ＴｒｉｃｌｉｎｉｃにおけるＯＤＦ

２００９年０６月２３日

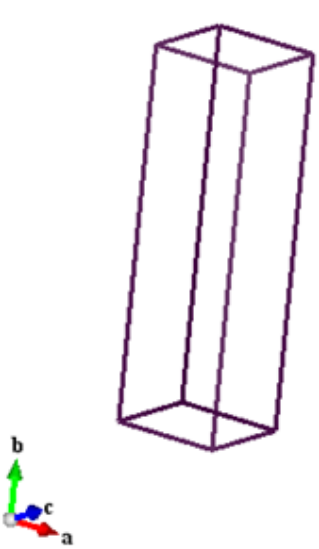
ＨｅｌｐｅｒＴｅｘ

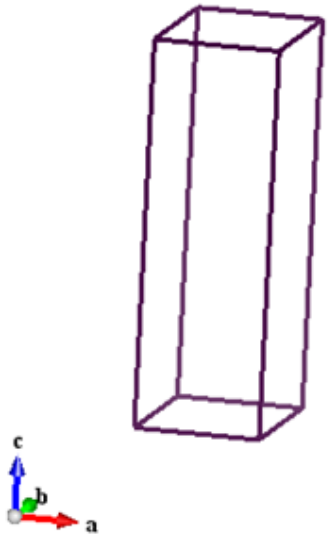
DOC-資料¥LaboTex¥Triclinic-LaboTex

ＬａｂｏＴｅｘでは格子定数　ａ　ｂ　ｃ　α　β　γに関して

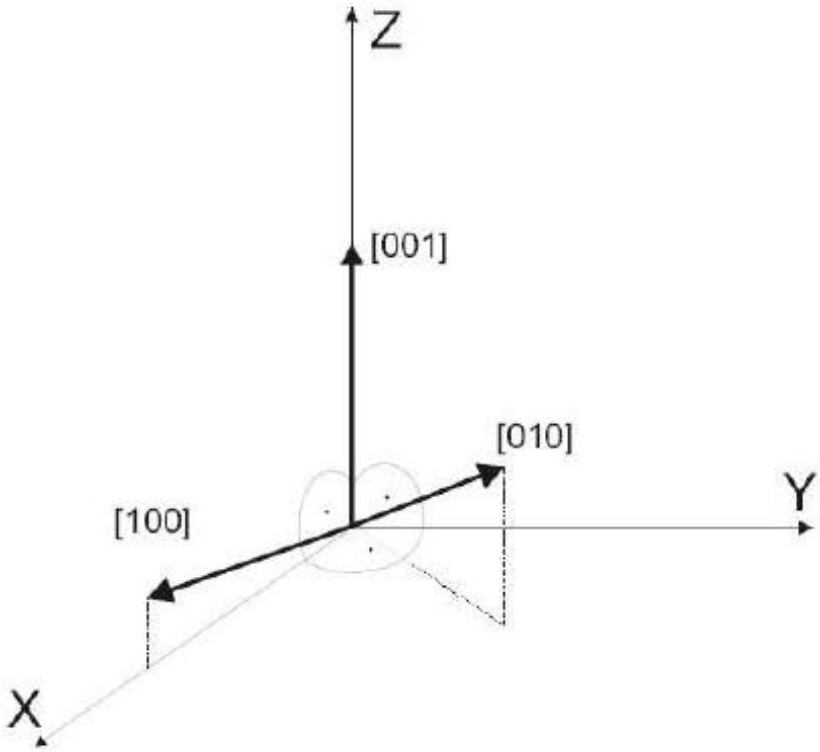
ａ　＜　ｂ　＜　ｃ　　α　β　γ　＜　９０．０の条件がある。

ICDD	LaboTex
P21/c(14)	
Cell: 6.63 20.78 6.5 90.0 99.5 90.0	6.5 6.32 20.78 90 90 80.5

