

C r y s t a l R o a t a t i o nによる結晶の回転

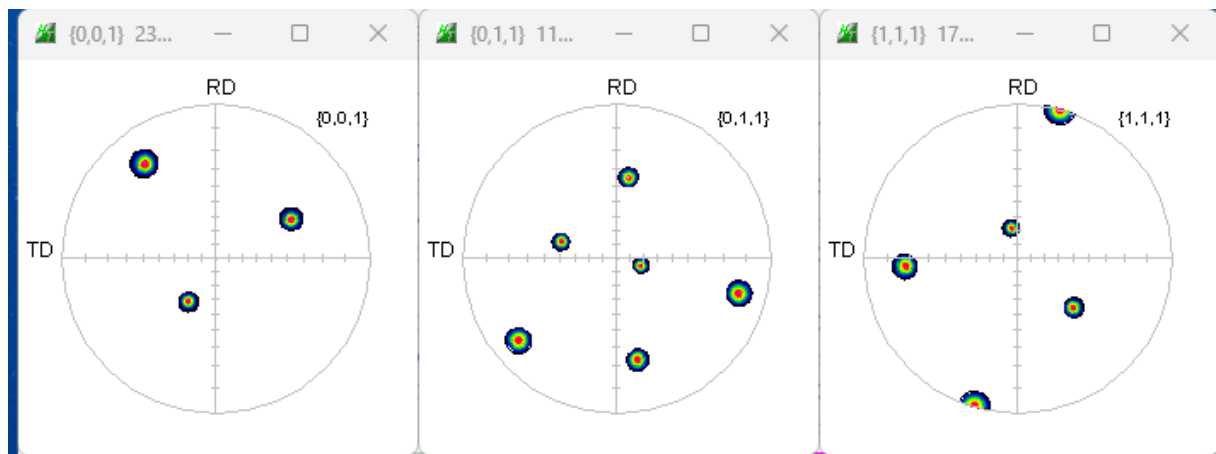
2025年12月10日

H e l p e r T e x O f f i c e

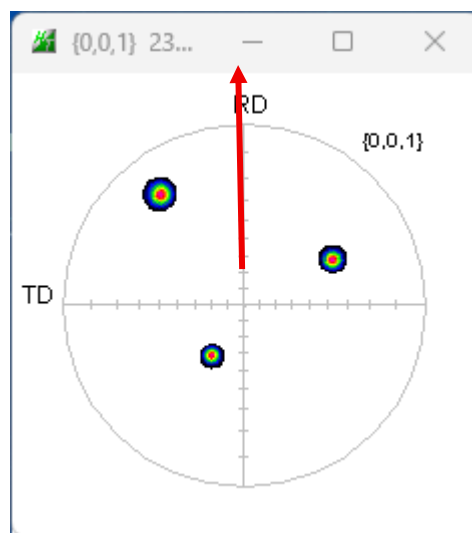
概要

極点図や結晶方位の回転を行う場合、回転軸を機械軸と結晶軸の選択があります。

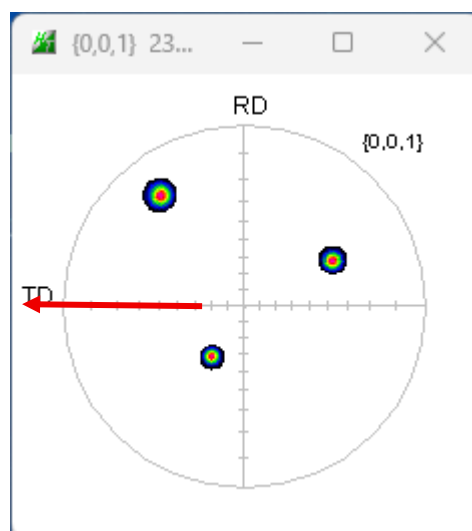
例えば、S方位 $(1\ 3\ 2)$ $[6\ -4\ 3]$ の場合



RD軸回転は、結晶軸は $[6\ -4\ 3]$



TD軸回転は、結晶軸は $[1\ 1\ 1\ 3\ -2\ 5]$



CrystalRotation機能

入力方位に読み込む

12/31] by CTR

File Help RD(TDroate) {uvw}<hkl> (132)[6-43] RV:Integer Free calcNew NewCubicCODisp

