

Tr i c l i n i cにおけるODF

2009年06月23日

He l p e r T e x

DOC-資料¥LaboTex¥Triclinic-LaboTex

LaboTexでは格子定数 a b c α β γ に関して
 $a < b < c$ $\alpha \beta \gamma < 90.0$ の条件がある。

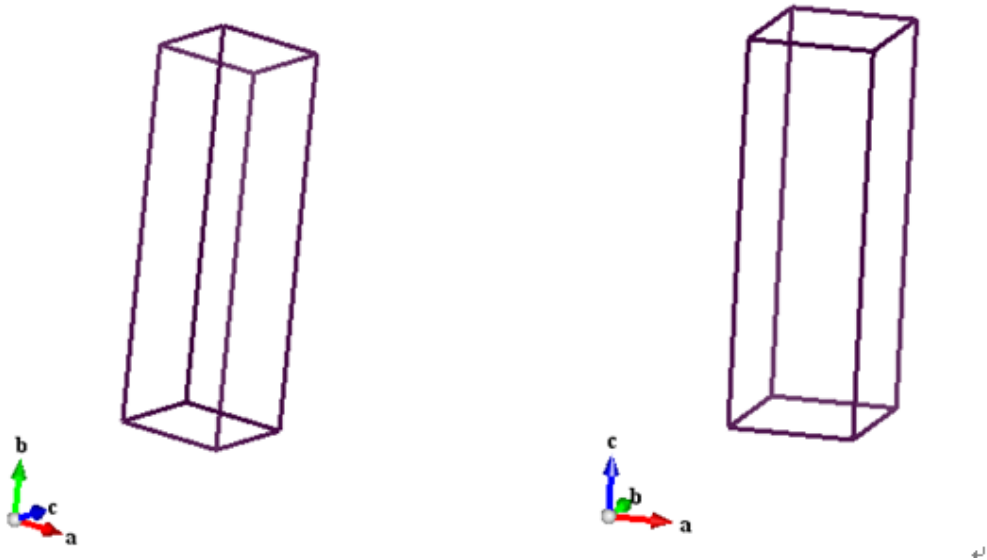
ICDD

P21/c(14)

