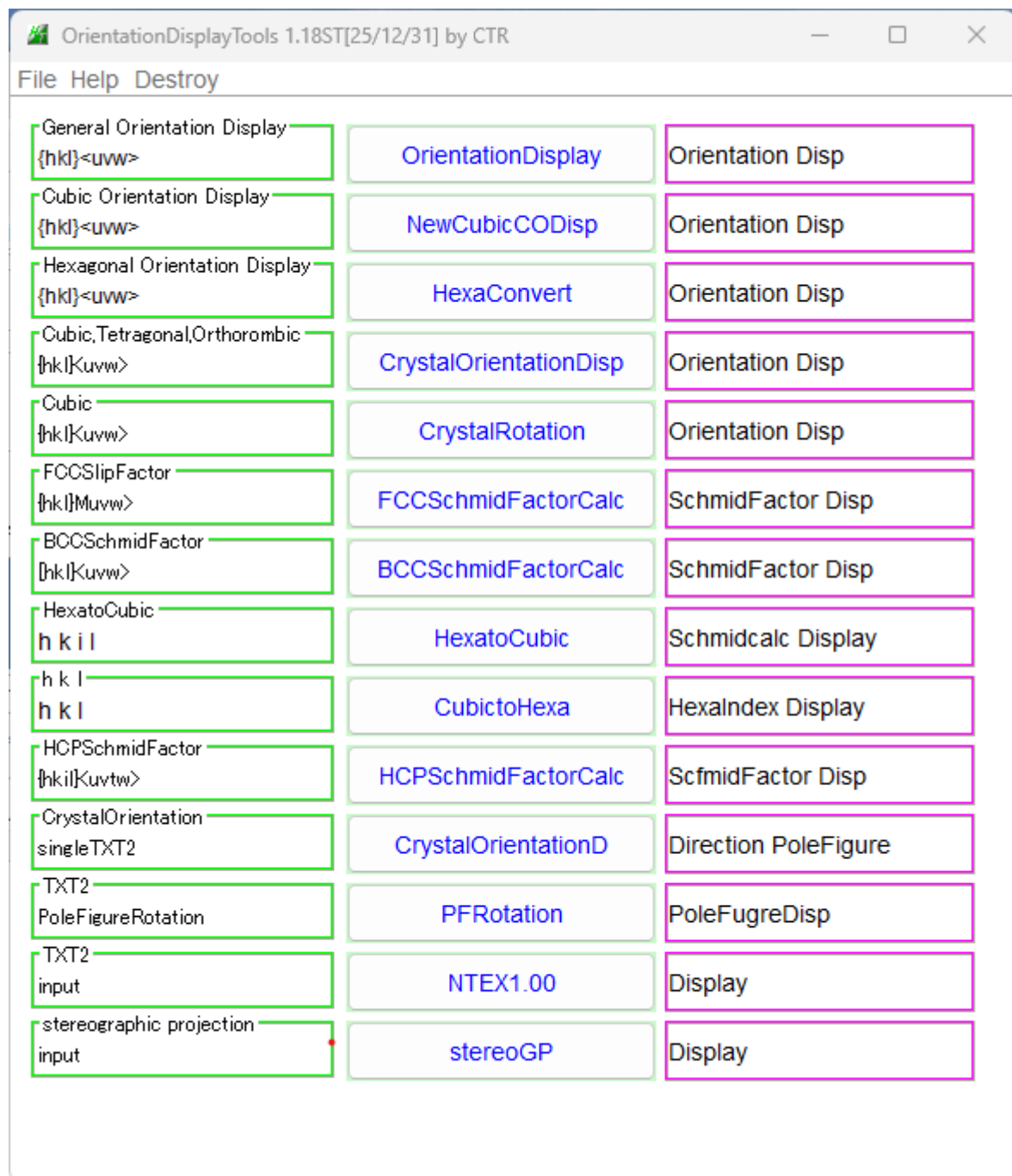


極点図のシュミレーション



2025年12月07日

HelperTex Office

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2. CrystalOrientationD
 2. 1 単結晶方位の計算 (Si単結晶、(220) 極点図より結晶方位計算)
 2. 2 標準ステレオ投影図の描画(計算した結晶方位による)
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 3. 3 ODF 図表示
 3. 4 Triclinic→Orthorhombic
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1. 概要

極点図は極点測定から得られるが、CTRソフトウェアでは以下のソフトウェアで極点図のシュミレーションが行える。

C r y s t a l O r i e n t a t i o n D

N e w C u b i c C O D i s p

C r y s t a l O r i e n t a t i o n D i s p

H e x a C o n v e r t

s t e r e o G P

C r y s t a l O r i e n t a t i o n D

C u b i c 標準ステレオ投影図の描画

単結晶方位の計算

N e w C u b i c C O D i s p

C u b i c 極点図のシュミレーション

極点図、ODF図、逆極点図描画

C r y s t a l O r i e n t a t i o n D i s p

C u b i c、T e t r a g o n a l、O r t h o r h o m b i c 対応

極点図シュミレーション

H e x a C o n v e r t

H e x a g o n a l 極点図シュミレーション

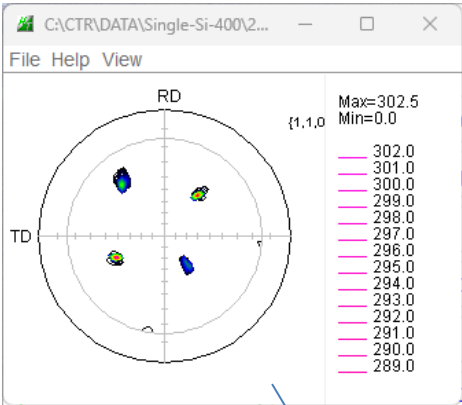
s t e r e o G P

C u b i c、T e t r a g o n a l、O r t h o r h o m b i c、H e x a g o n a l 対応

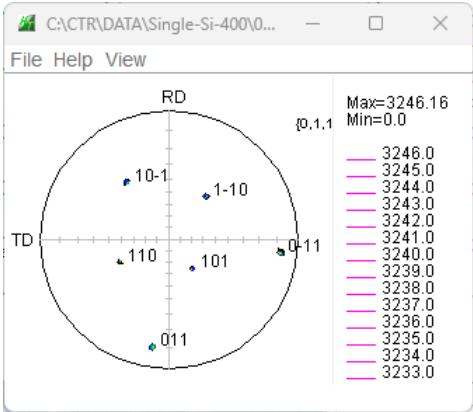
極点図シュミレーション

2. CrystalOrientationD

2. 1 単結晶方位の計算（Si単結晶、(220)極点図より結晶方位計算）



データ選択



指数付け完了

CrystalOrientationD 2.16T[25/12/31] by CTR

File Help Blind-10 CreatePFStep:1.0 hkl disp=true a0->90 X-Axis:South

PoleFigure

Select file

011 ☒ Center of gravity PoleFigure(TXT2) RD input mode is South. Maxindex 20 ExtentAngle 3.0

C:\CTR\DATA\Single-Si-400\220 chB00D8S 2.TXT

Data input area

Alpha(center=0) Xaxis(South: Beta=0)(RD: Beta=180) hkl

45.011 -64.989 1 1 0 to Stack

Reset 45.038 139.993 1 -1 0 Stack

Calculation

ND rotate 0.0 degree calc U-matrix ☐ notContour CalcPoleFigure FWHM 0.1 degree

calc{hkl}<uvw> maxIndex 15 extentAngle 2.0

Calculate Index

CalcPoleFigure

1 1 0 011

1 0 1 Clear

1 0 -1 Set

1 -1 0 Append

0 1 1 All

-1 1 0

0 1 -1

☐ Other(h,k,l) 1,1,1

55.07 -140.45 1 0 -1

sqrtdelete: (1 1 0),(1 -1 0) -> (1 0 -1) temporarily {19 0 4}<4 -16 -19>

Xaxis(South: Beta=0)(RD: Beta=180)

ND rotate =0.0

Alpha	Beta	
45.011	-64.989	1 1 0
45.038	139.993	1 -1 0

U-matrix

-0.18193451993510923	0.6048079349834435	0.7753110293534099
-0.11035308023070894	-0.7960475195436751	0.5950886860896928
0.9770987811575533	0.022709214196552974	0.2115709418871103

Direction Alpha Beta center=90

1 1 0	45.01	-64.99	44.99	115.011
0 1 1	80.46	-8.28	9.54	171.715
1 0 1	32.81	39.25	57.19	219.246
0 -1 1	82.33	83.01	7.67	263.012
1 -1 0	47.56	138.93	42.44	318.926
1 0 -1	57.23	-143.61	32.77	36.388

CalcPoleFigure

Direction	Alpha	Beta	Center=90
1 1 0	45.01	-64.99	115.011
1 0 1	32.81	39.25	219.246
1 0 -1	57.23	-143.61	36.388
1 -1 0	47.56	138.93	318.926
0 1 1	80.46	-8.28	171.715
0 -1 1	82.33	83.01	263.012

PoleFigure holder

Holder C:\CTR\work\CrystalOrientationD

Initialize File

CrystalOrientationD 2.16T[25/12/31] by CTR

File Help Blind-10 CreatePFStep:1.0 hkl disp=true a0->90 X-Axis:South

PoleFigure

Select file
 ☒ Center of gravity PoleFigure(TXT2) RD input mode is South. Maxindex ExtentAngle

C:\CTR\DATA\Single-Si-400\220 chB00D3S 2.TXT
 Data input area

Alpha(center=0) Xaxis(South: Beta=0)(RD: Beta=180) hkl

Calculation

ND rotate degree ☐ notContour FWHM degree

{hkl}<uvw>

maxIndex extentAngle

Calculate Index

CalcPoleFigure

☐ Other(h,k,l)

0.0 -176.99 11 0 2
 0.0 96.38 0 0 3
 0.0 132.62 0 0 3

結晶方位計算結果

calcuw
 chiangle phiangle calcuw

89.3	-178.85	1	-3	-4
91.52	179.13	1	-4	-5
90.54	-179.98	2	-7	-9
88.42	178.87	3	-9	-11
89.4	178.24	3	-10	-12
90.16	-179.63	3	-10	-13
90.89	179.7	3	-11	-14
91.5	-178.48	3	-11	-15
88.54	-178.16	4	-11	-15
88.65	179.46	4	-12	-15

{hkl}<uvw>(extentAngle=2.0)
 (4 0 1)[1 -3 -4] (306.04 75.96 90.0)
 (4 0 1)[3 -10 -12] (308.95 75.96 90.0)
 (5 0 1)[1 -4 -5] (308.11 78.69 90.0)
 (5 0 1)[3 -11 -15] (305.72 78.69 90.0)
 (9 0 2)[2 -7 -9] (307.21 77.47 90.0)
 (13 0 3)[3 -10 -13] (306.85 77.01 90.0)
 (14 0 3)[3 -11 -14] (307.53 77.91 90.0)

