関してＭｏｎｏｃｌｉｎｉｃは

ａ ＜ ｂ　ｃ　９０．０　９０．０　γ ＜ ９０．０の条件がある。

ＩＣＤＤ　５０－２３９７（ＧＡ－Ｐｏｌｙｐｒｏｐｙｌｅｎｅ）

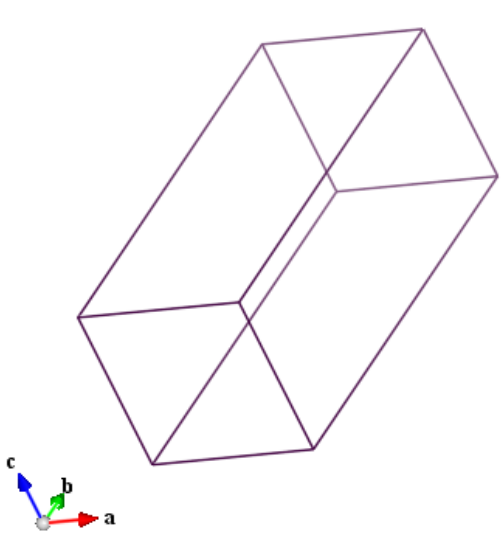
Ｐ２１／ｃ（１４）

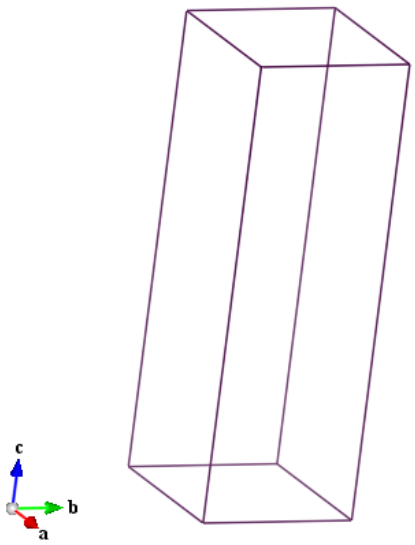
ICDD

6.63　20.78 6. 5　90.0　99.5　90.0

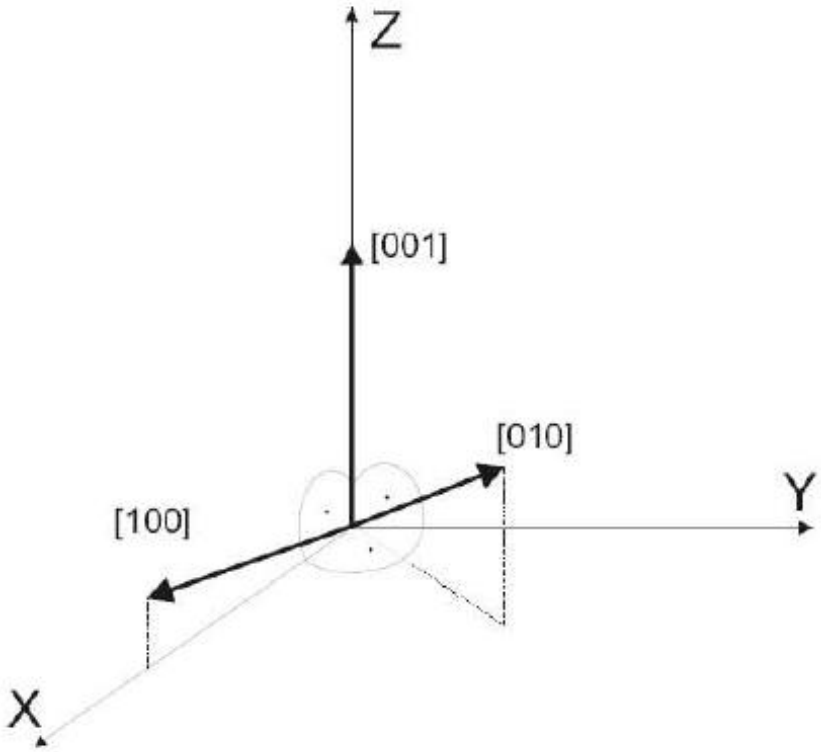
LaboTex

6.5　6.63　20.78　90.0　90.0　80.5



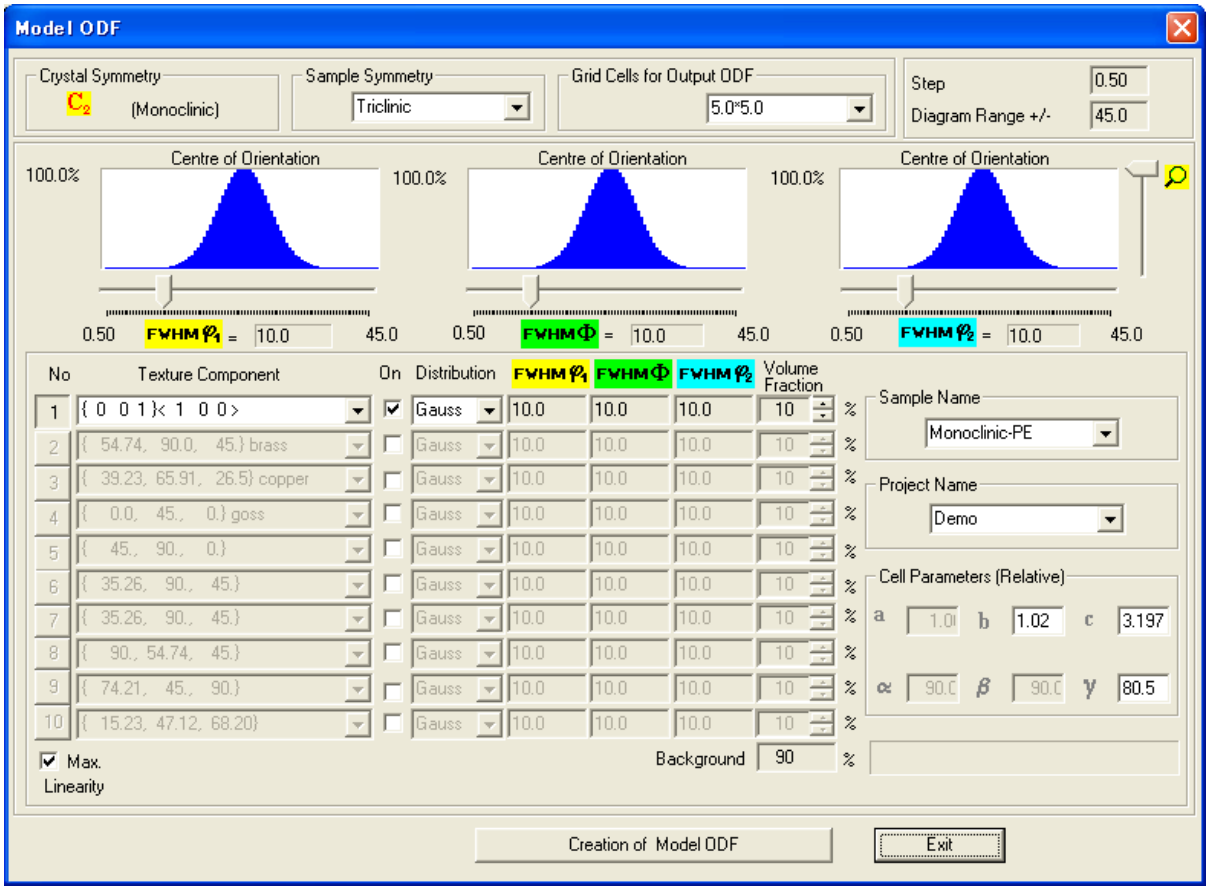


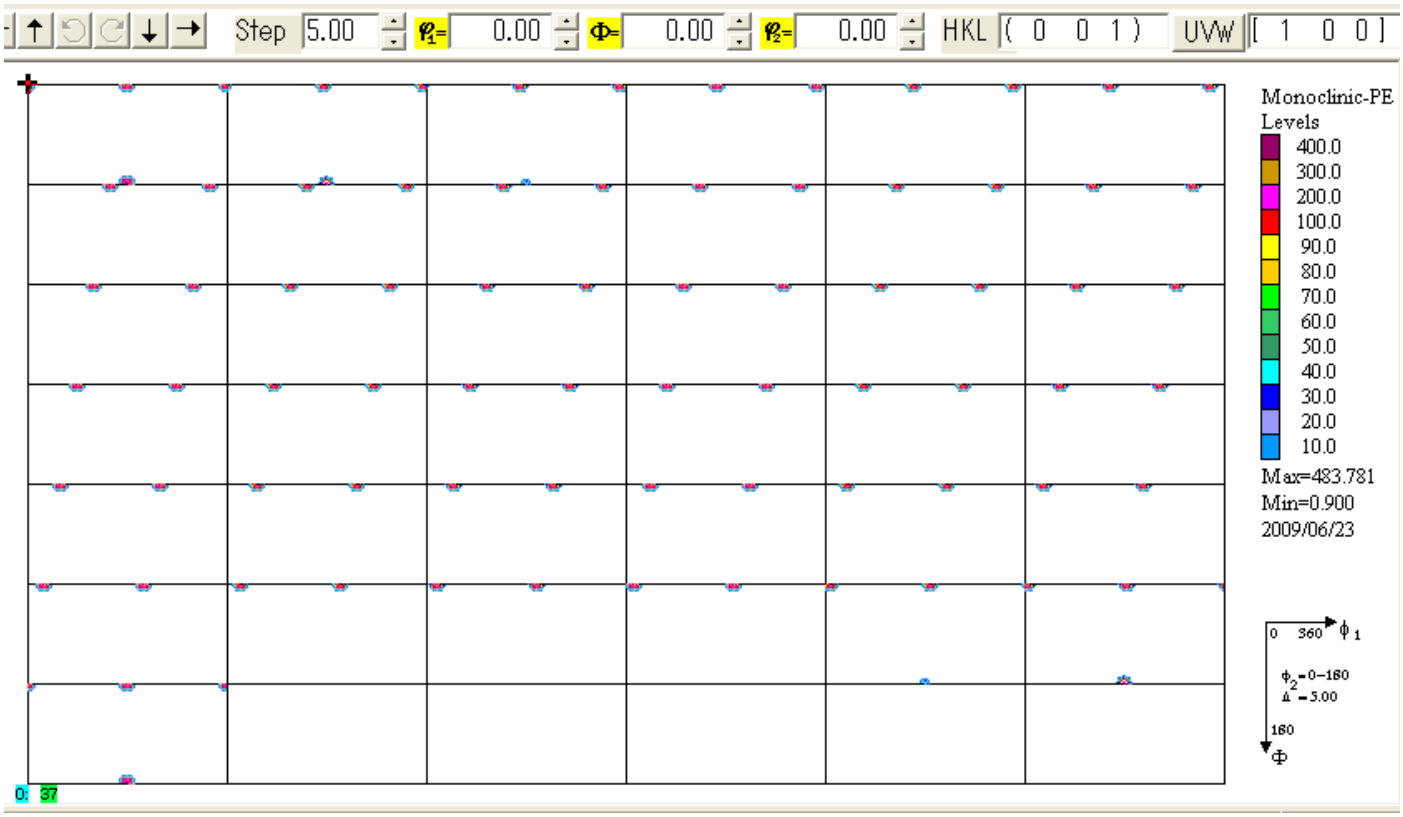
又、Ｃｒｙｓｔａｌとｓａｍｐｌｅの関係はＺ軸は[001]になる。

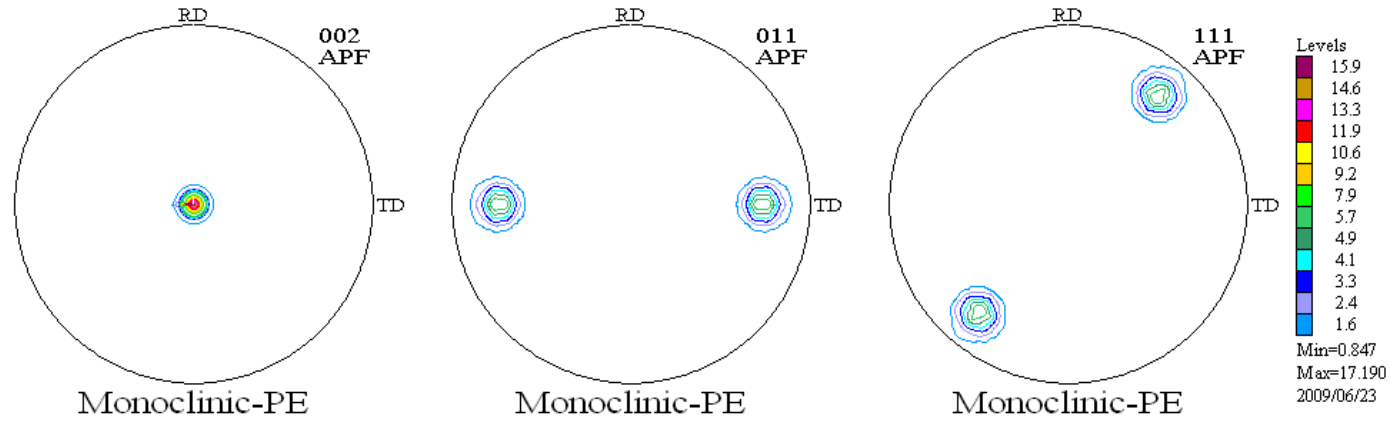