Material

MaterialCubic

1.0 1.0 1.0 90.0 90.0 90.0

入力方位

{hkl|Kuvw>

1 3 2 6 -4 3

ODF

NewCubicCODisp

Rotation vector of crystal axis

☐ 6 -4 3

SET

CT

回転条件

Rotation vector of machine axis(LaboTex,MTEX)

☒ 1 0 0

SET

Rotation angle

90

Calc

Result

6.0 17.0 1.0
-4.0 9.0 3.0
3.0 -22.0 2.0
RDaxis [6 -4 3]
TDaxis [17 9 -22]
NDaxis [1 3 2]
6.0 -4.0 3.0 (6 -4 3)
(132)[6-43] eulerangle:(27.032,57.689,18.435)
Eulerangle g(ψ 1 ϕ ψ 2)=
0.7682 0.5817 0.2673
-0.5121 0.308 0.8018
0.3841 -0.7528 0.5345
Rotation [6,-4,3] angle:90.0
Calc-d=(0.7682,-0.5121,0.3841)
a(6.0,-4.0,3.0),90.0
Rotated Eulerangle
0.5902 -0.0093 0.8072
-0.7776 0.2623 0.5715
-0.2171 -0.9649 0.1475
Rotated RD TD ND
0.7682 -0.2673 0.5817
-0.5121 -0.8018 0.308
0.3841 -0.5345 -0.7528
Calc Miller indices
(1.8889 1.0 -2.4444)[2.0 -1.333 1.0]
(17 9 -22)[6 -4 3] (35.7 138.84 62.1)
INT/DOUBL

回転でえられた方位

入力方位に読み込む

(17 9 -22)[6 -4 3]

ODF

set{hkl|Kuvw>

NewCubicCODisp

ResultCreat

極点図表示

Result (179-22)[6-43] (35.7 138.84 62.1)

確認手順

CrystalRotationで方位選択

NewCubicCODispで極点図作成(CTRYwork¥NewCubicCODisp)

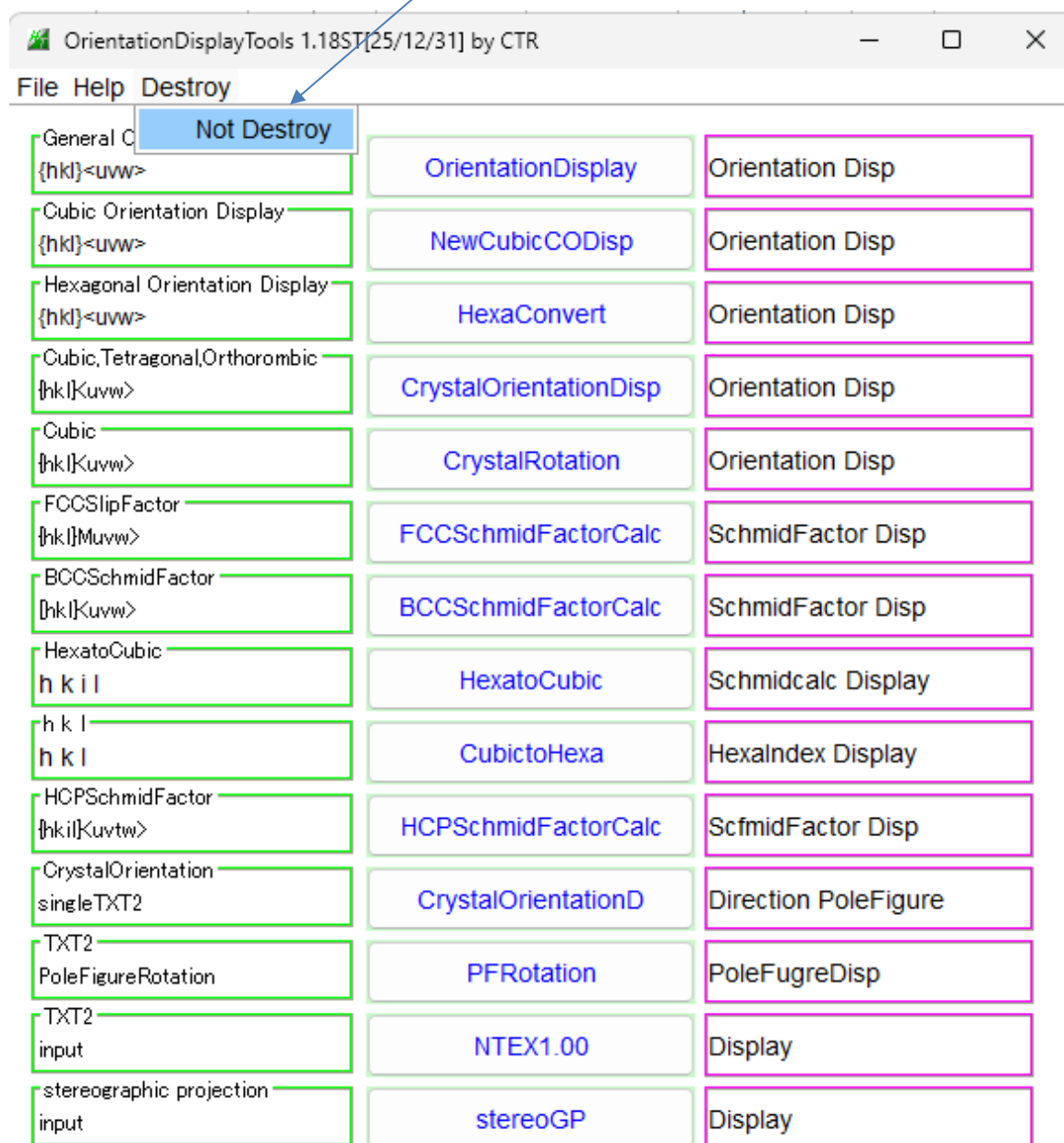
CTRYwork¥NewCubicCODispで作成された極点図(TXT)を他の場所に copy