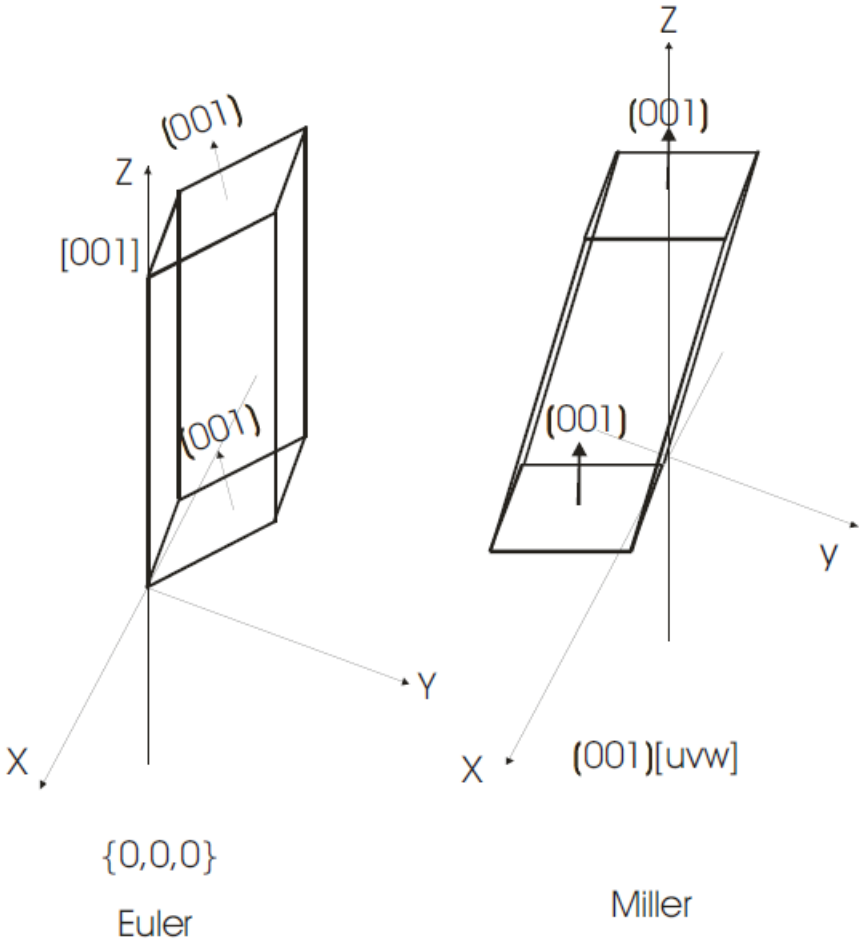




又、Ｃｒｙｓｔａｌとｓａｍｐｌｅの関係はＺ軸は[001]になる。



この為、Ｔｒｉｃｌｉｎｉｃでは

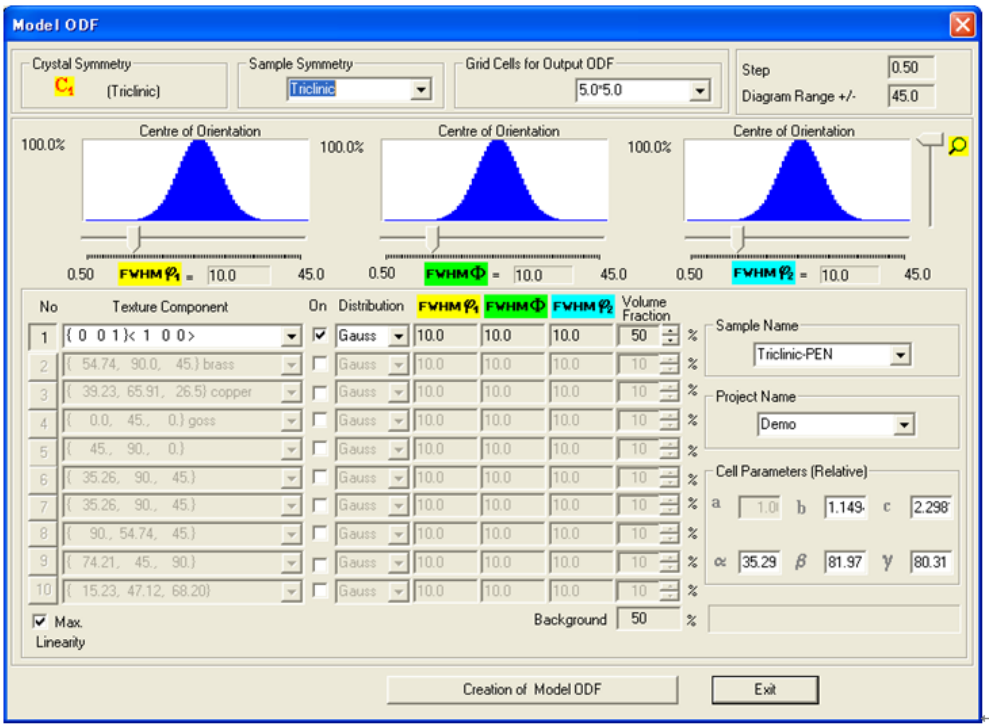


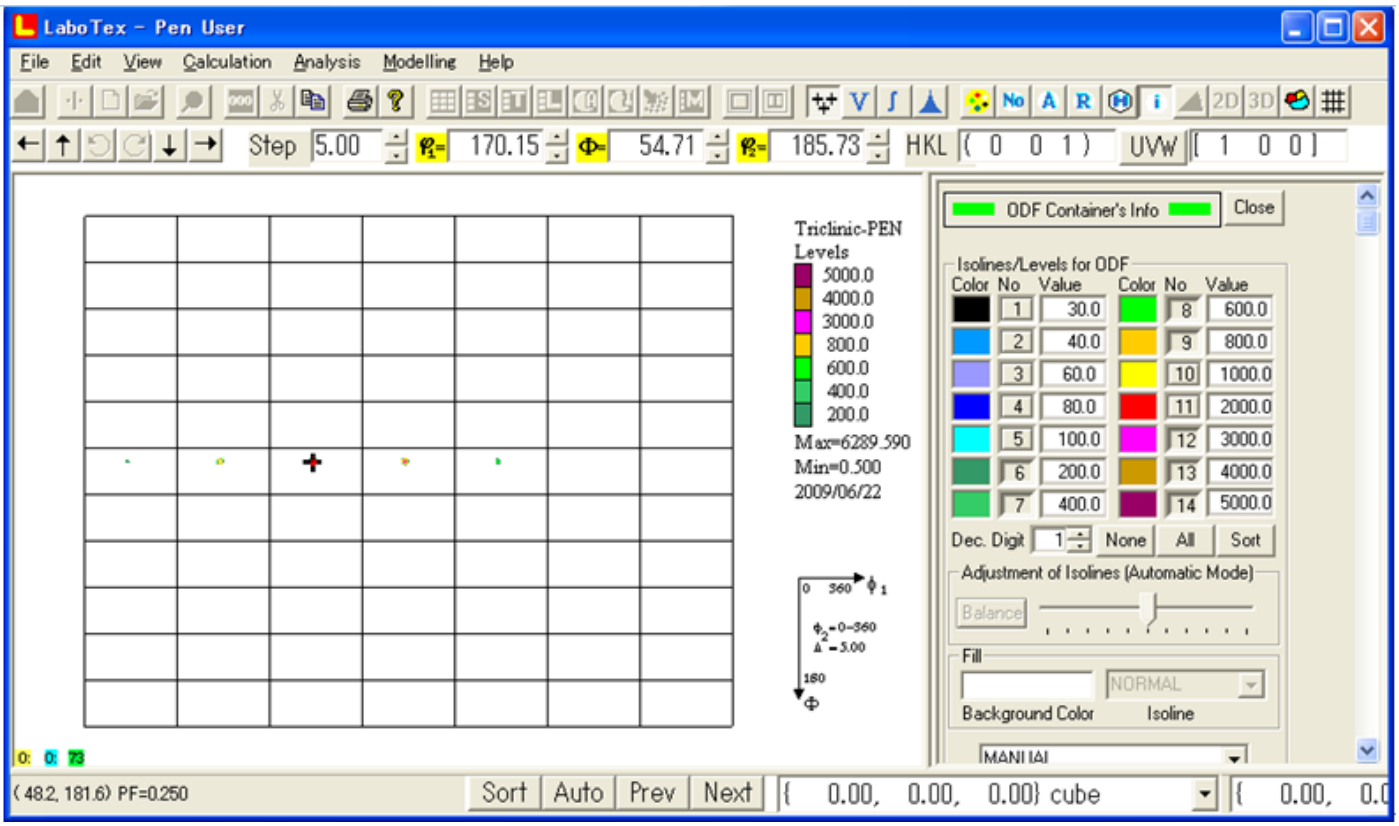
よって、{００１}＜１００＞のＥｕｌｅｒ角度は{０，０，０}にならない

軸変換

ICDD						LaboTex			
h	k	l	d	2θ	I	h	k	l	d
0	0	1	7.652	11.56	25.4	0	0	1	7.651
−1	0	2	6.228	14.21	3.8	0	1	2	6.228
0	1	0	5.681	15.59	95.1	1	0	0	5.681
−1	1	2	4.582	19.35	9.5	1	1	2	4.582
0	−1	1	4.552	19.48	7.7	−1	0	1	4.552
−1	1	1	4.373	20.29	11.3	1	1	1	4.373
−1	0	3	4.246	20.90	2.8	0	1	3	4.246
−1	−1	2	3.895	22.81	10.8	−1	1	2	3.895
1	0	0	3.810	23.33	100.0	0	−1	0	3.810
−1	−1	1	3.774	23.55	17.1	−1	1	1	3.774
−1	1	3	3.601	24.70	2.0	1	1	3	3.601
−1	1	0	3.313	26.89	92.1	1	1	0	3.313
0	−1	2	3.167	28.15	3.1	−1	0	2	3.167
−2	0	4	3.114	28.64	3.6	0	2	4	3.114
−2	1	4	2.938	30.39	0.4	1	2	4	2.938
−2	0	2	2.874	31.09	4.6	0	2	2	2.874