ICDD			LaboTex		
(0 2 0)	10.3900	8.503	(0 0 2)	10.390000	
(1 0 0)	6.5391	13.53	(0 1 0)	6.539074	
(1 1 0)	6.2375	14.187	(0 1 1)	6.237529	=(0 −1 1)
(0 4 0)	5.1950	17.054	(0 0 4)	5.195000	
(1 3 0)	4.7549	18.646	(0 1 3)	4.754944	=(0 −1 3)
(−1 2 1)	4.5126	19.657	(1 1 2)	4.512605	
(1 1 1)	4.1556	21.364	(1 −1 1)	41.555670	
(−1 3 1)	4.0593	21.877	(1 1 3)	4.059328	
(1 2 1)	3.9267	22.626	(1 −1 2)	3.926685	
(1 3 1)	3.6170	21.877	(1 −1 3)	3.617048	
(−1 4 1)	3.6170	24.592	(1 1 4)	3.606155	
(1 5 0)	3.5075	25.372	(0 1 5)	3.507527	=(0 −1 5)
(0 6 0)	3.4633	25.701	(0 0 6)	3.463333	
(2 0 0)	3.2695	27.253	(0 2 0)	3.269537	
(1 4 1)	3.2695	27.253	(1 −1 4)	3.285392	
(−1 5 1)	3.1986	27.869	(1 1 5)	3.198630	
(0 1 2)	3.1680	28.145	(2 0 1)	3.167959	
(2 2 0)	3.1188	28.598	(0 2 2)	3.118765	=(0 −2 2)
(−2 1 1)	3.0942	28.829	(1 2 1)	3.094250	
(−1 0 2)	3.0866	28.902	(2 1 0)	3.086596	