結晶方位の回転

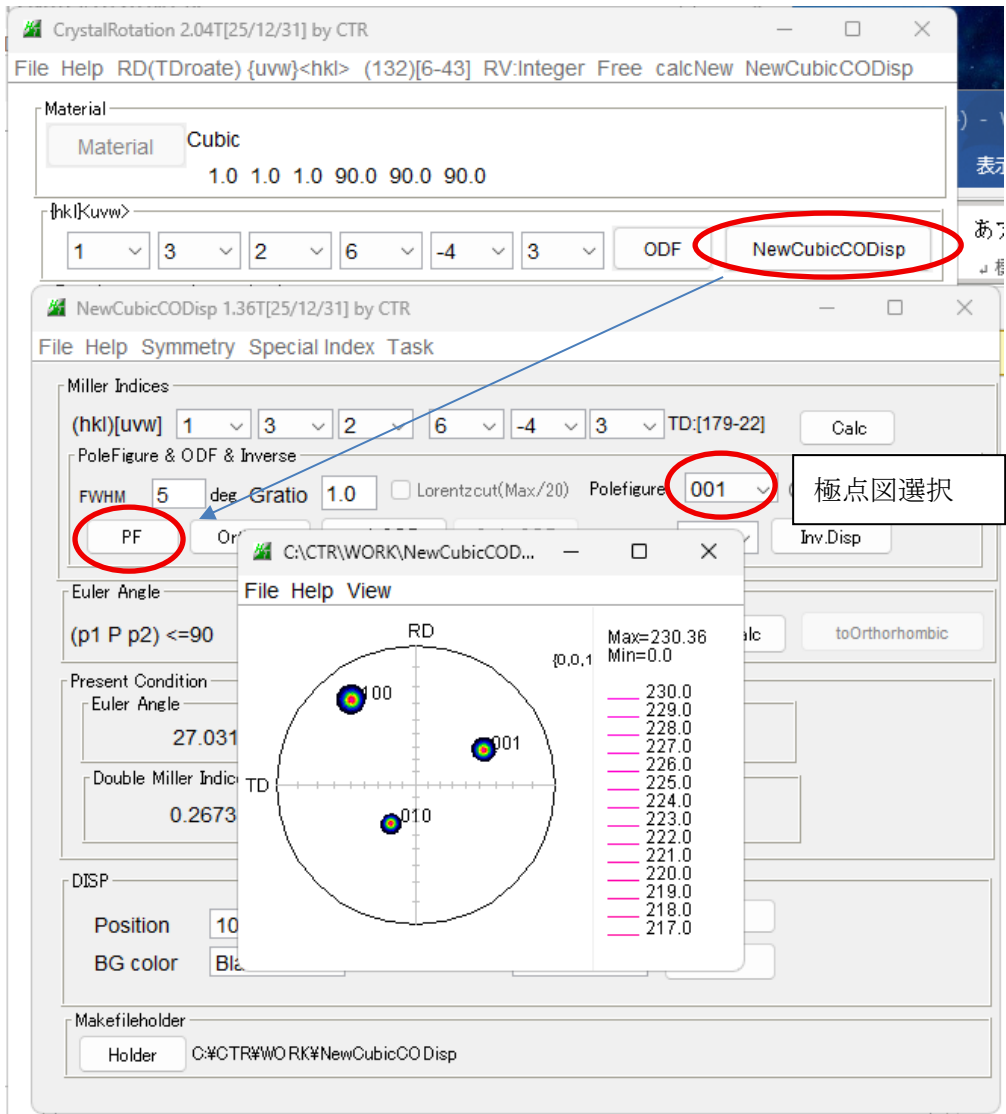
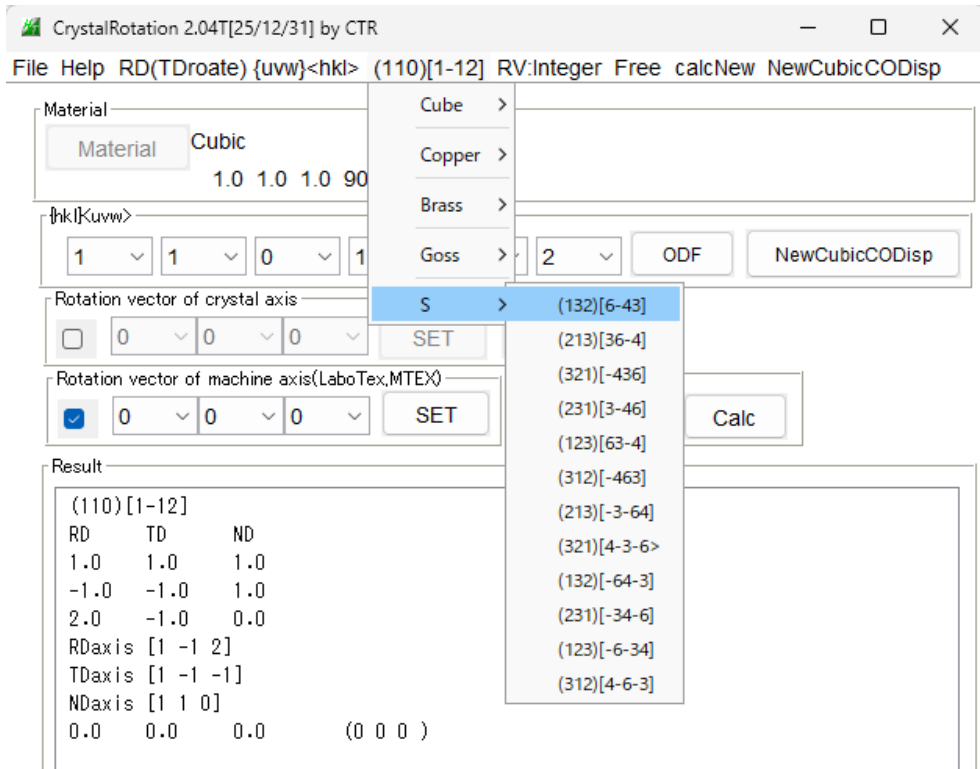
回転した方位からNewCubicCODispで極点図表示

Copyした極点図をPFRotationで回転し、極点図の比較

同一カテゴリの複数ソフトウェア起動のため



S 方位の入力データ選択



作成した極点図を他の場所にコピー

S 方位を RD 軸に 90 度回転

CrystalRotation 2.04T[25/12/31] by CTR

File Help TD(RDrotate) {TD}<uvw> (132)[6-43] RV:Integer Free calcNew NewCubicCODisp