PoleFigure holder
 C:\CTR\work\CrystalOrientationD

2. 2 標準ステレオ投影図の描画(計算した結晶方位による)

C:\CTR\DATA\Single-Si-400\220 chB00D3S 2.TXT
 Data input area

Alpha(center=0) Xaxis(South: Beta=0)(RD: Beta=180) hkl

Calculation

ND rotate degree ☒ notContour FWHM degree

{hkl}<uvw>

maxIndex extentAngle

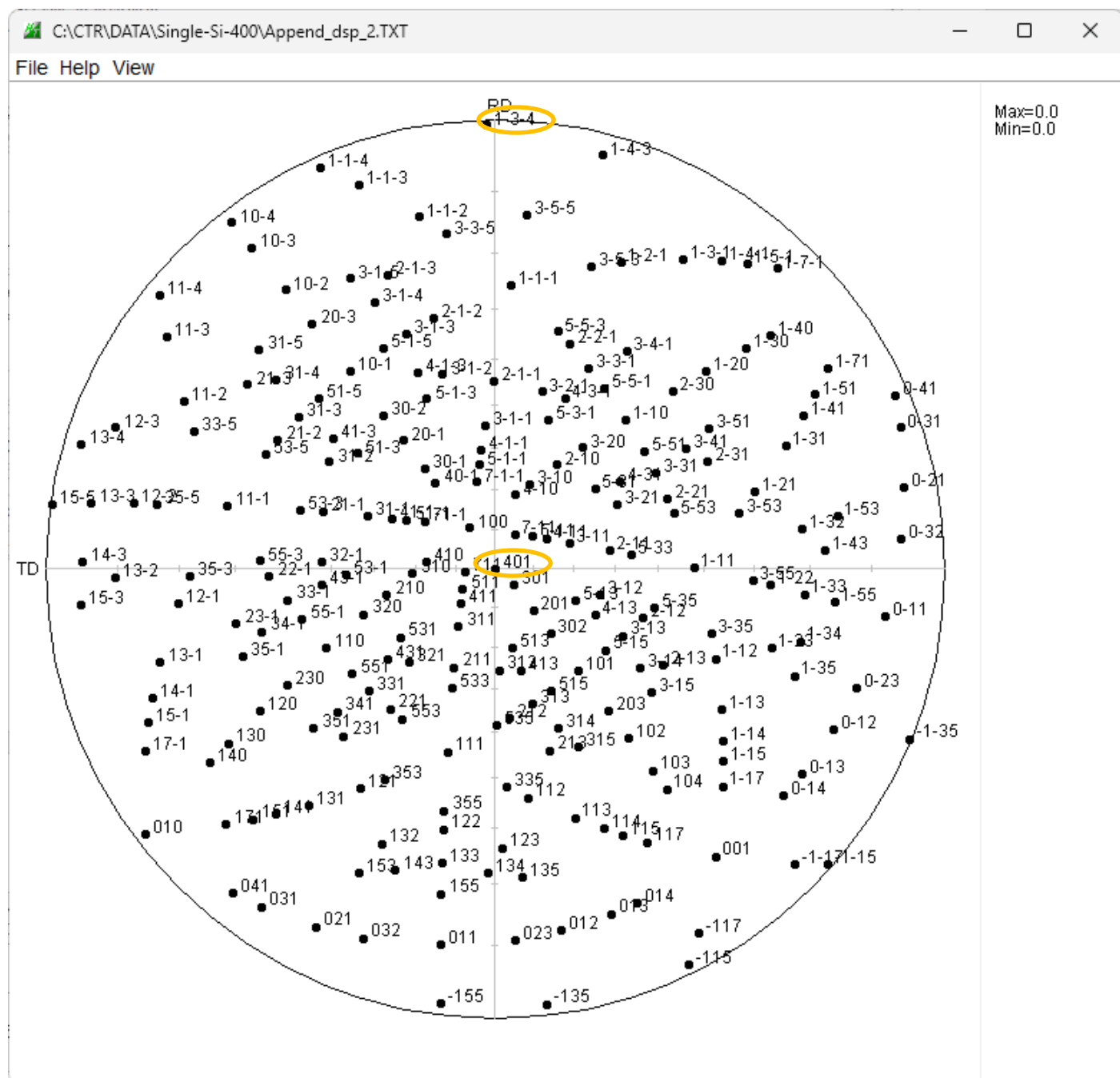
Calculate Index

CalcPoleFigure

☒ Other(h,k,l)

All + Append (1, 3, 4)

(4 0 1) [1 - 3 - 4] ステレオ投影図



3. NewCubicCODisp

3.1 方位選択、方位入力

NewCubicCODisp 1.36T[25/12/31] by CTR

File Help Symmetry Special Index Task

Miller Indices

(hkl)[uvw] 1

PoleFigure & ODF & Inverse

FWHM 5 deg

PF OrthoPF

OrthoODF Inverse ND Inv.Disp

Euler Angle

(p1 P p2) <=90 0.0 54.7356 45.0

Calc toOrthorhombic

Present Condition

Euler Angle

Double Miller Indices

DISP

Position 10 Disp size 400 DISP

BG color Black Line size 2.0 Minus

Makefileholder

Holder C:\CTR\WORK\NewCubicCODisp

NewCubicCODisp 1.36T[25/12/31] by CTR

File Help Symmetry Special Index Task

Miller Indices

(hkl)[uvw] 1 3 2 6 -4 3 TD:[179-22]

Calc

PoleFigure & ODF & Inverse

FWHM 5 deg Gratio 1.0

☒ Lorentzcut(Max/20) Polefigure 001 ☐ Other 1,2,3

PF OrthoPF calcODF OrthoODF Inverse ND Inv.Disp

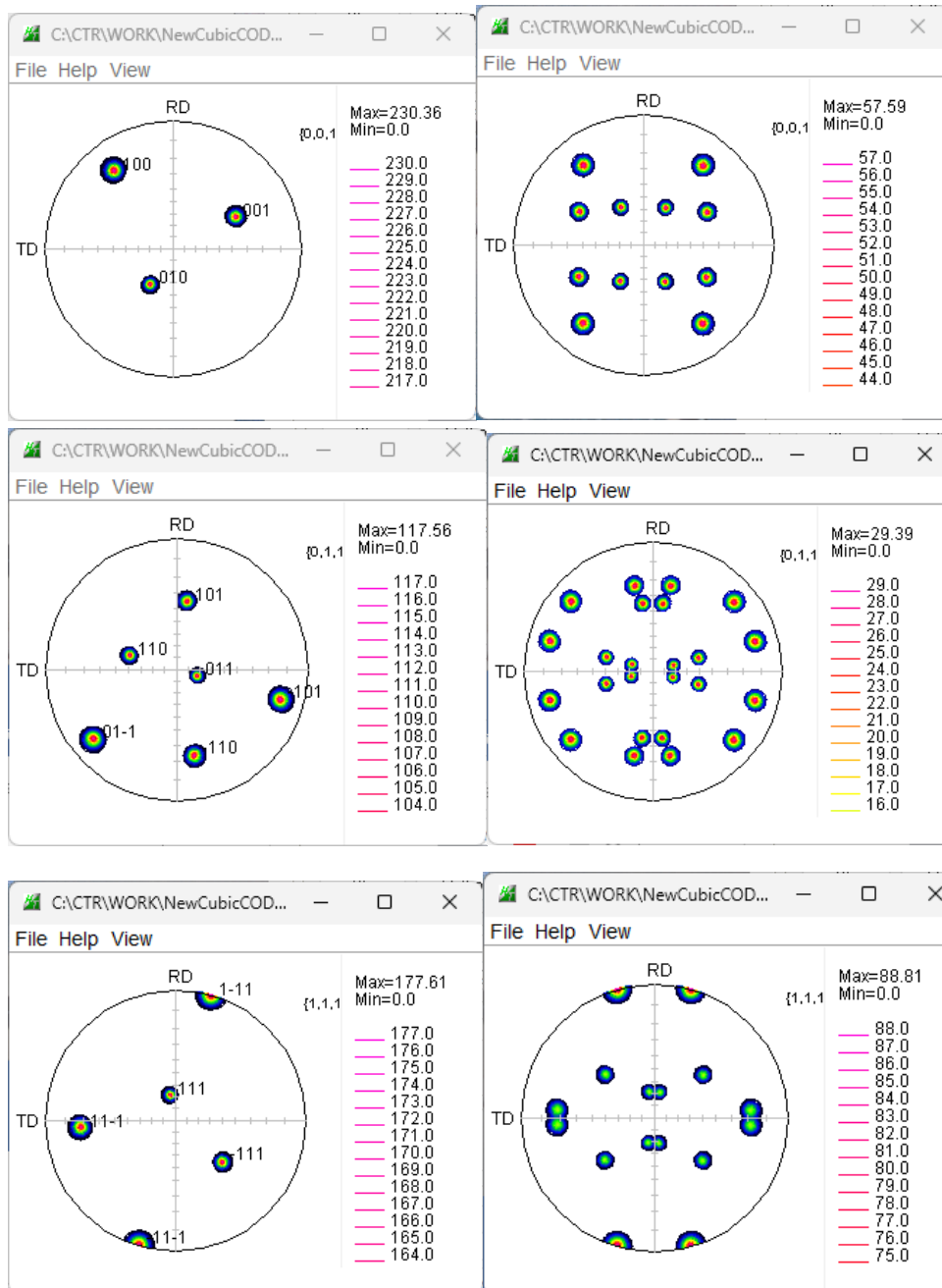
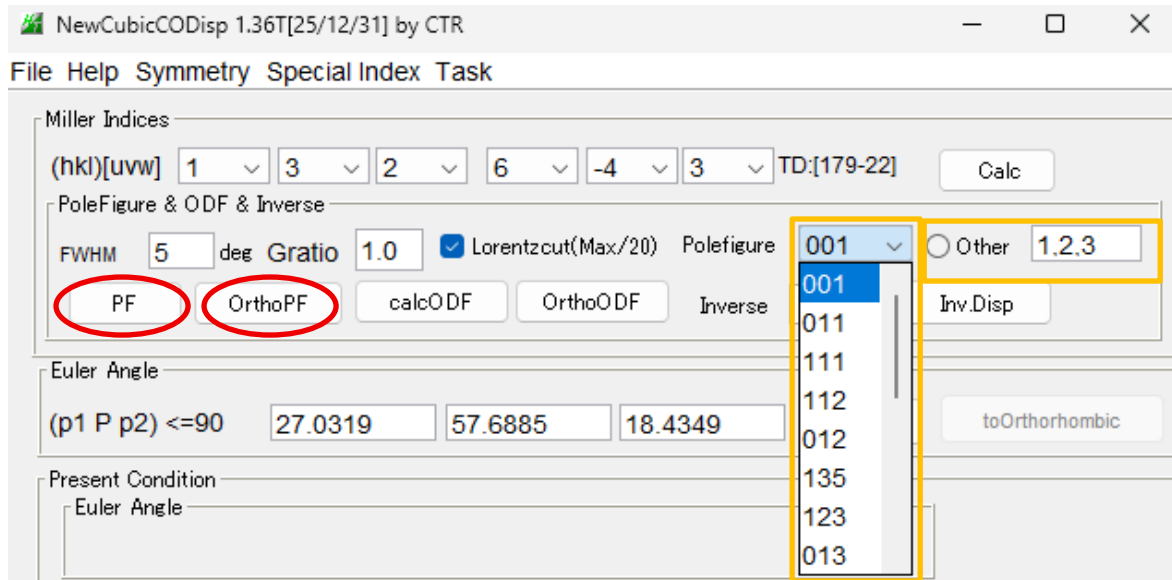
Euler Angle