(−1 1 2)	3.0531	29.13	(2 1 1)	3.053100	
(0 2 2)	3.0630	29.13	(2 0 2)	3.062975	
(−2 2 1)	2.9962	29.794	(1 2 2)	2.996203	
(1 5 1)	2.9684	30.08	(1 −1 5)	2.968414	

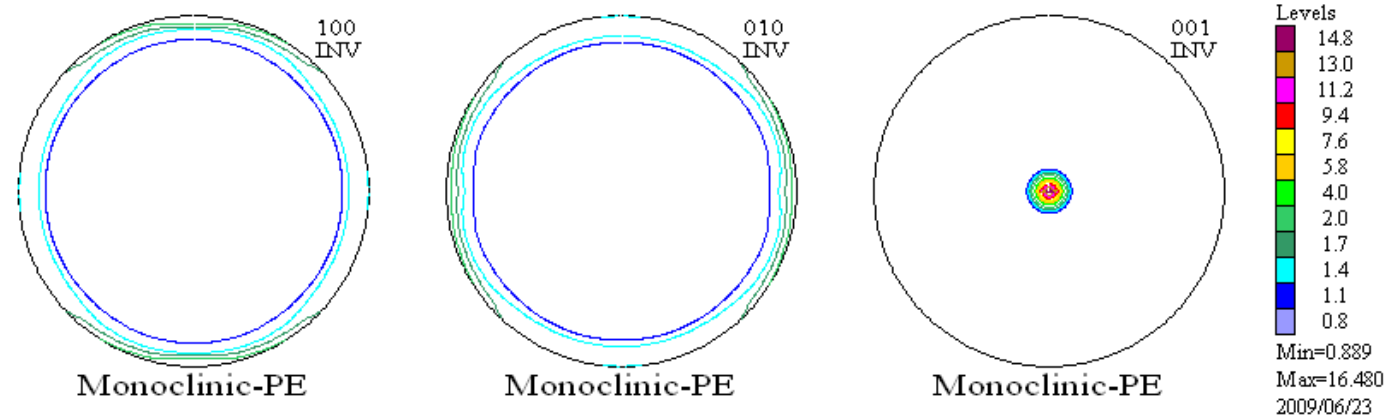
{001}<100>の計算




Step 5.00
φ1= 0.00
Φ= 0.00
φ2= 0.00
HKL (0 0 1)
UVW [1 0 0]
Monoclinic-PE
Levels
400.0
300.0
200.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
Max=483.781
Min=0.900
2009/06/23
0 360 φ1
φ2=0-180
Δ=5.00
180 Φ
0 37