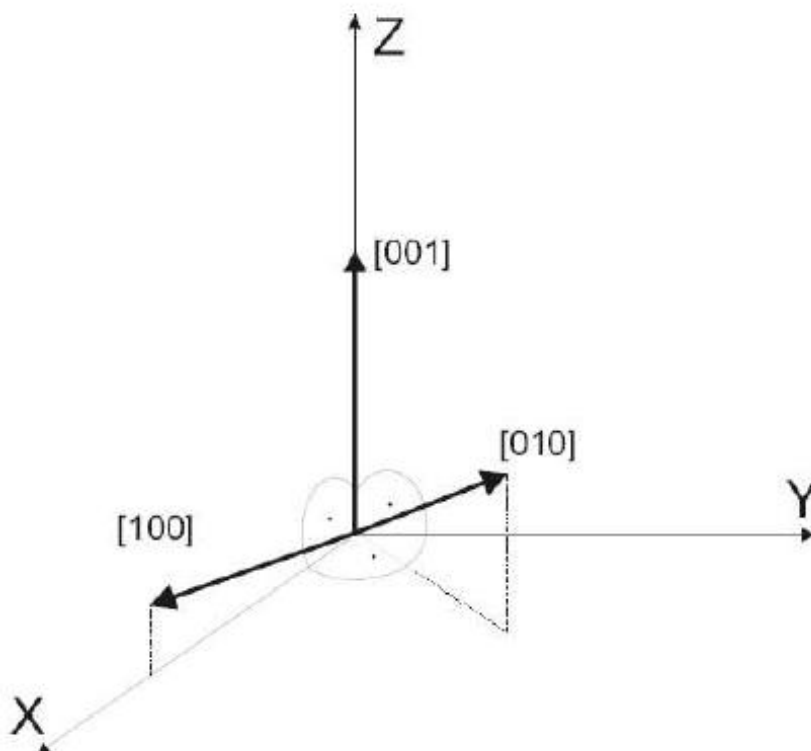
Cell: 6.63 20.78 6.5 90.0 99.5 90.0

LaboTex

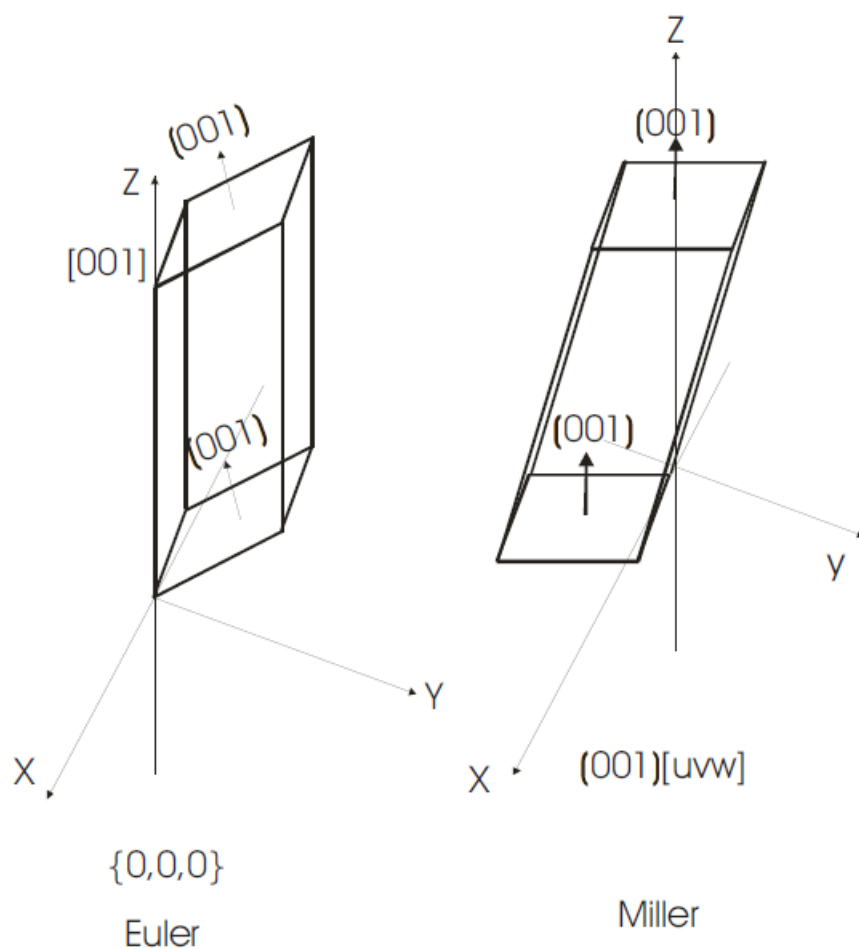
6.5 6.32 20.78 90 90 80.5



又、Crystalとsampleの関係はZ軸は[001]になる。



この為、Triclinicでは



よって、 $\{001\} \langle 100 \rangle$ 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 $\{001\}\langle 100\rangle$

Model ODF

Crystal Symmetry: Triclinic
 Sample Symmetry: Triclinic
 Grid Cells for Output ODF: 5.0x5.0
 Step: 0.50
 Diagram Range +/-: 45.0

Centre of Orientation plots (FWHM $\phi_1 = 10.0$, FWHM $\Phi = 10.0$, FWHM $\phi_2 = 10.0$)

No	Texture Component	On	Distribution	FWHM ϕ_1	FWHM Φ	FWHM ϕ_2	Volume Fraction
1	{ 0 0 1 } < 1 0 0 >	<input checked="" type="checkbox"/>	Gauss	10.0	10.0	10.0	50 %
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: Triclinic-PEN
 Project Name: Demo
 Cell Parameters (Relative): a=1.0, b=1.149, c=2.298
 $\alpha=35.29$, $\beta=81.97$, $\gamma=80.31$