(p1 P p2) <=90 27.0319 57.6885 18.4349

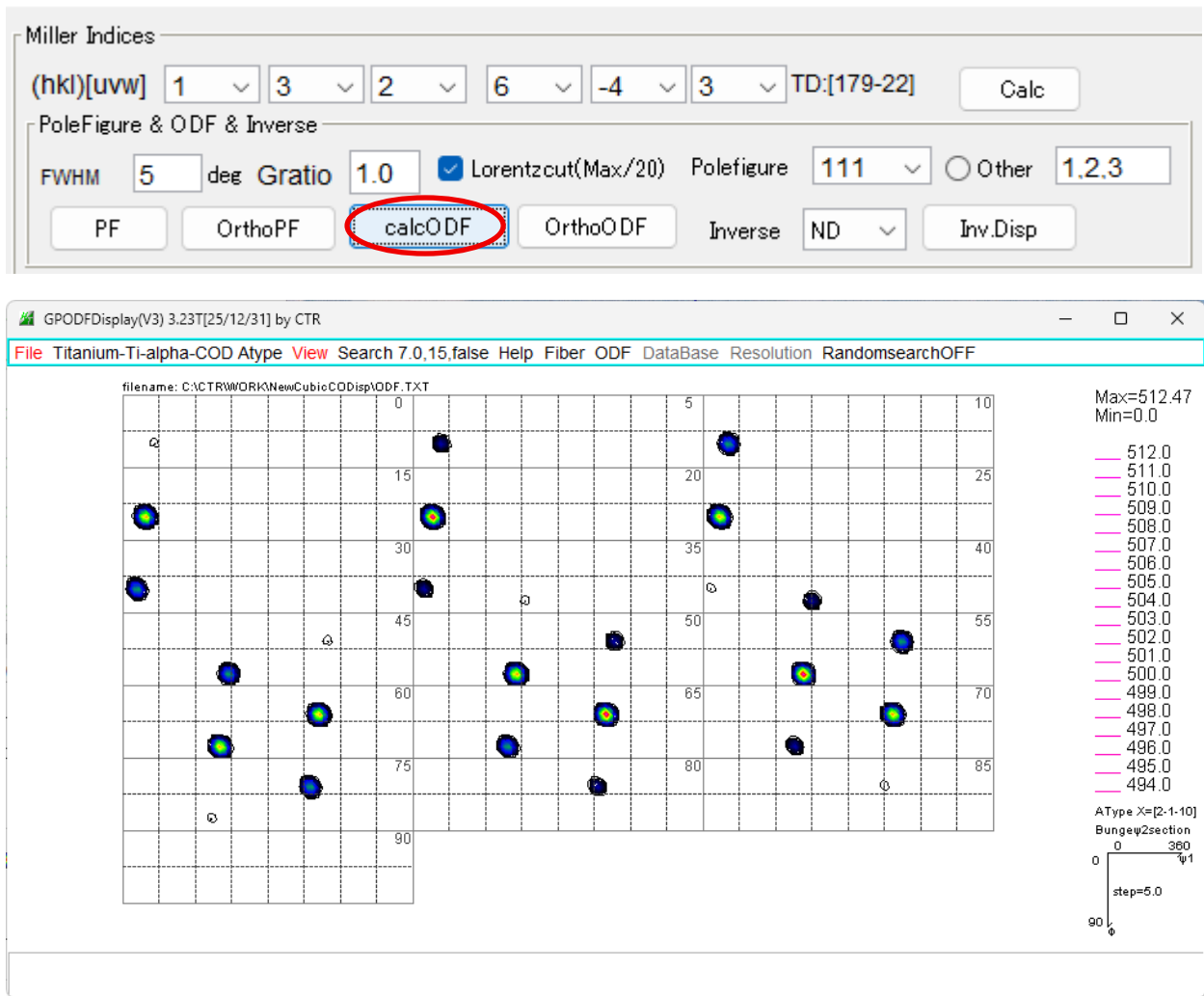
Calc toOrthorhombic

極点図、ODF図、逆極点図表示

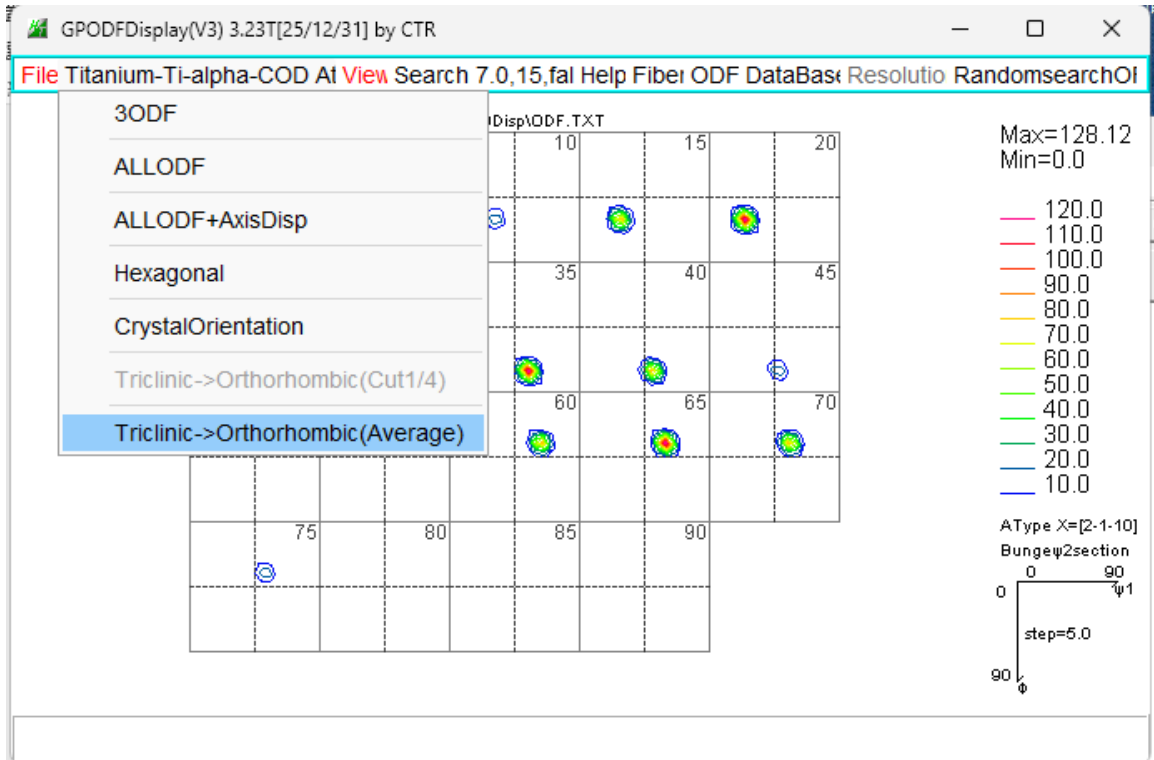
3. 2 極点图表示



3. 3 ODF 图表示



3. 4 Triclinic—>Orthorhombic



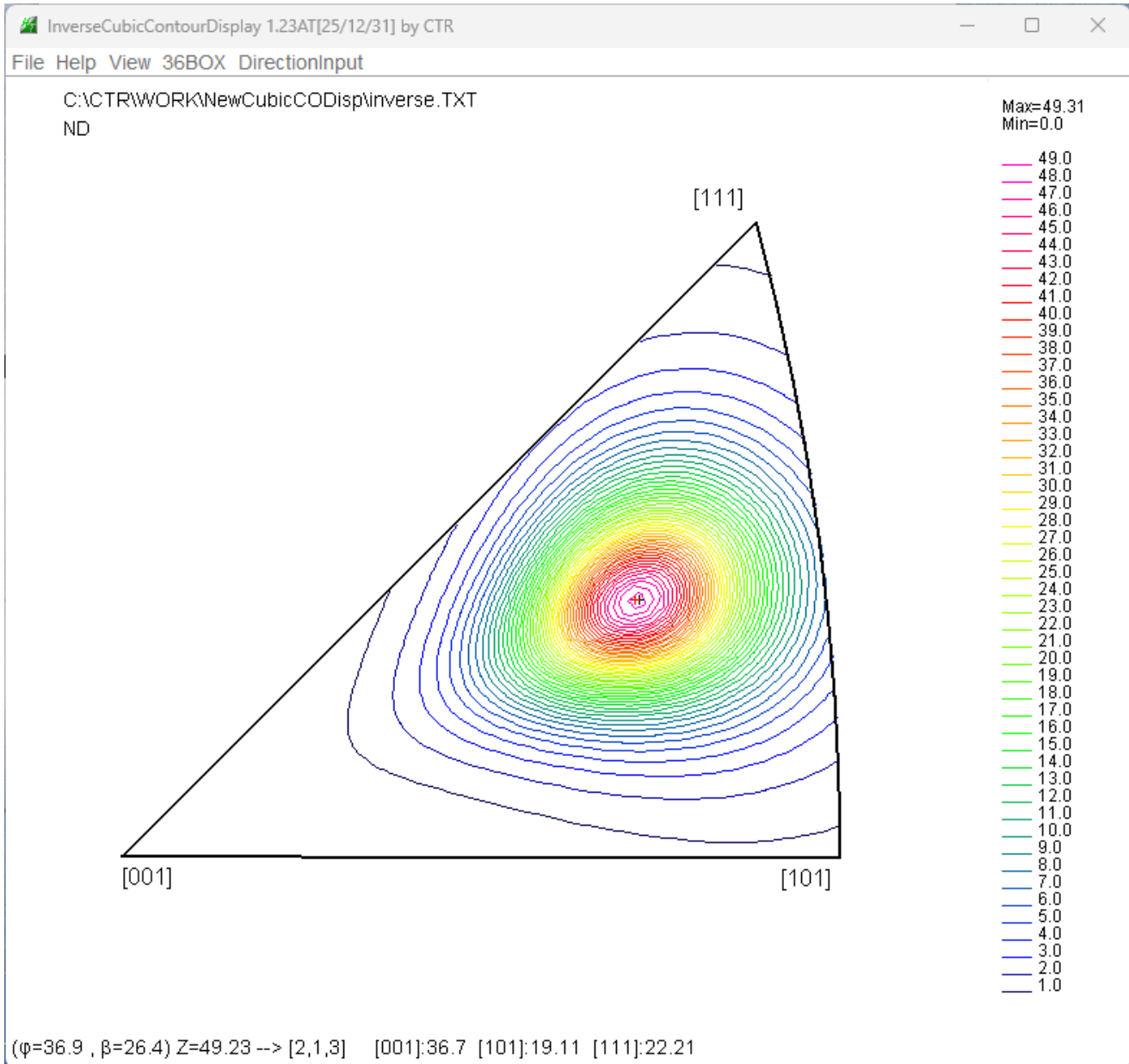
3. 5 逆極点图表示

Miller Indices
(hkl)[uvw] 1 3 2 6 -4 3 TD:[179-22] Calc

PoleFigure & ODF & Inverse