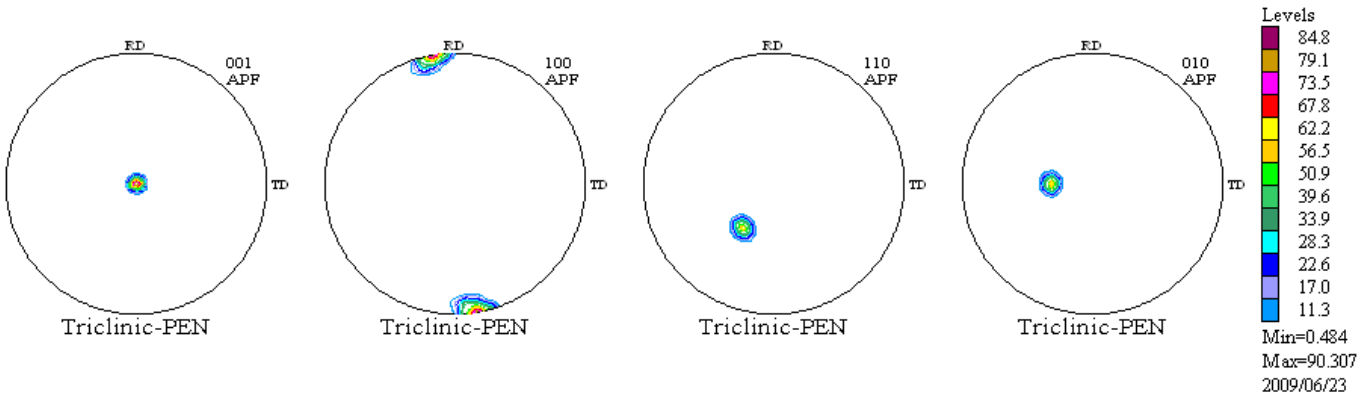
Create {001}<100>



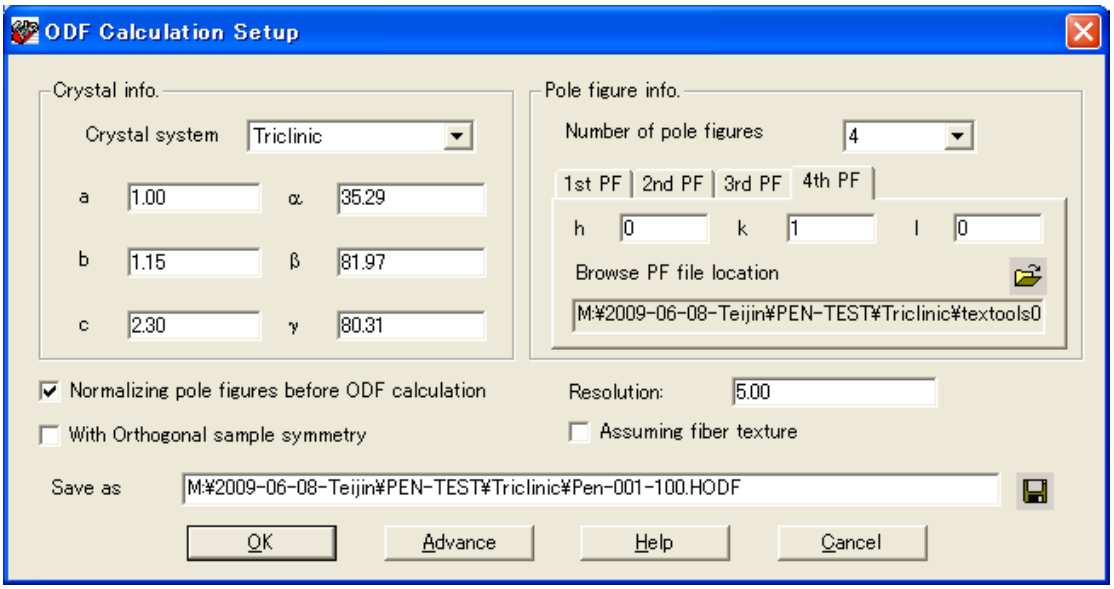


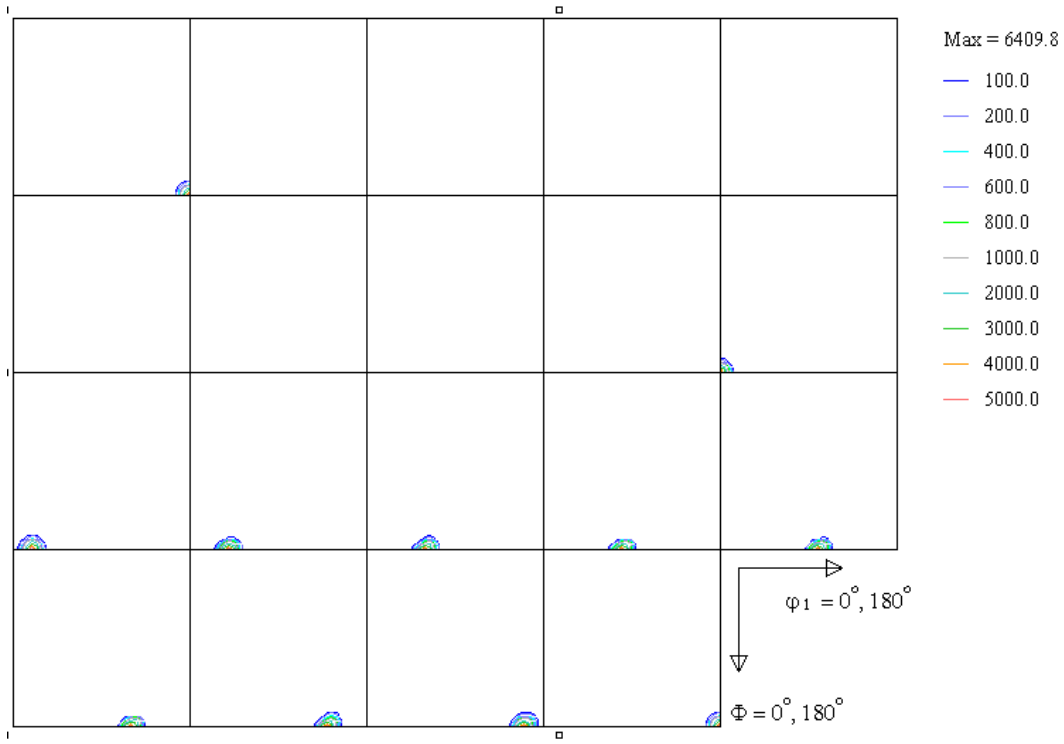
(001)[100] = （φ１、Φ、φ２）＝（170.15,54.71,185.73）