Max Linearity: Background: 50 %

Buttons: Creation of Model ODF, Exit

LaboTex - Pen User

File Edit View Calculation Analysis Modelling Help

Step: 5.00
 $\phi_1 = 170.15$, $\Phi = 54.71$, $\phi_2 = 185.73$
 HKL (0 0 1) UYW [1 0 0]

Triclinic-PEN Levels
 5000.0
 4000.0
 3000.0
 800.0
 600.0
 400.0
 200.0
 Max=6289.590
 Min=0.500
 2009/06/22

ODF Container's Info Close

Color No	Value	Color No	Value
1	30.0	8	600.0
2	40.0	9	800.0
3	60.0	10	1000.0
4	80.0	11	2000.0
5	100.0	12	3000.0
6	200.0	13	4000.0
7	400.0	14	5000.0

Dec. Digit: 1 None All Sort

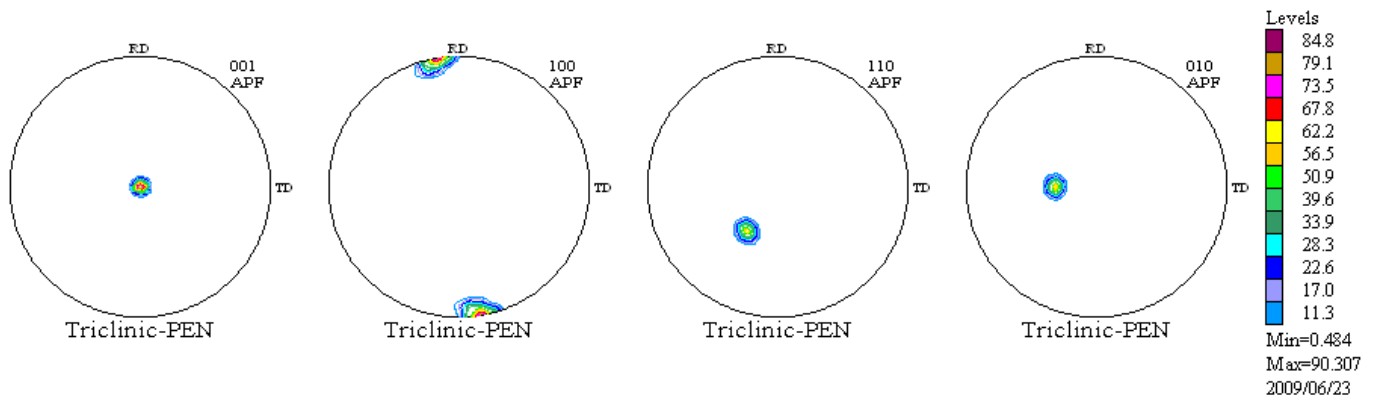
Adjustment of Isolines (Automatic Mode)
 Balance: [Slider]
 Fill: NORMAL
 Background Color: Isoline