FWHM 5 deg Gratio 1.0 ☒ Lorentzcut(Max/20) Polefigure 001 ☐ Other 1.2.3

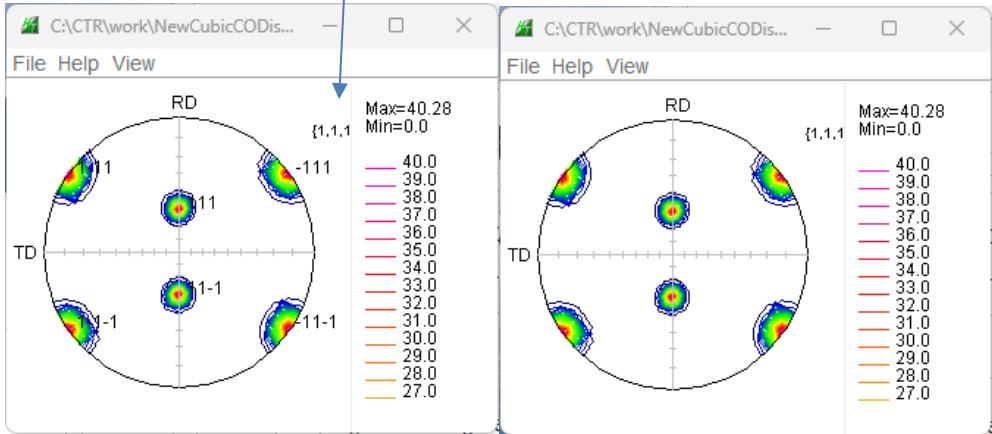
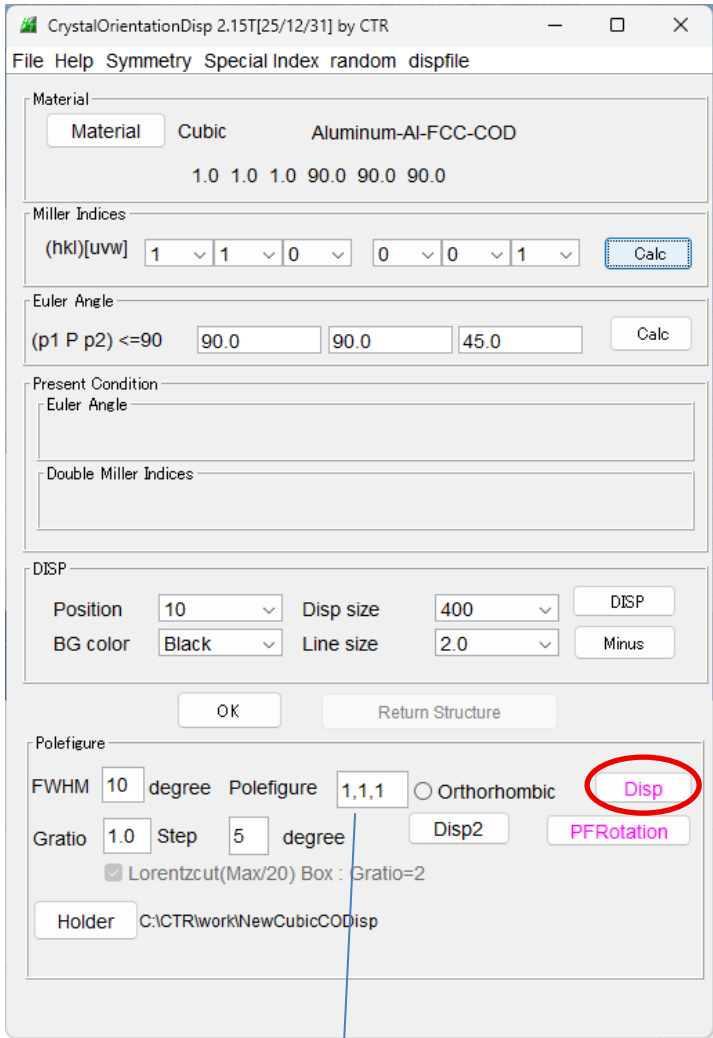
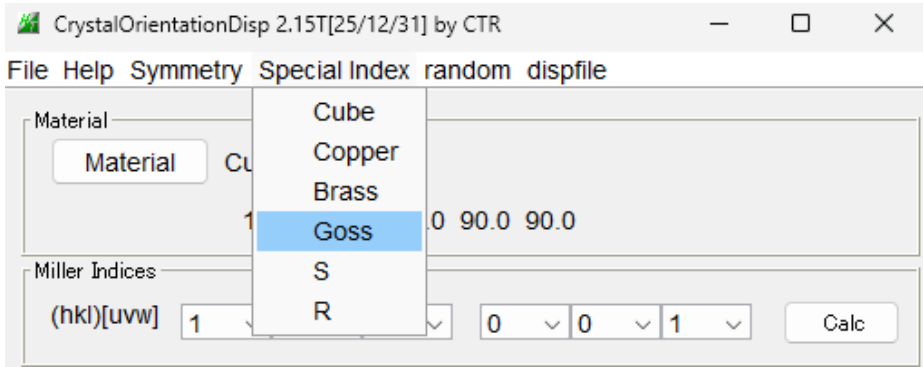
PF OrthoPF calcODF OrthoODF Inverse ND **Inv.Disp**

Euler Angle

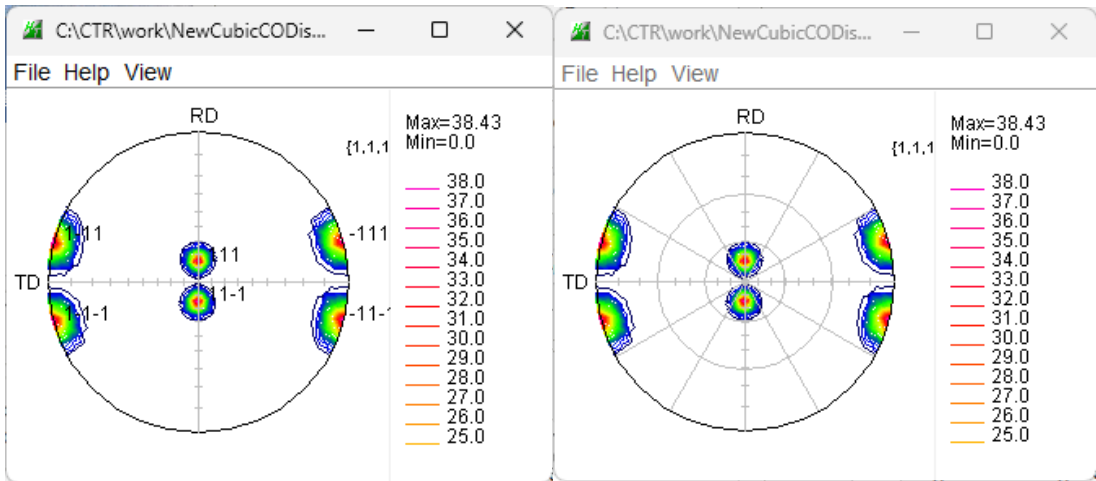
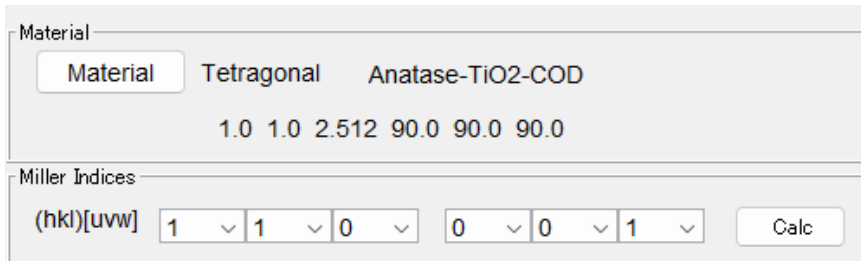
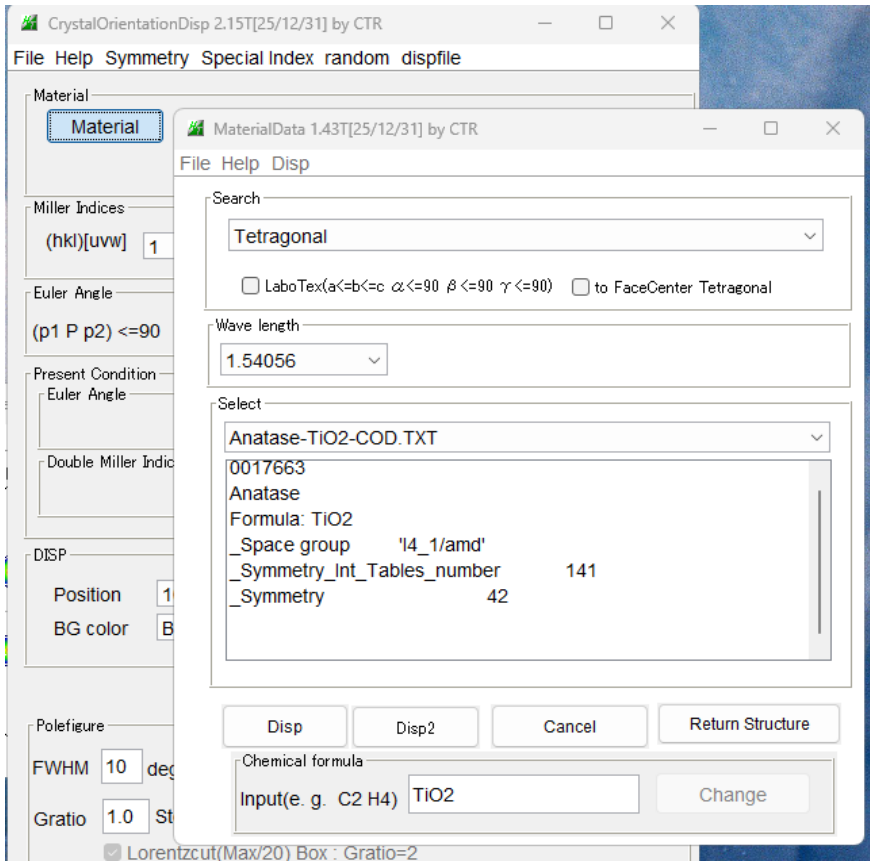