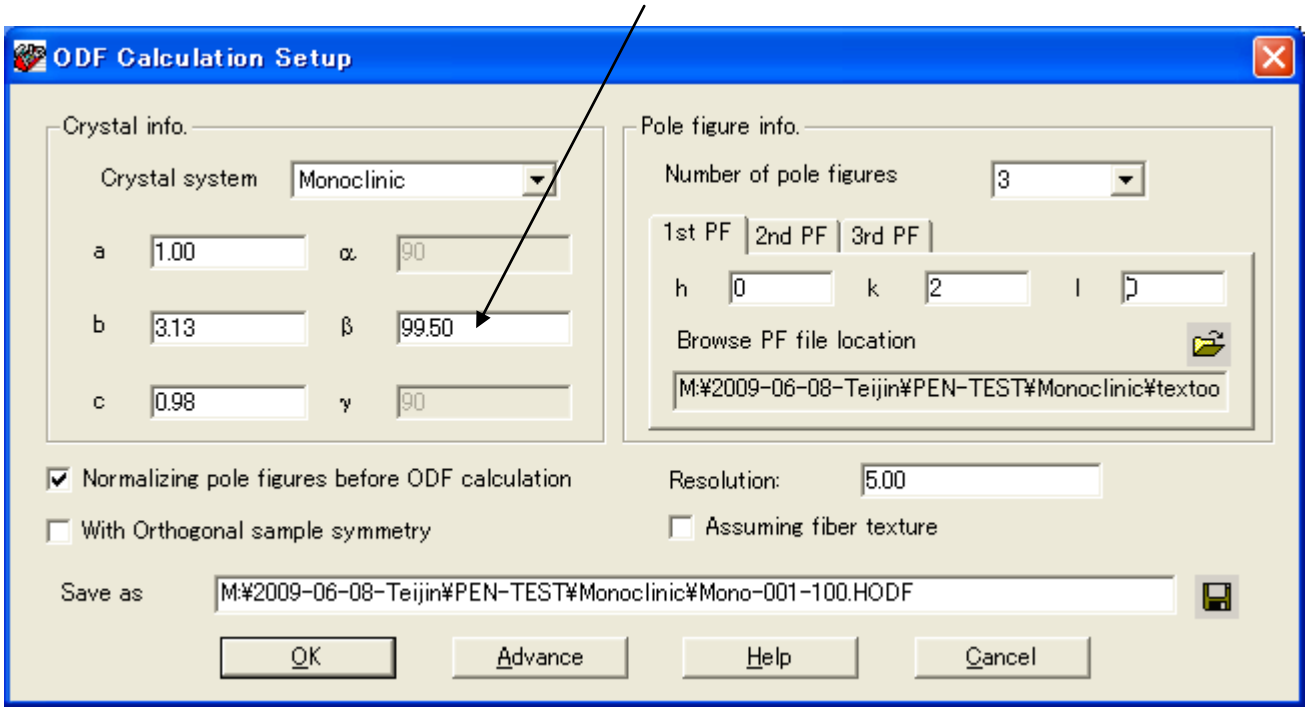

RD
002
APF
TD
Monoclinic-PE
RD
011
APF
TD
Monoclinic-PE
RD
111
APF
TD
Monoclinic-PE
Levels
15.9
14.6
13.3
11.9
10.6
9.2
7.9
5.7
4.9
4.1
3.3
2.4
1.6
Min=0.847
Max=17.190
2009/06/23