MANI IAI

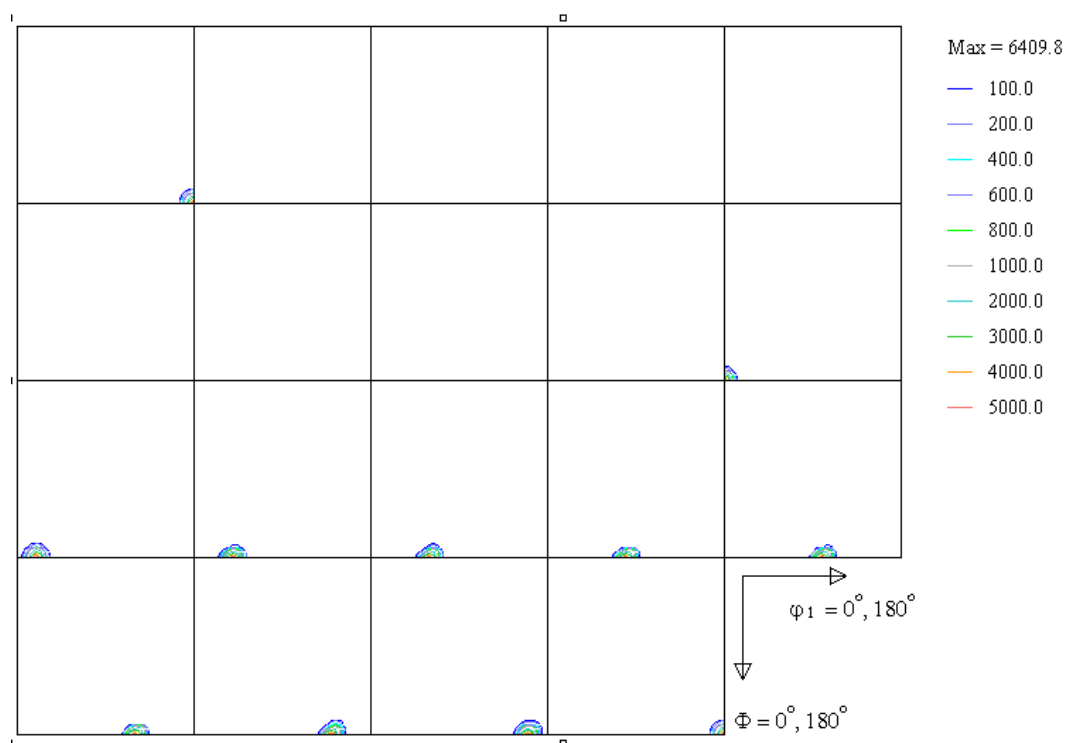
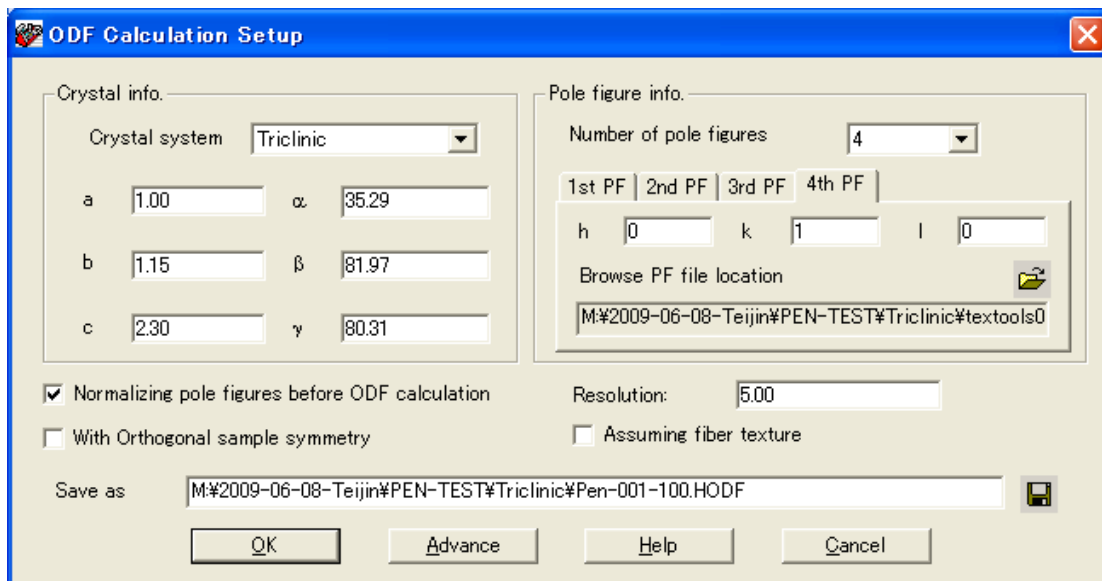
(482, 181.6) PF=0.250
 Sort Auto Prev Next { 0.00, 0.00, 0.00 } cube { 0.00, 0.00