4. CrystalOrientationDisp

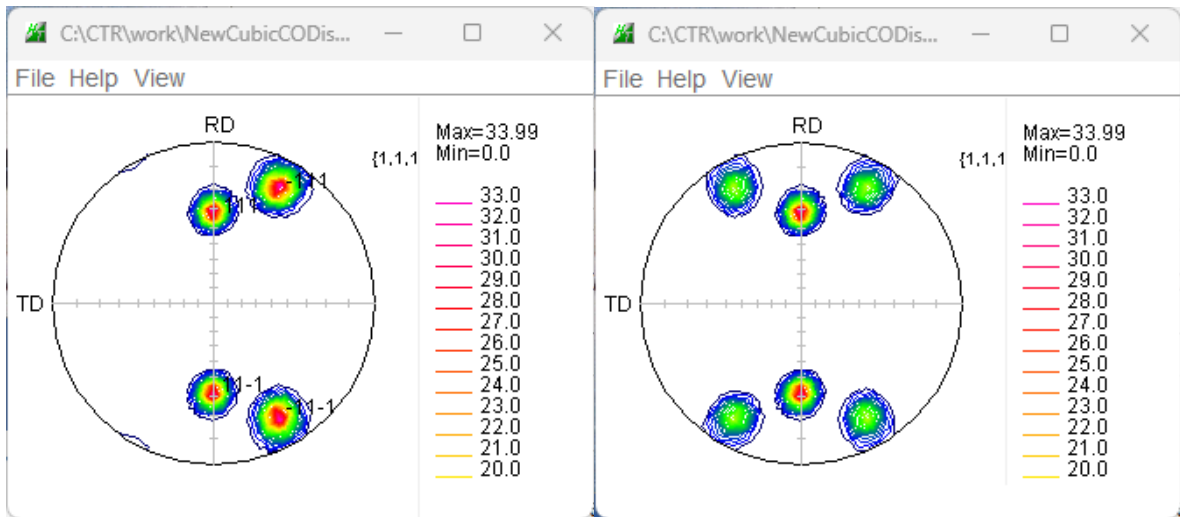
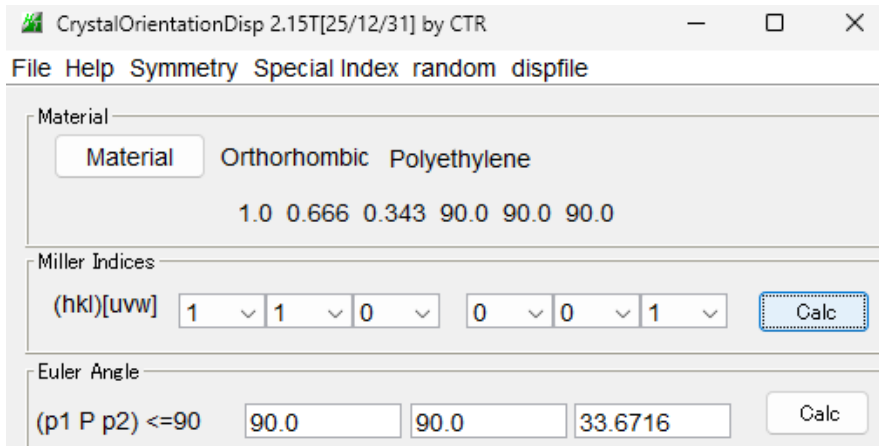
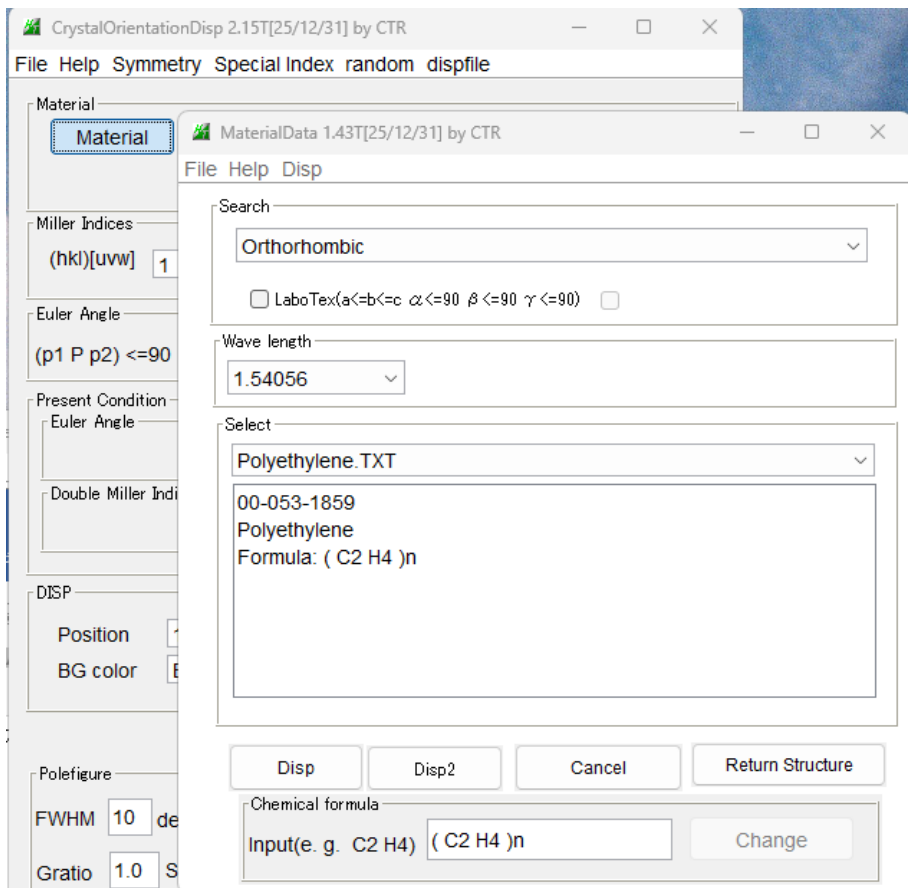
4. 1 Cubic(Goss)



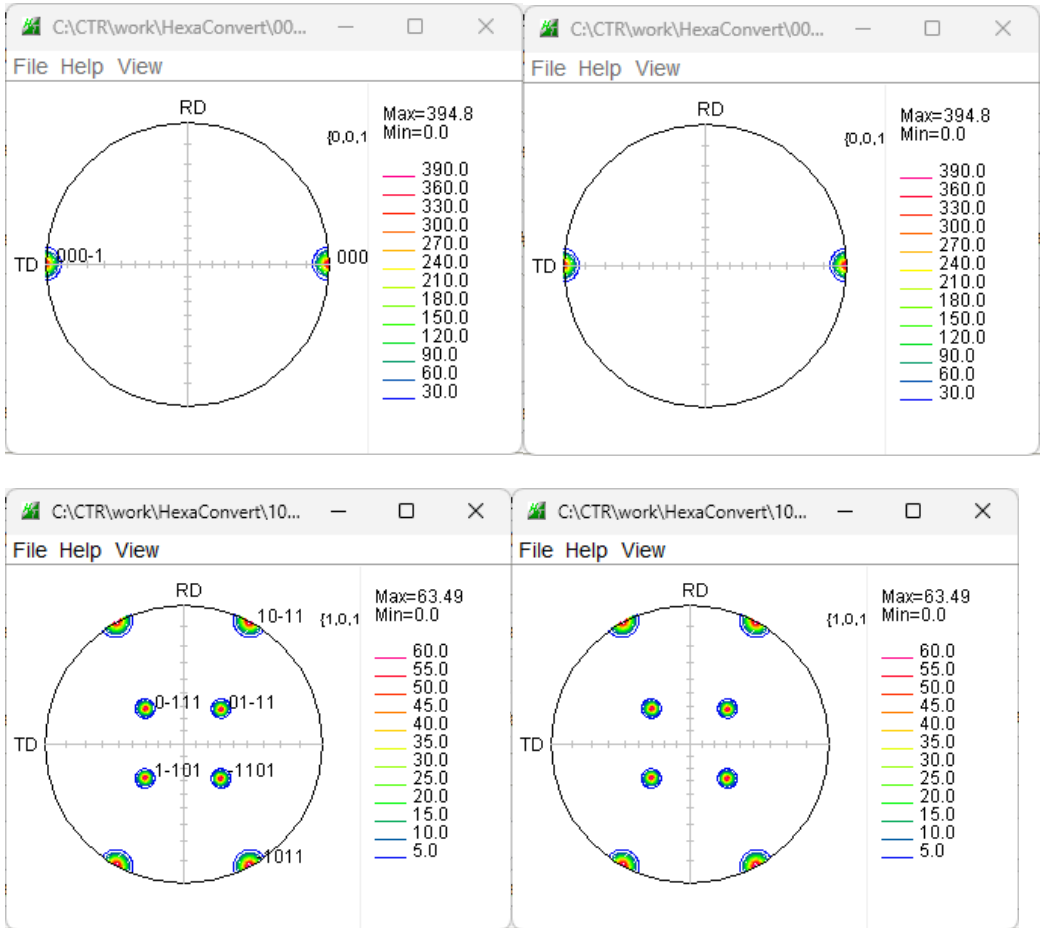
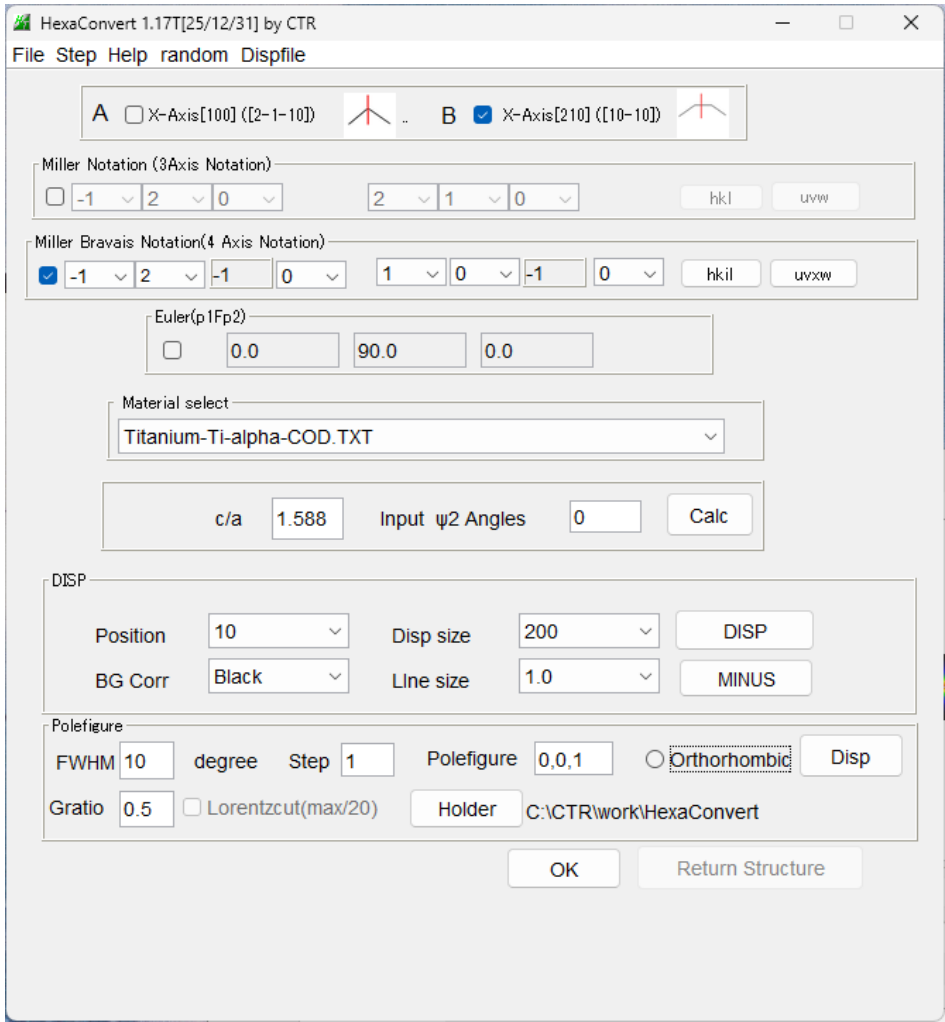
4. 2 Tetragonal