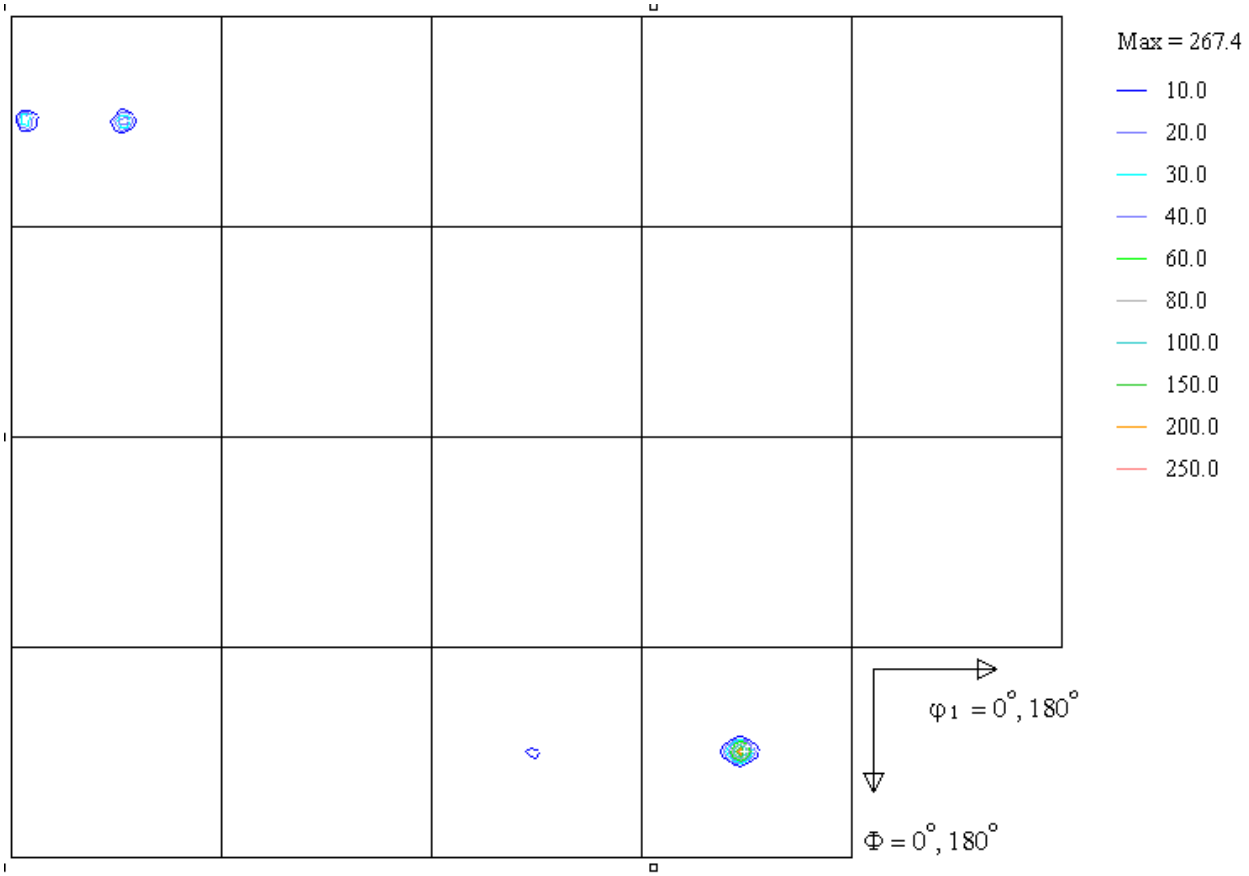
逆極点

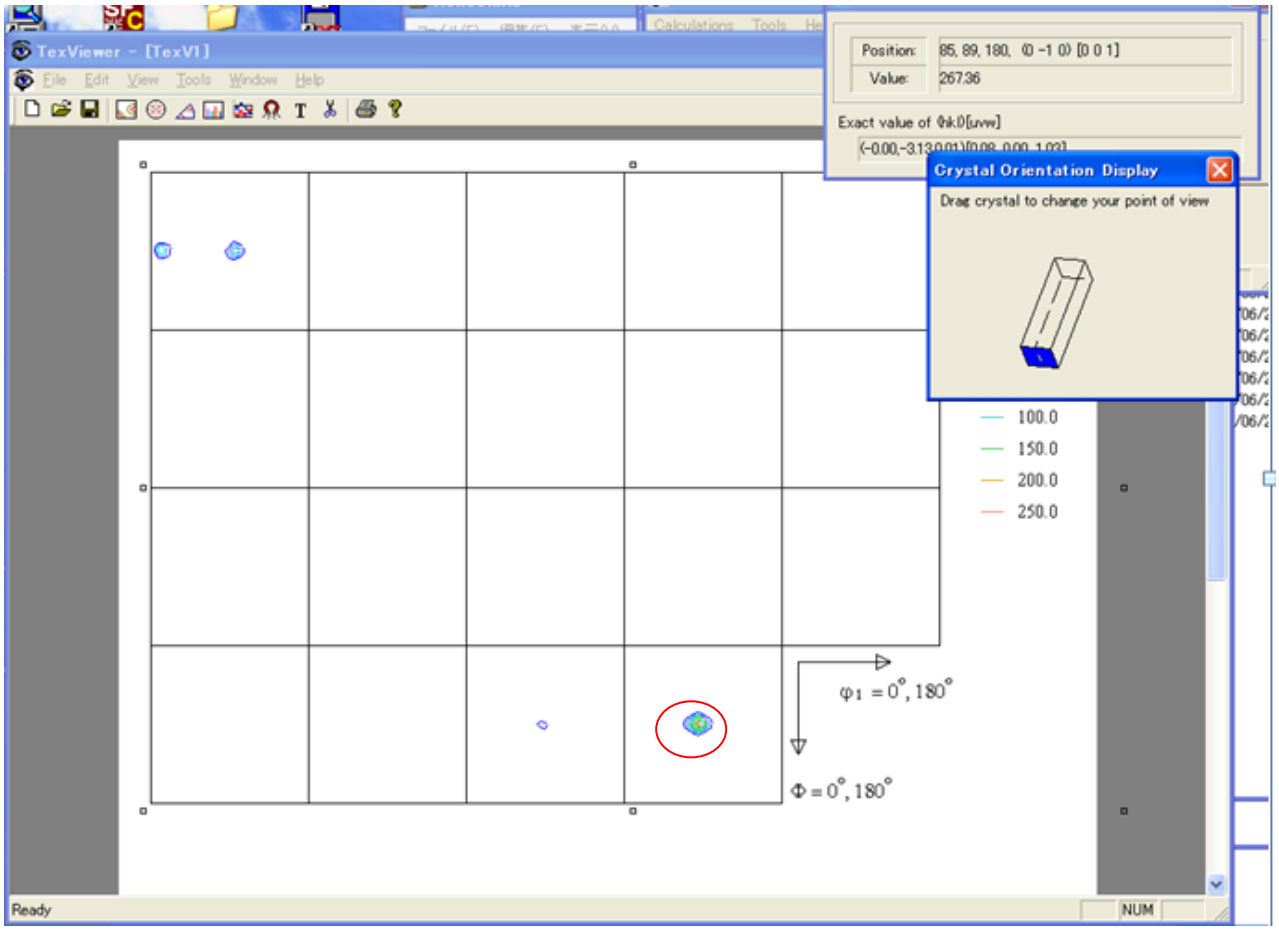

100
INV
Monoclinic-PE
010
INV
Monoclinic-PE
001
INV
Monoclinic-PE
Levels
14.8
13.0
11.2
9.4
7.6
5.8
4.0
2.0
1.7
1.4
1.1
0.8
Min=0.889
Max=16.480
2009/06/23