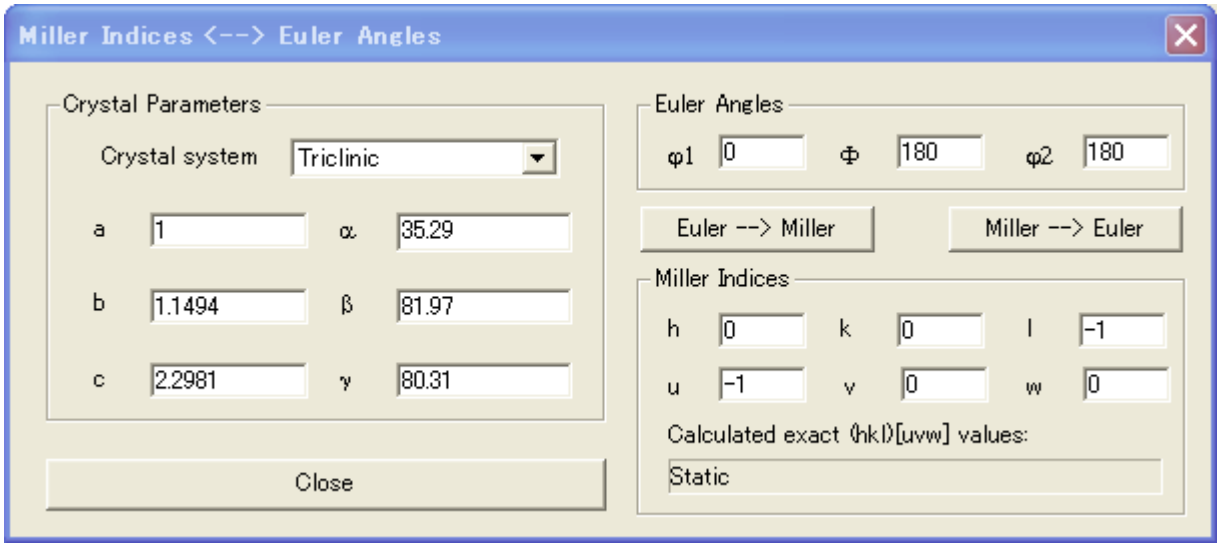
｛００１｝＜１００＞の再計算極点図

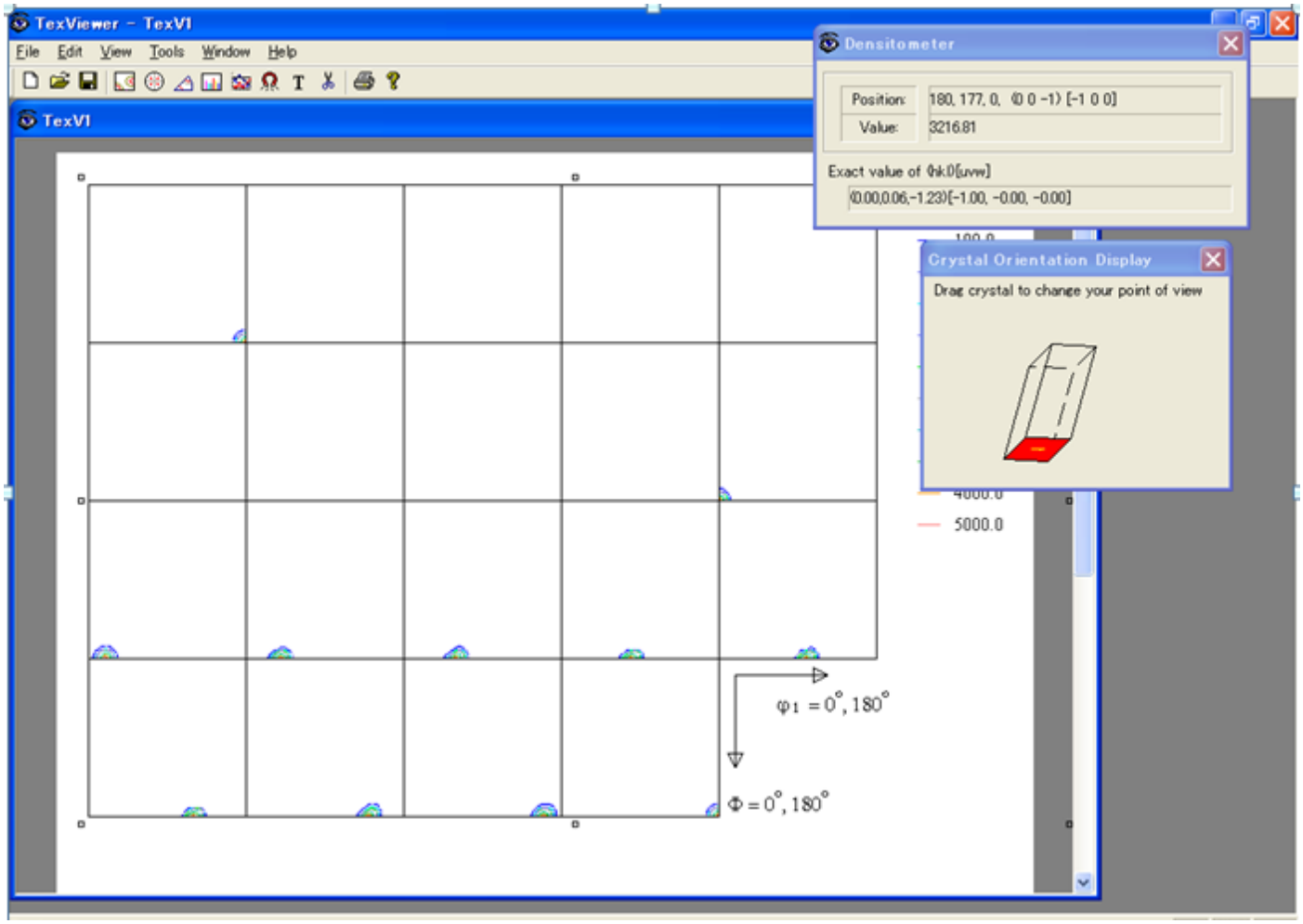


この極点データをＥｘｐｏｒｔｓｉ，ＴｅｘＴｏｏｌｓで解析すると

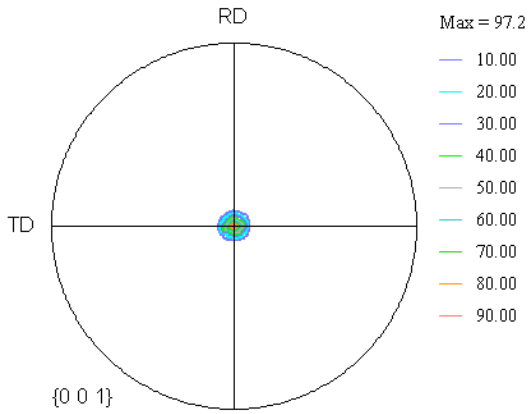


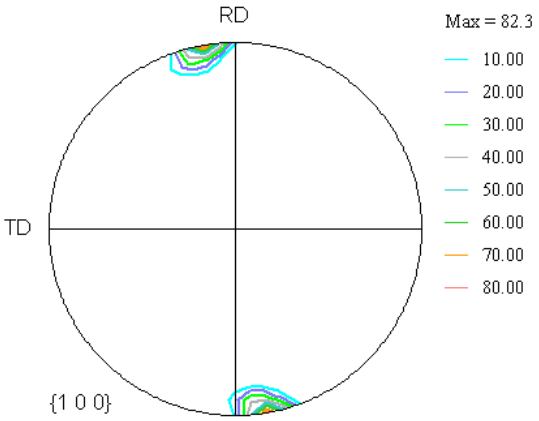