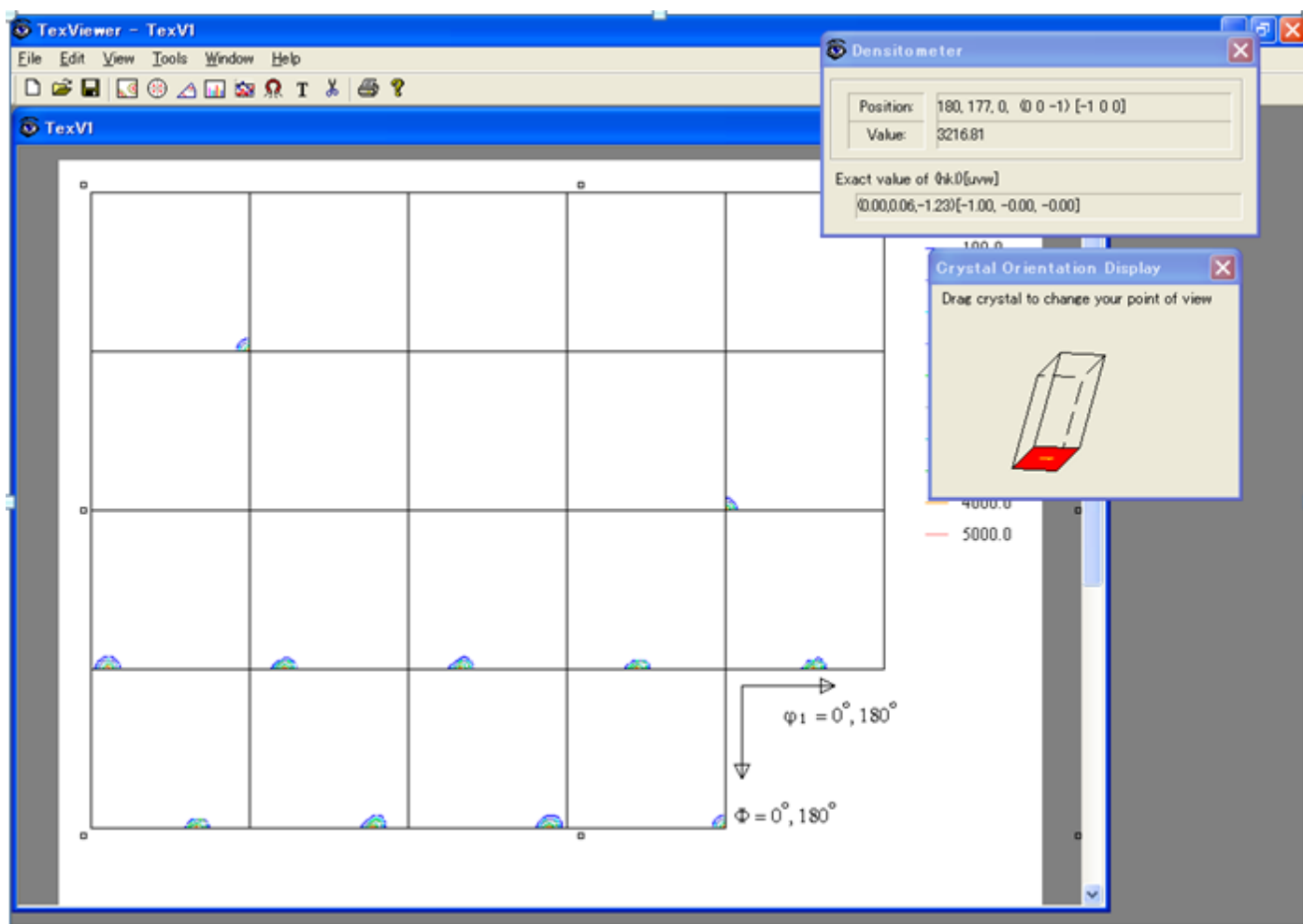
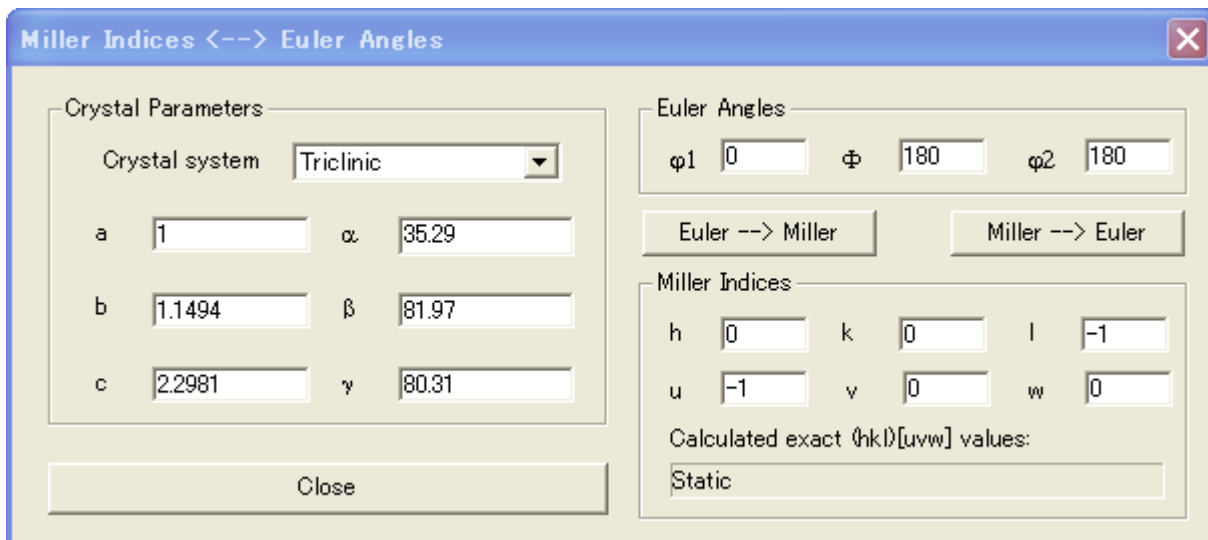
$$(001)[100] = (\phi_1, \Phi, \phi_2) = (170.15, 54.71, 185.73)$$