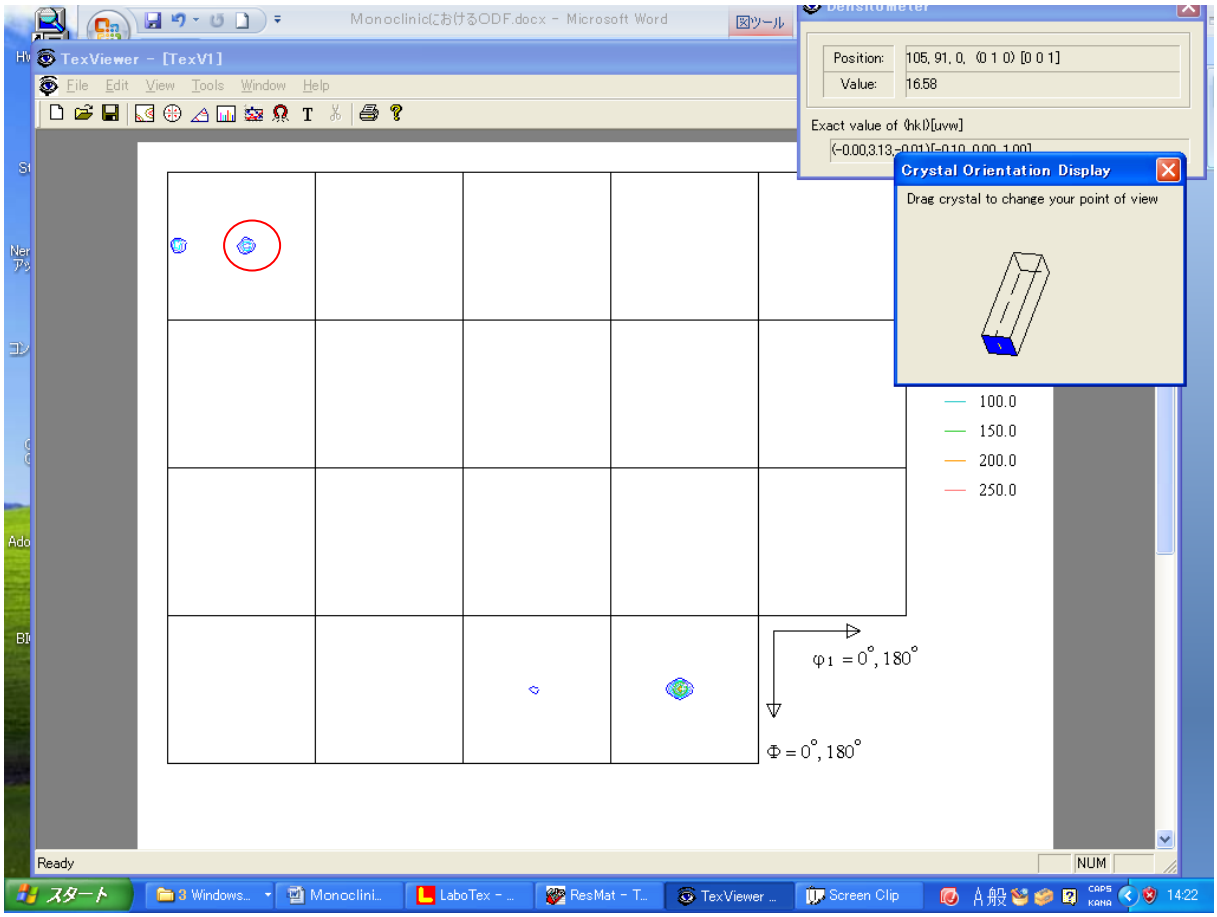
極点図のＥｘｐｏｒｔをＴｅｘＴｏｏｌｓで解析

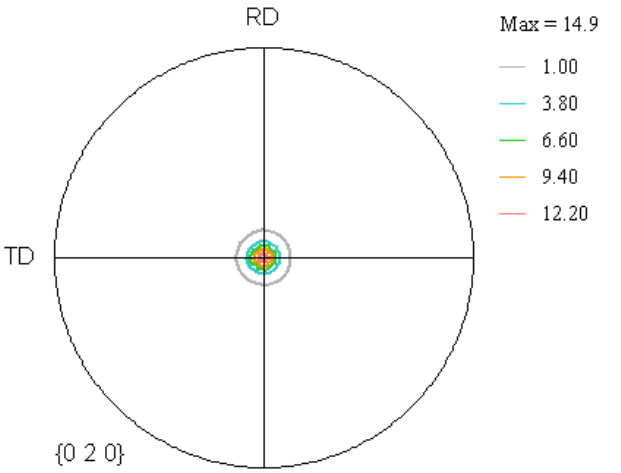
ＴｅｘＴｏｏｌｓでは、ＩＣＤＤ形式の入力になる。

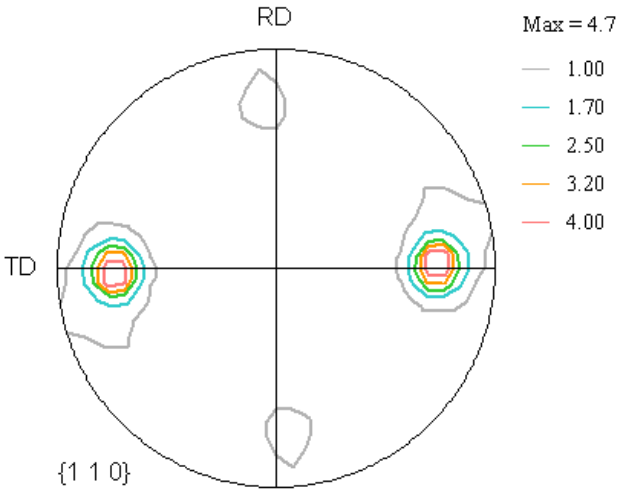


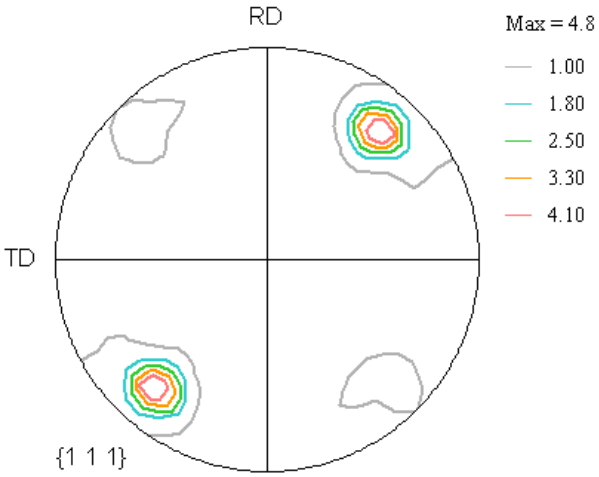



TexViewer - [TexV1]
File Edit View Tools Window Help
Position: 85, 89, 180, (0 -1 0) [0 0 1]
Value: 267.36
Exact value of {hkl}[uvw]
Crystal Orientation Display
Drag crystal to change your point of view
100.0
150.0
200.0
250.0
φ1 = 0°, 180°
Φ = 0°, 180°
Ready
NUM


MonoclinicにおけるODF.docx - Microsoft Word
TexViewer - [TexV1]
File Edit View Tools Window Help
Position: 105, 91, 0, (0 1 0) [0 0 1]
Value: 16.58
Exact value of {hkl}[uvw]
Crystal Orientation Display
Drag crystal to change your point of view
100.0
150.0
200.0
250.0
φ1 = 0°, 180°
Φ = 0°, 180°
Ready
NUM
スタート
3 Windows...
Monoclini...
LaboTex - ...
ResMat - T...
TexViewer ...
Screen Clip
14:22


RD
TD
{0 2 0}
Max = 14.9
1.00
3.80
6.60
9.40
12.20


RD
TD
{1 1 0}
Max = 4.7
1.00
1.70
2.50
3.20
4.00


RD
TD
{1 1 1}
Max = 4.8
1.00
1.80
2.50
3.30
4.10