Material

Material Cubic

1.0 1.0 1.0 90.0 90.0 90.0

hkl|Kuvw>

1 3 2 6 -4 3 ODF NewCubicCODisp

Rotation vector of crystal axis

☐ 6 -4 3 SET

Rotation vector of machine axis(LaboTex,MTEX)

☒ 1 0 0 SET

Rotation angle

90 Calc

RD 軸を 90 度回転

Result

```

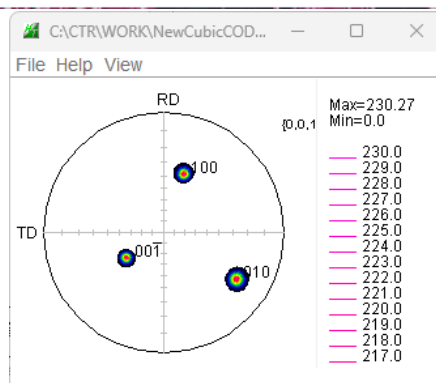
6.0 17.0 1.0
-4.0 9.0 3.0
3.0 -22.0 2.0
RDaxis [6 -4 3]
TDaxis [17 9 -22]
NDaxis [1 3 2]
6.0 -4.0 3.0 (6 -4 3)
(132)[6-43] eulerangle:(27.032,57.689,18.435)
Eulerangle g(ψ1φψ2)=
0.7682 0.5817 0.2673
-0.5121 0.308 0.8018
0.3841 -0.7528 0.5345
Rotation [6,-4,3] angle:90.0
Calc-d=(0.7682,-0.5121,0.3841)
a(6.0,-4.0,3.0),90.0
Rotated Eulerangle
0.5902 -0.0093 0.8072
-0.7776 0.2623 0.5715
-0.2171 -0.9649 0.1475
Rotated RD TD ND
0.7682 -0.2673 0.5817
-0.5121 -0.8018 0.308
0.3841 -0.5345 -0.7528
Calc Miller indices
(1.8889 1.0 -2.4444)[2.0 -1.333 1.0]
(17 9 -22)[6 -4 3] (35.7 138.84 62.1)
INT/DOUBLE= (9.0 9.0 9.0)[3.0 3.0 3.0]