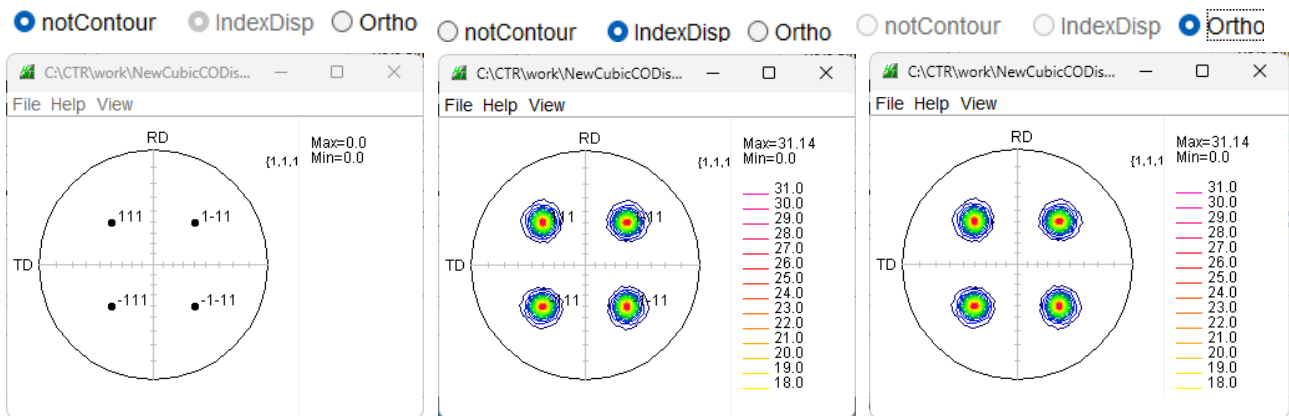
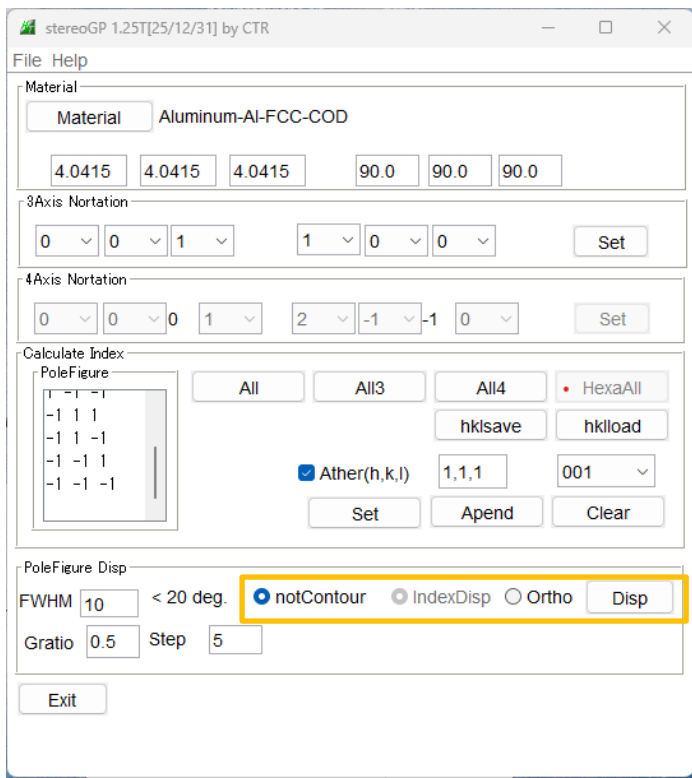
4. 3 Orthorhombic