{001} <100>の再計算極点図

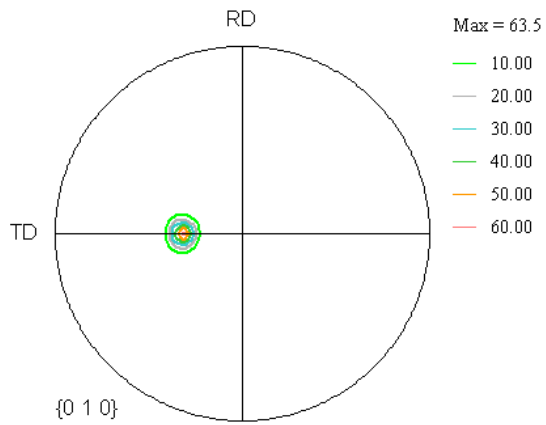
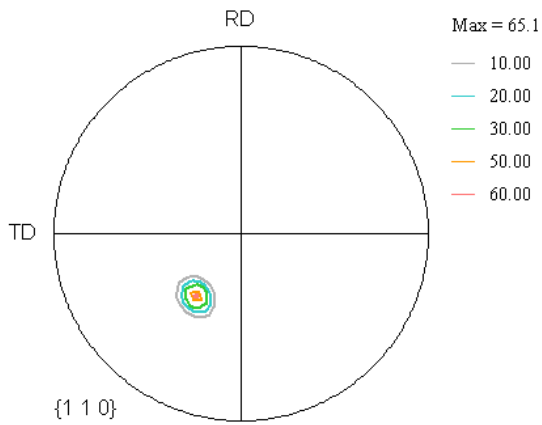
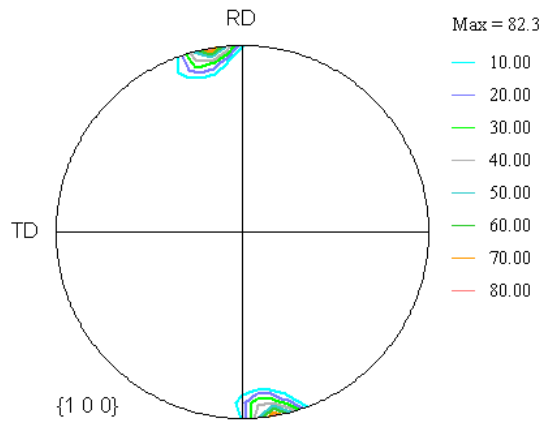
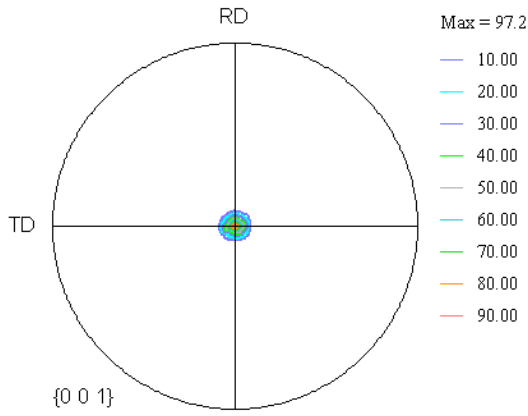