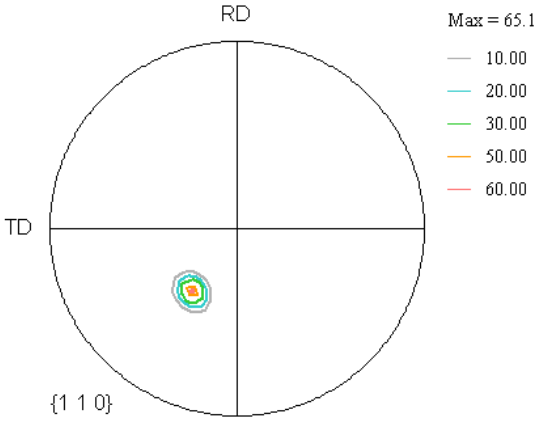


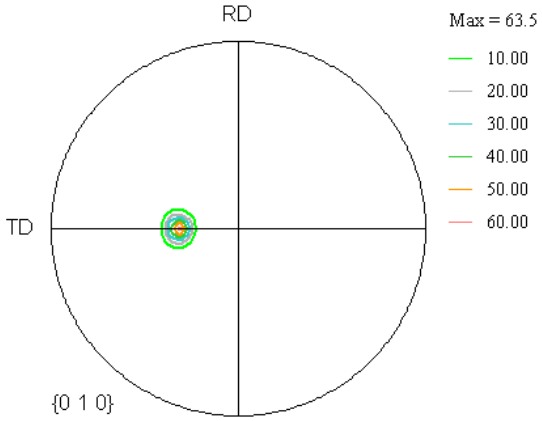


こちらの表現が分かりやすい。



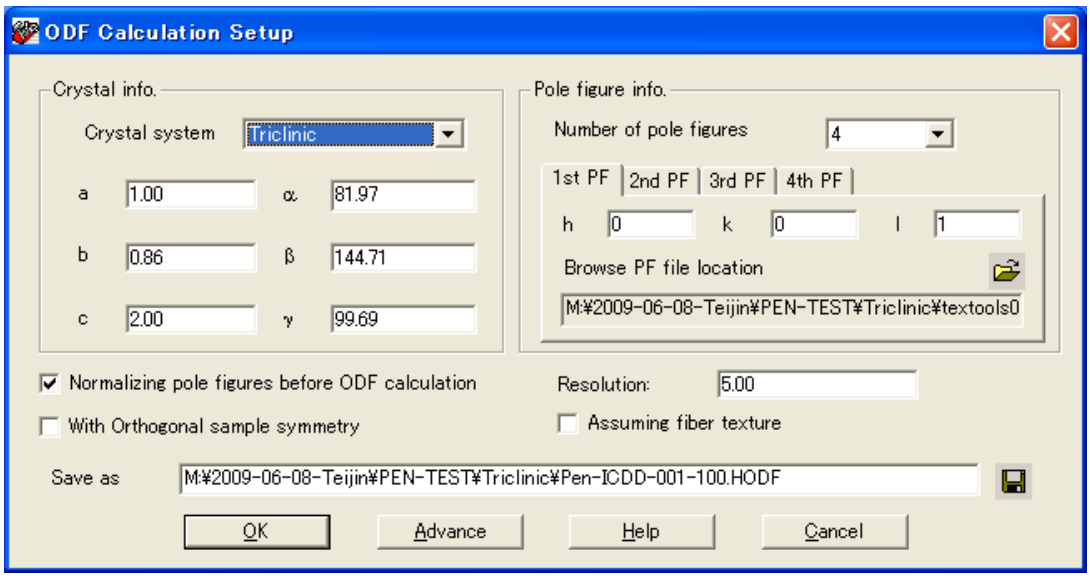


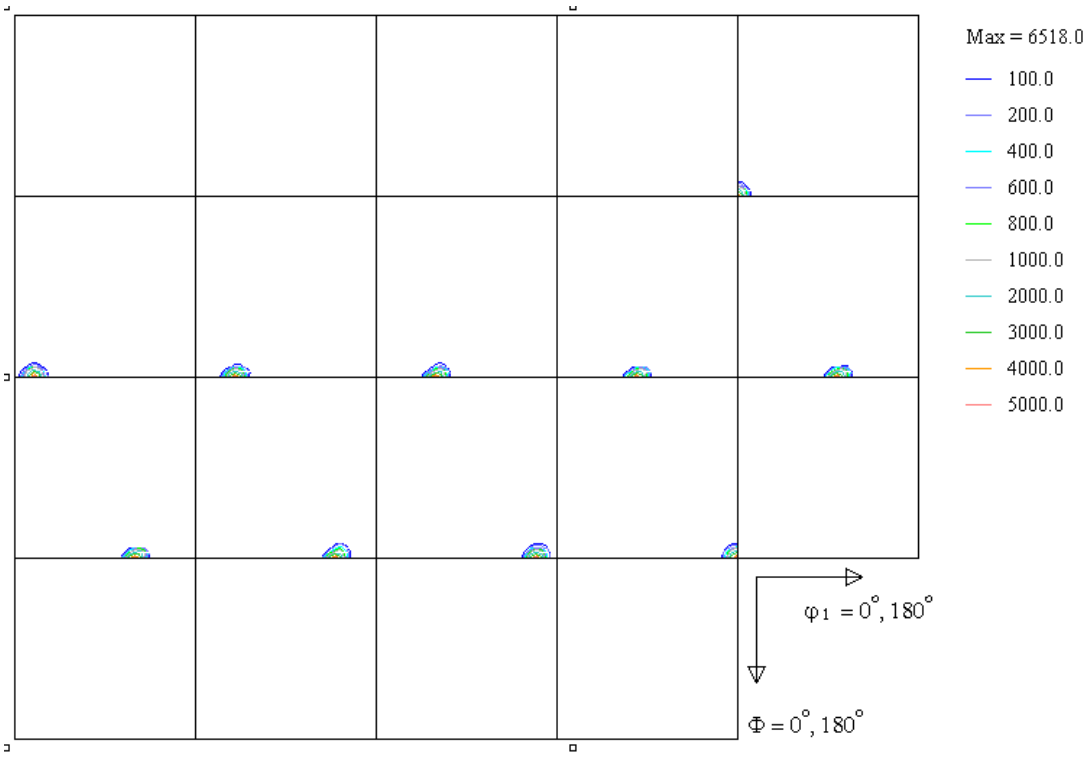


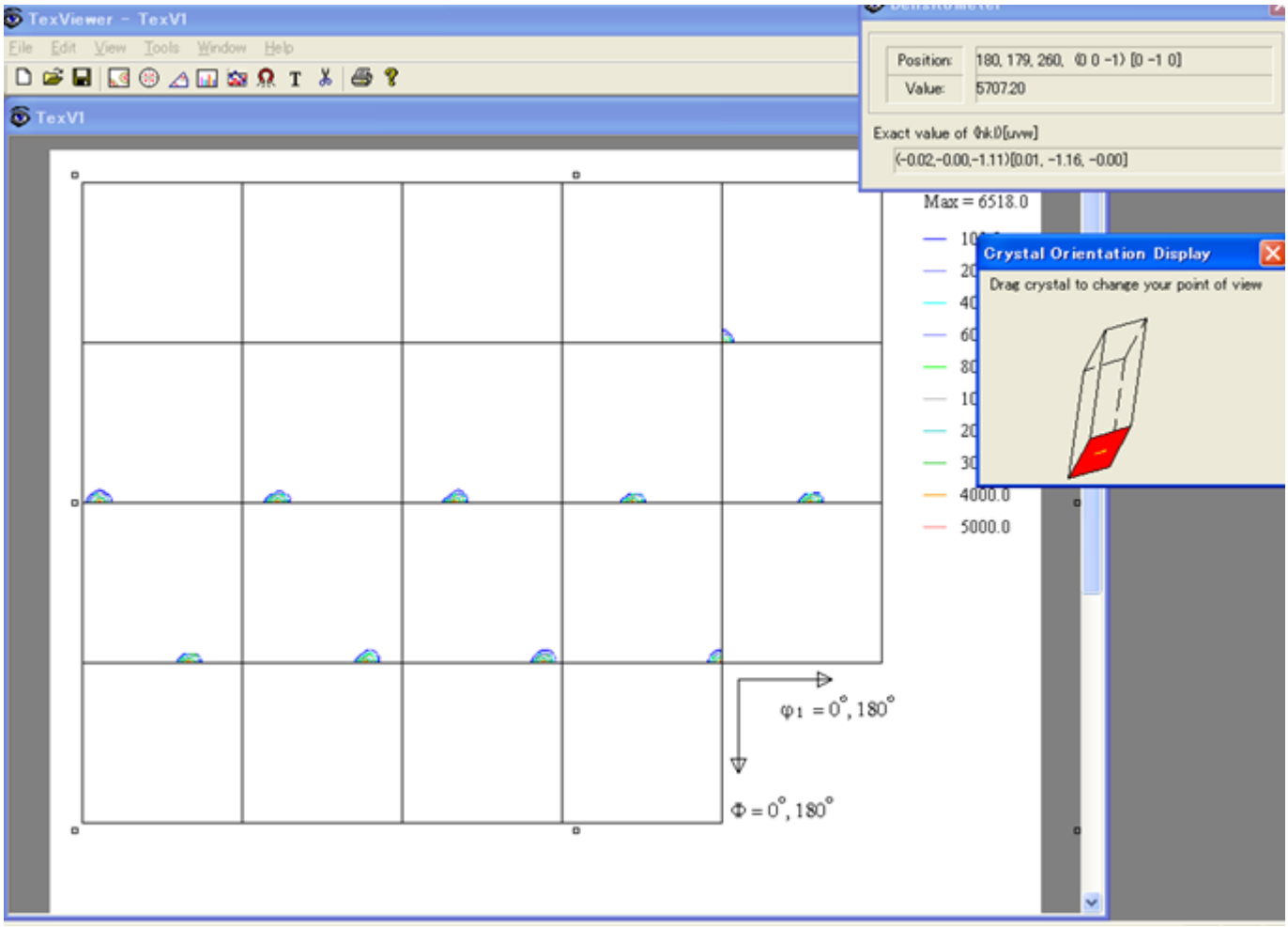


残念ながら逆極点表示には問題があり表示出来ない

軸変換（ＩＣＤＤと同じ）では




Max = 6518.0
100.0
200.0
400.0
600.0
800.0
1000.0
2000.0
3000.0
4000.0
5000.0
φ1 = 0°, 180°
Φ = 0°, 180°


TexViewer - TexV1
File Edit View Tools Window Help
TexV1
Position: 180, 179, 260, (0 0 -1) [0 -1 0]
Value: 5707.20
Exact value of Φ[uvw]
(-0.02,-0.00,-1.11)[0.01, -1.16, -0.00]
Max = 6518.0
Crystal Orientation Display
Drag crystal to change your point of view
4000.0
5000.0
φ1 = 0°, 180°
Φ = 0°, 180°

となる。