```

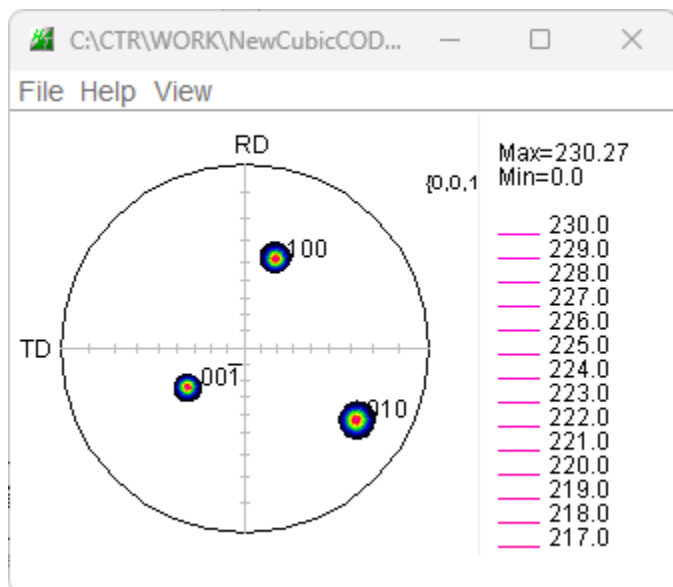
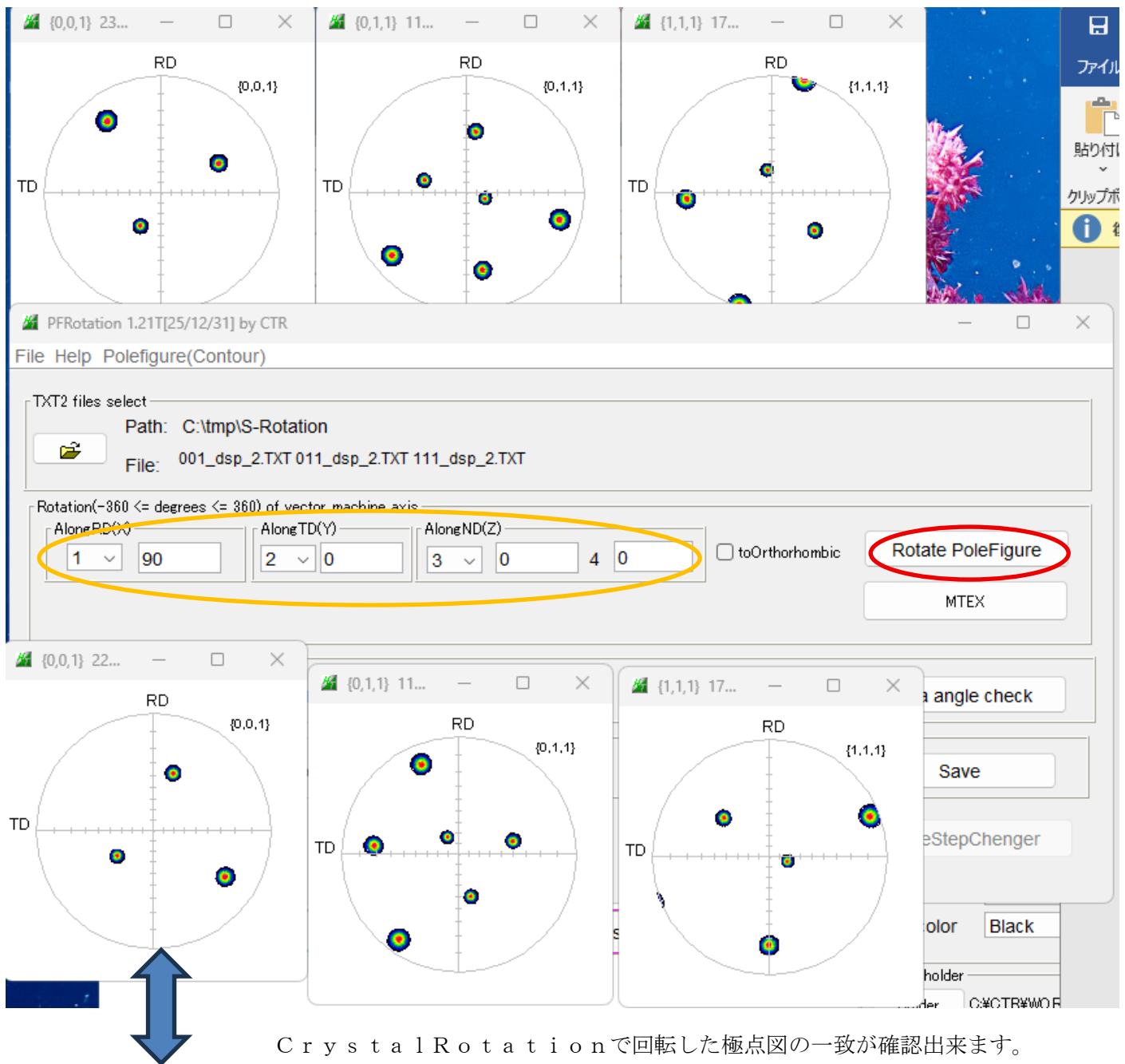
(17 9 -22)[6 -4 3] ODF set|hkl|Kuvw> NewCubicCODisp ResultCreat

Result (179-22)[6-43] (35.7 138.84 62.1)