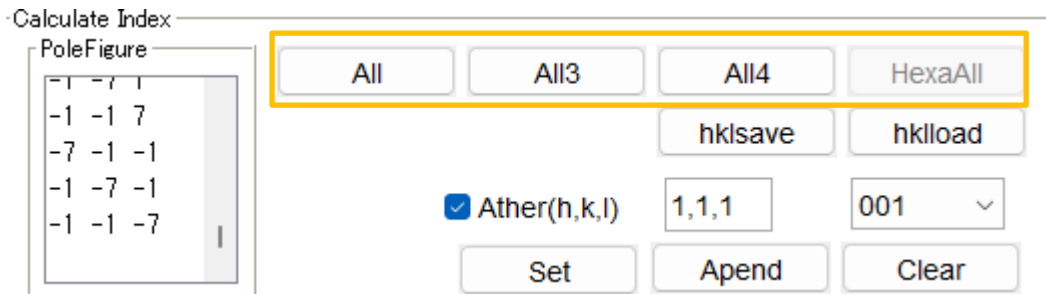
5. HexaConvert



6. stereoGP



ステレオ投影指定



6. 1 C u b i c ステレオ投影

stereoGP 1.25T[25/12/31] by CTR

File Help

Material

Material Aluminum-Al-FCC-COD

4.0415 4.0415 4.0415 90.0 90.0 90.0

3Axis Nortation

0 0 1 1 0 0 Set

4Axis Nortation

0 0 0 1 2 -1 -1 0 Set

Calculate Index

PoleFigure

All All3 All4 HexaAll

hklsave hkload

☒ Ather(h,k,l) 1,1,1 001

Set Apend Clear

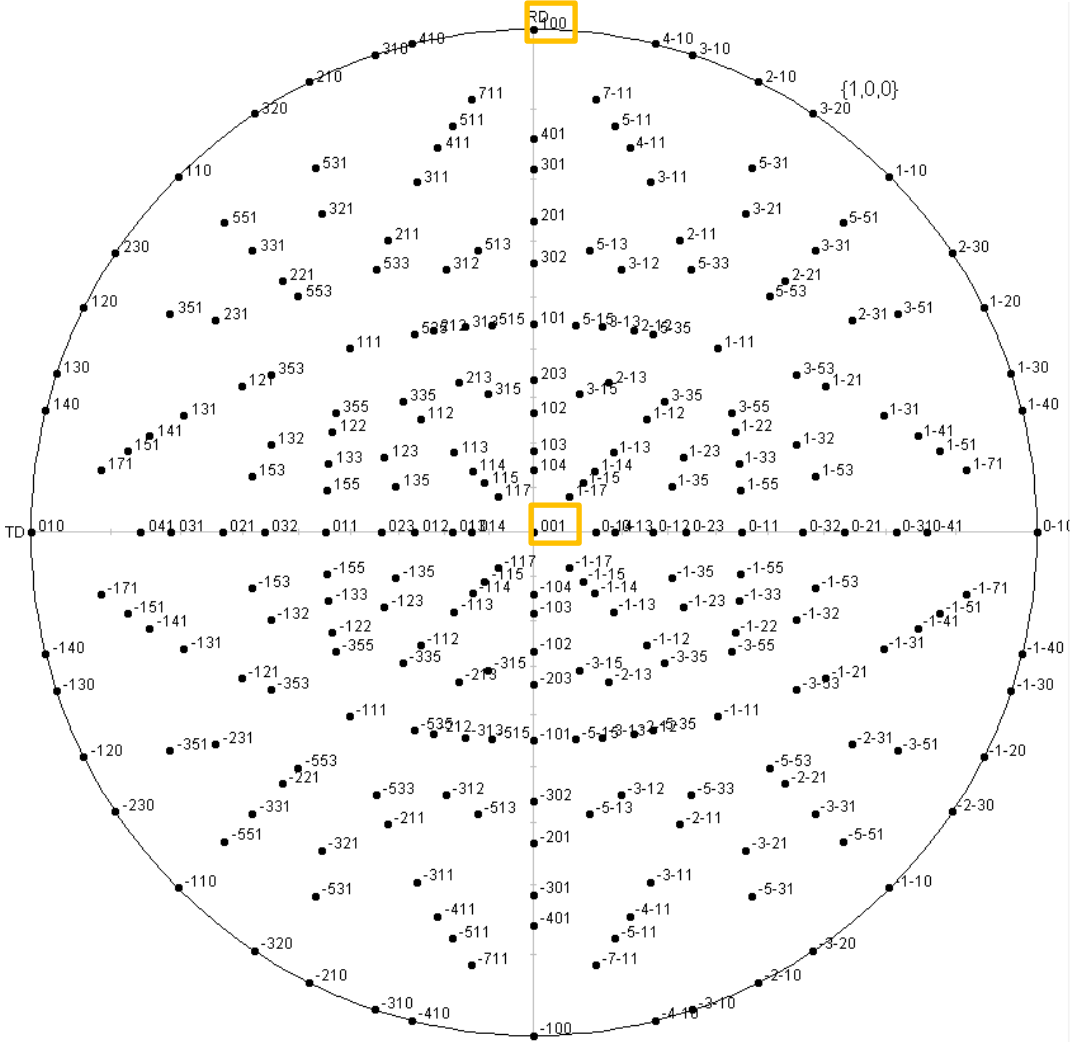
PoleFigure Disp

FWHM 10 < 20 deg. ☒ notContour ☐ IndexDisp ☐ Ortho Disp

Gratio 0.5 Step 5

Exit

(0 0 1) [1 0 0] 投影図



6. 2 Tetragonalステレオ投影

stereoGP 1.25T[25/12/31] by CTR

File Help

Material

Anatase-TiO2-COD

3.733.739.3790.090.090.0

3Axis Nortation

001100

Set

4Axis Nortation

00012-1-10

Set

Calculate Index

PoleFigure

-1-17

-7-1-1

-1-7-1

-1-1-7

AllAll3All4HexaAll

hklsavehkload

☒ Ather(h,k,l)1,1,1001

SetApendClear

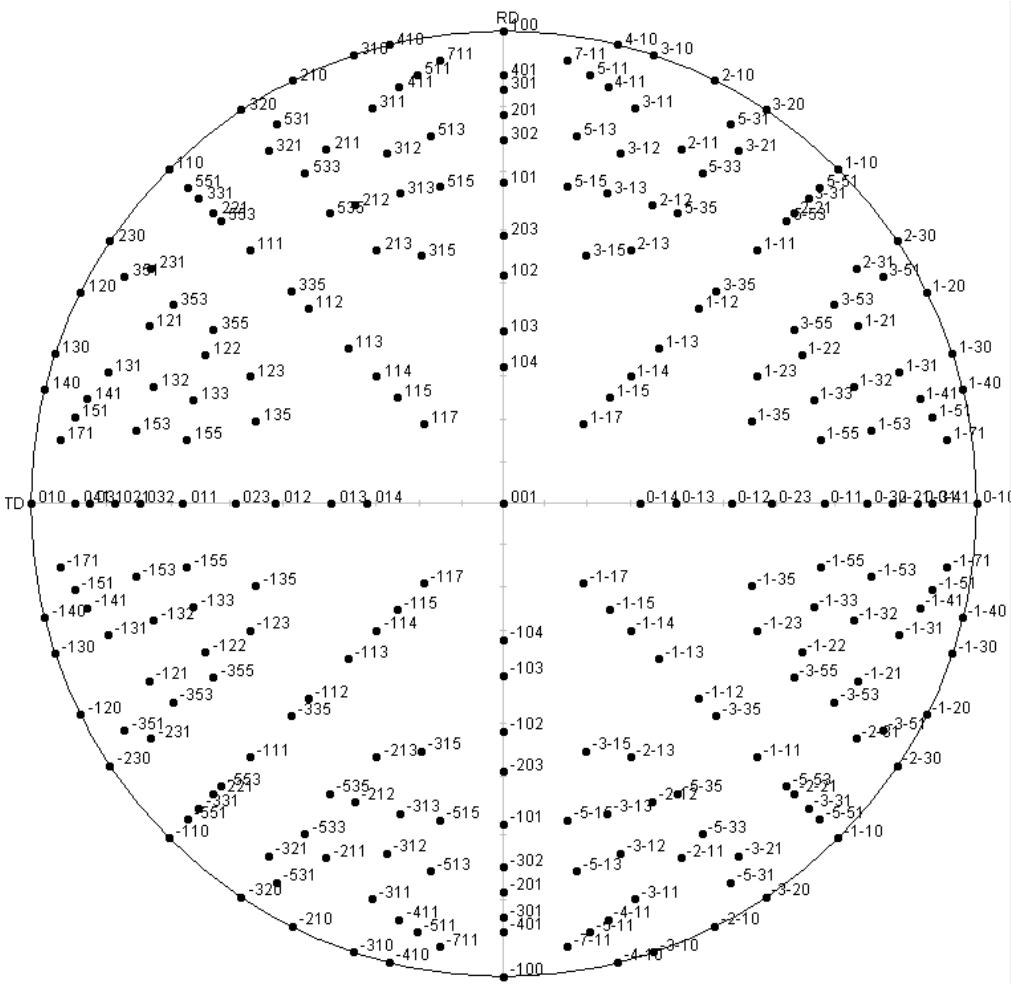
PoleFigure Disp

FWHM10< 20 deg. ☒ notContour ☐ IndexDisp ☐ OrthoDisp

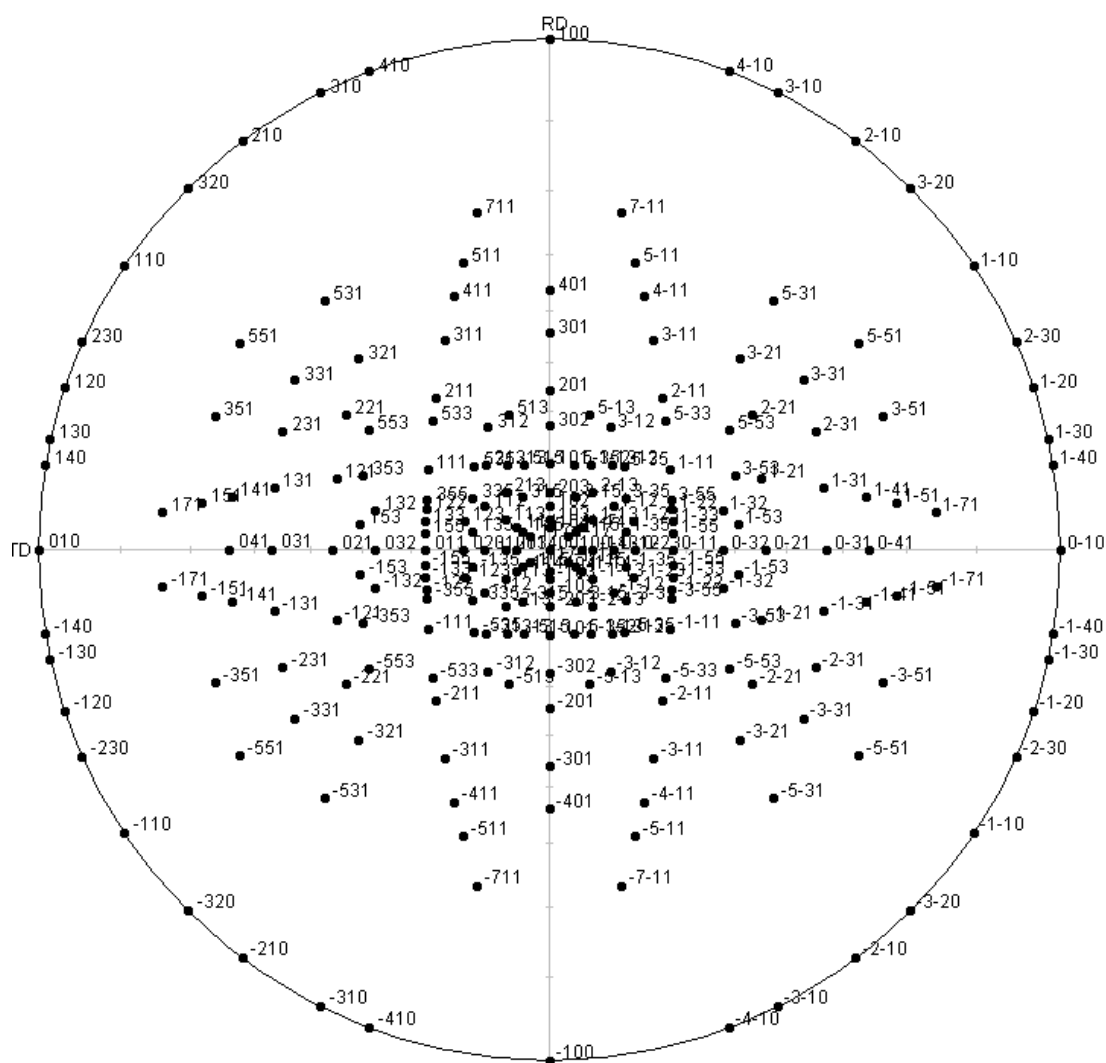
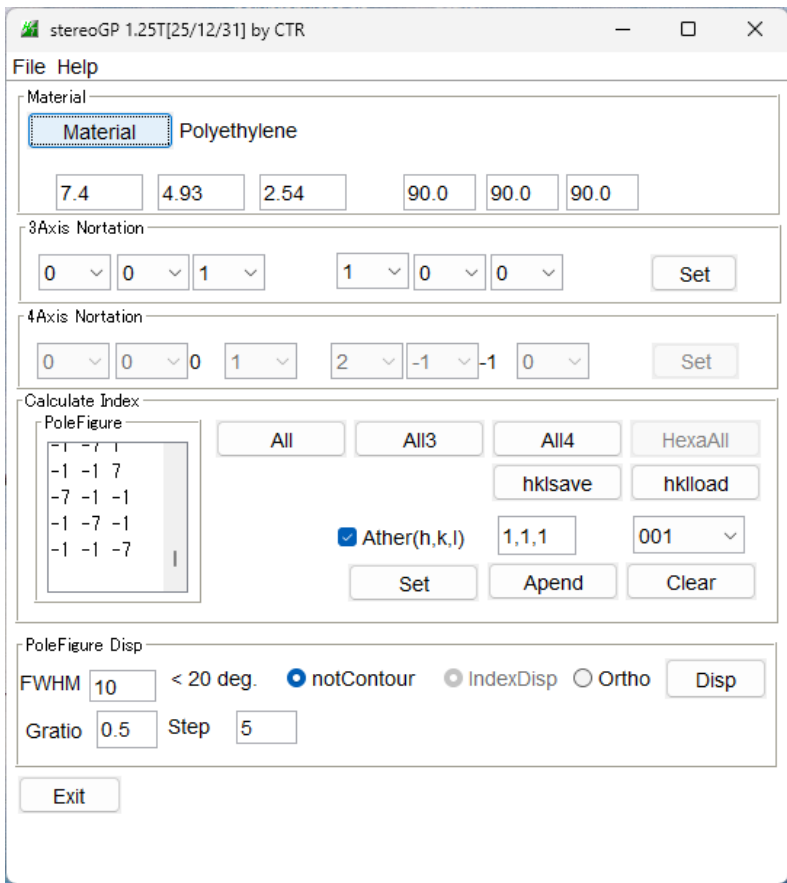
Gratio0.5Step5