この極点データをExport si, TextToolsで解析すると





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

ODF Calculation Setup

Crystal info.

Crystal system: **Triclinic**

a: 1.00 α: 81.97

b: 0.86 β: 144.71

c: 2.00 γ: 99.69

Pole figure info.

Number of pole figures: 4

1st PF | 2nd PF | 3rd PF | 4th PF

h: 0 k: 0 l: 1

Browse PF file location: M:\2009-06-08-Teijin\PEN-TEST\Triclinic\textools0

Normalizing pole figures before ODF calculation

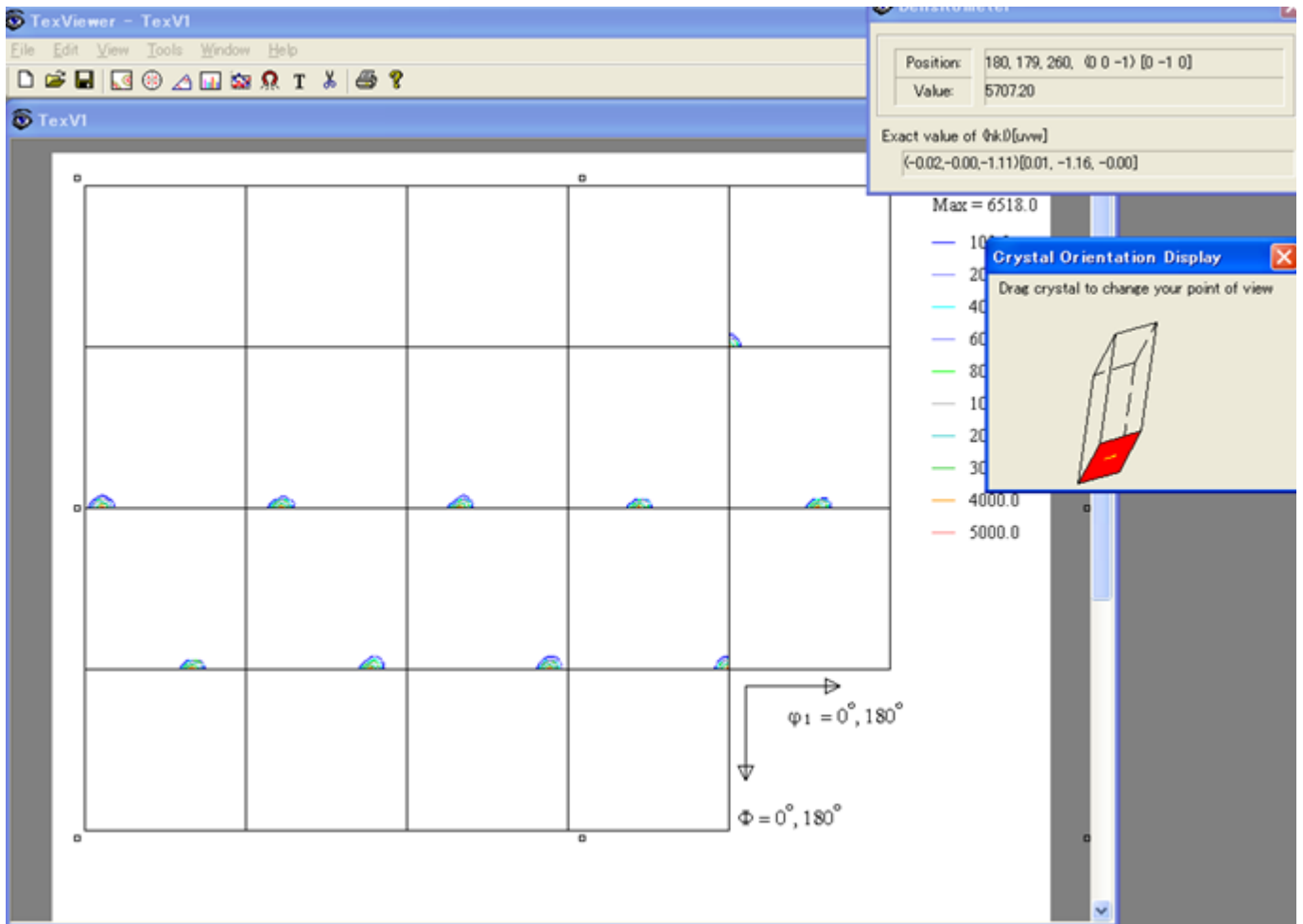
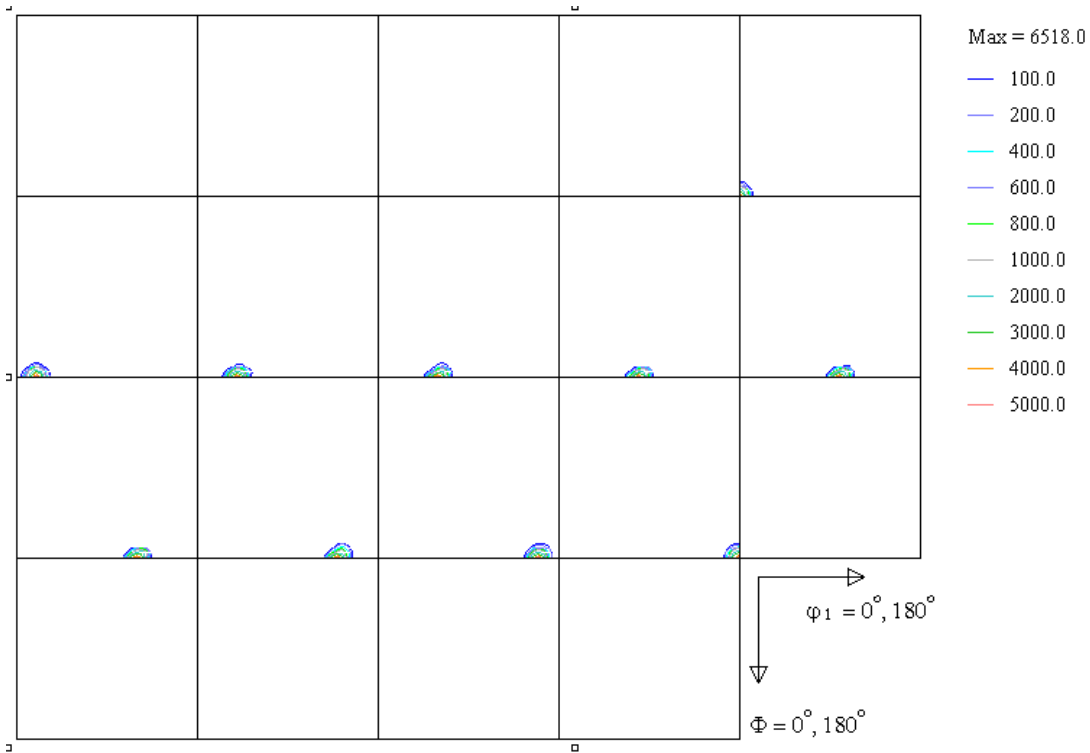
With Orthogonal sample symmetry

Resolution: 5.00

Assuming fiber texture

Save as: M:\2009-06-08-Teijin\PEN-TEST\Triclinic\Pen-ICDD-001-100.HODF

OK Advance Help Cancel



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