Exit

(001) [100] 投影図



6. 3 Orthorhombic ステレオ投影



6. 4 H e x a g o n a l スレテオ投影

stereoGP 1.25T[25/12/31] by CTR

File Help

Material

Material Titanium-Ti-alpha-COD

2.952.954.68690.090.0120.0

3Axis Nortation

001100

Set

4Axis Nortation

00012-1-10

Set

Calculate Index

PoleFigure

-210

2-1-10

-2110

-12-10

-1-120

AllAll3All4HexaAll

hklsavehkload

☒ Ather(h,k,l)1,1,1001

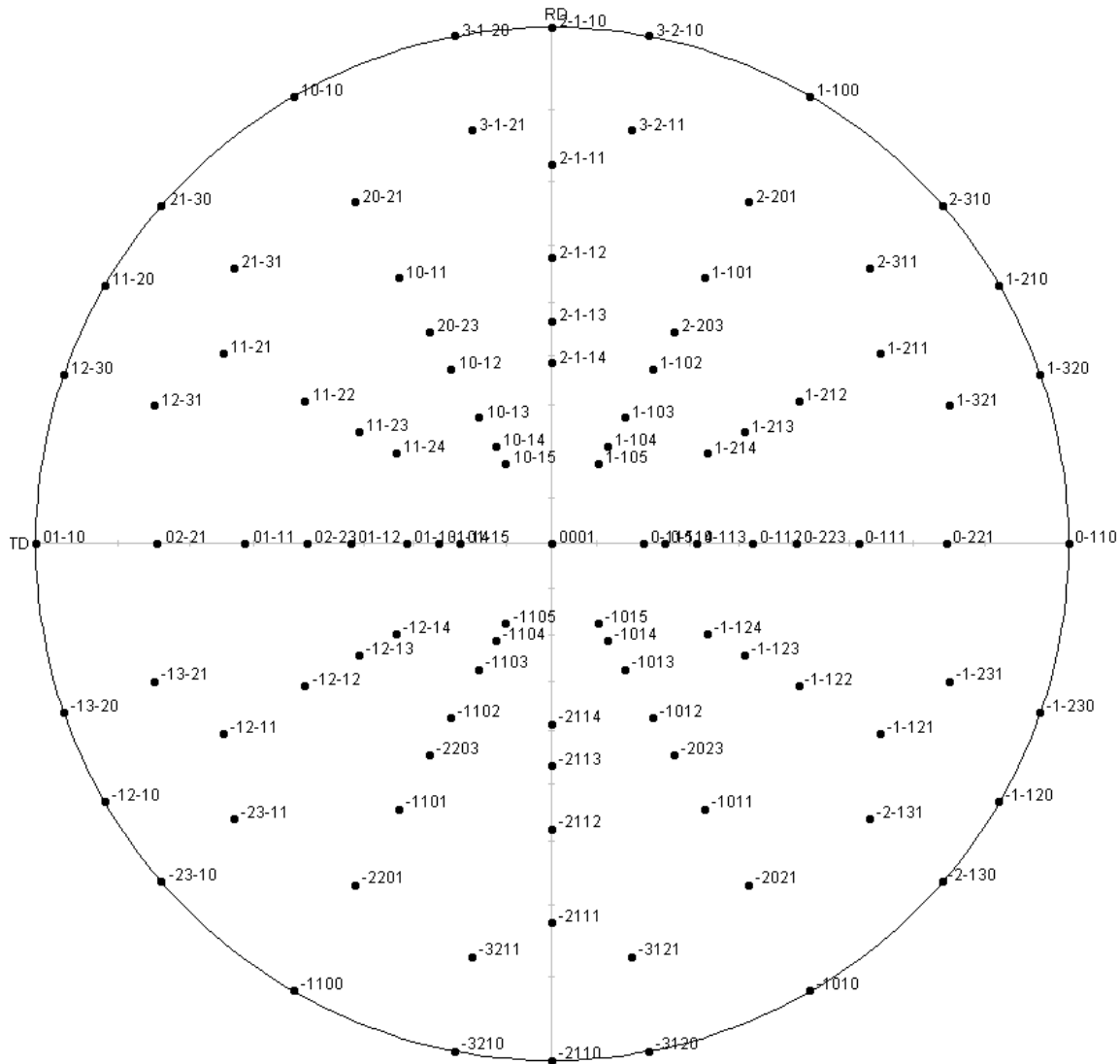
SetApendClear

PoleFigure Disp

FWHM 10< 20 deg. ☒ notContour ☐ IndexDisp ☐ OrthoDisp

Gratio 0.5Step 5

Exit



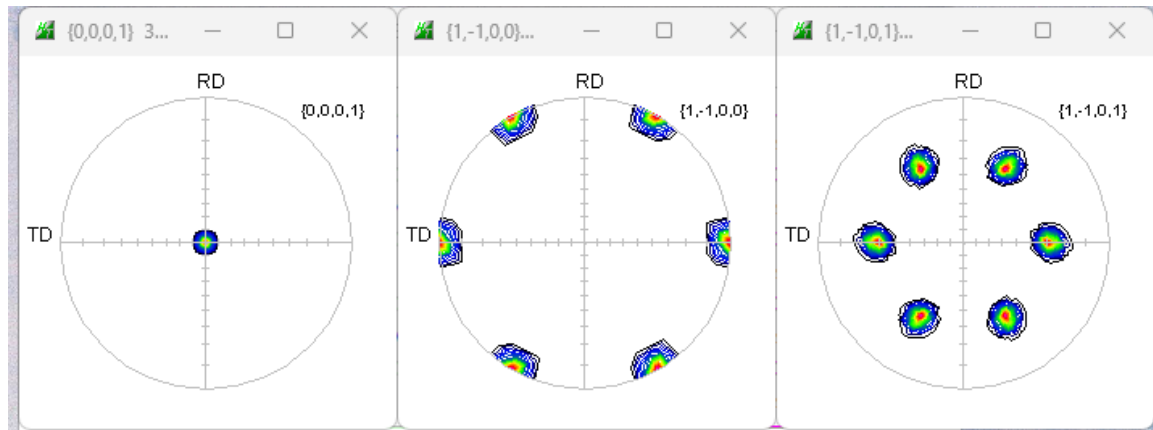
7. 極点図の回転

stereoGPによるTitanium (001) [100] から

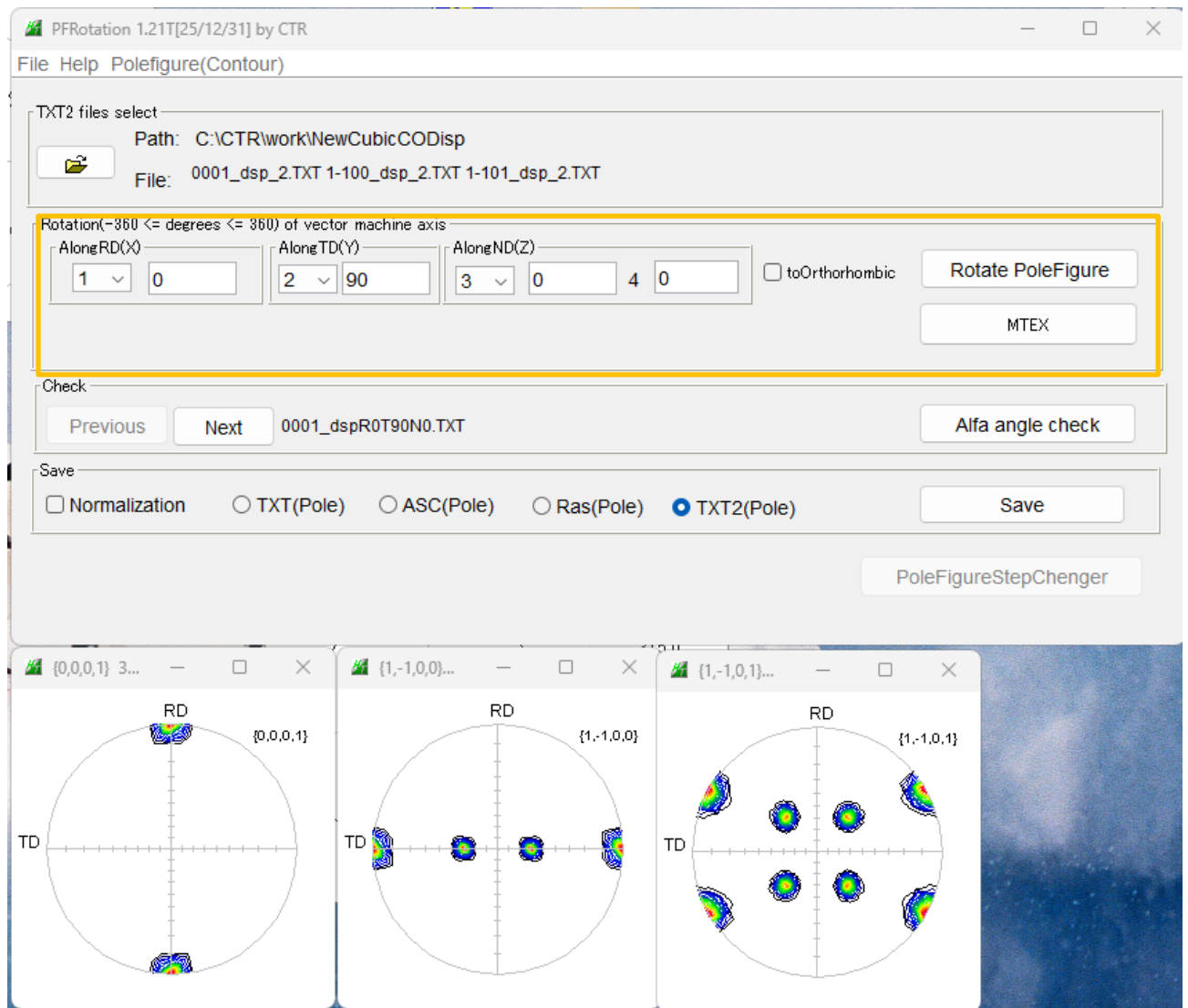
(001),

(100)、

(101) を作成極点図



TD 軸に 90 度回転を計算



本ソフトウェアでは、RD測定結果をODF解析し、Export極点図をND変換し再度ODF解析することで、サイド測定からND方向の方位解析が可能になります。