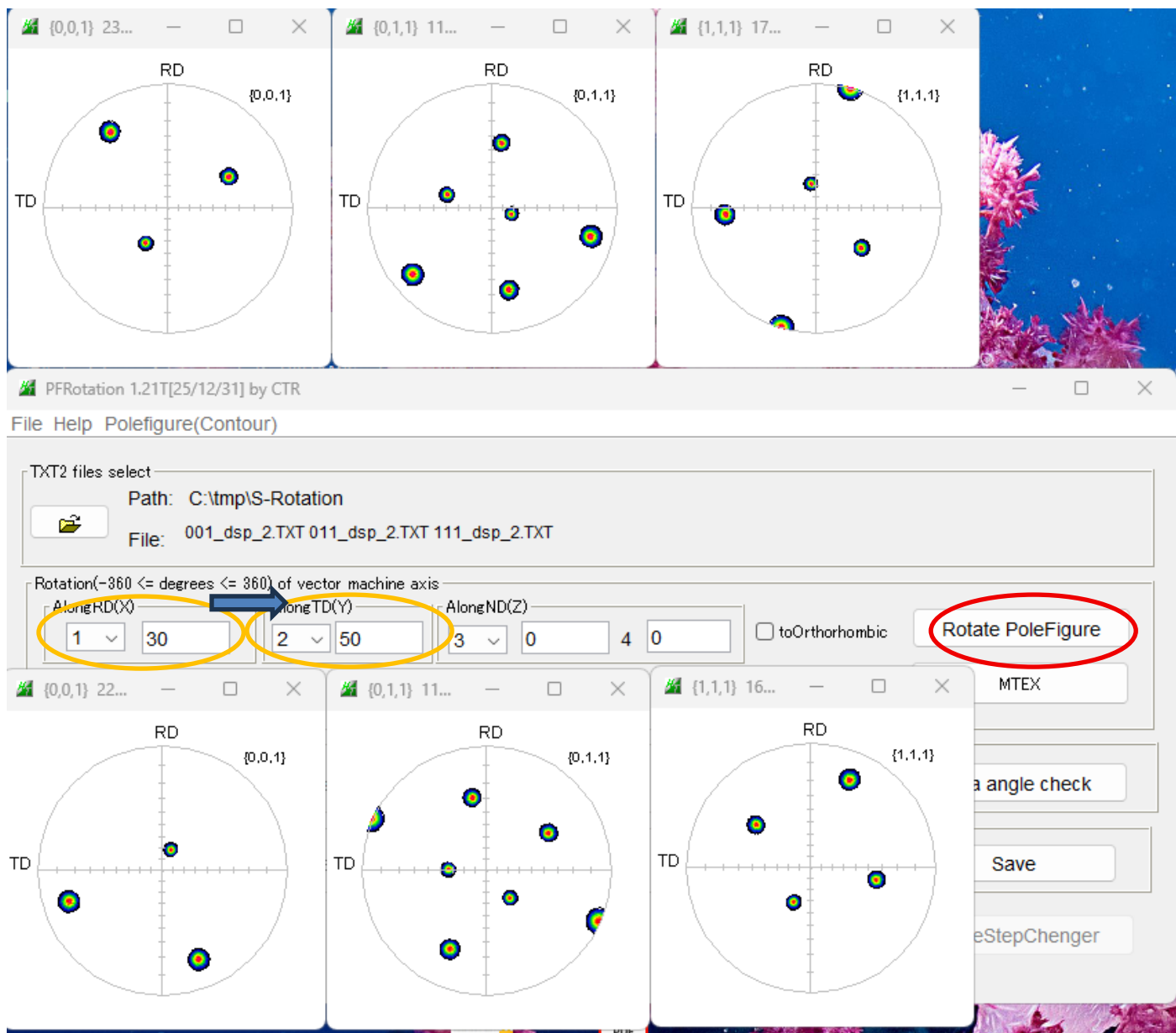
回転された方位の極点図確認



C o p y した極点図を P F R o t a t i o n で回転し、極点図の比較



RD軸(30度)→TD軸(50)の場合



CrystalRotationでは

CrystalRotation 2.04T[25/12/31] by CTR

File Help RD(TDroate) {uvw}<hkl> (132)[6-43] RV:Integer Free calcNew NewCubicCODisp

Material

Material Cubic

1.0 1.0 1.0 90.0 90.0 90.0

hkl|Kuvw>

1 3 2 6 -4 3 ODF NewCubicCODisp

Rotation vector of crystal axis

☐ 6 -4 3 SET RD軸30度回転

Rotation vector of machine axis(LaboTex,MTEX)

☒ 1 0 0 SET

Rotation angle

30 Calc

Result

```
6.0 17.0 1.0
-4.0 9.0 3.0
3.0 -22.0 2.0
RDaxis [6 -4 3]
TDaxis [17 9 -22]
NDaxis [1 3 2]
6.0 -4.0 3.0 (6 -4 3)
(132)[6-43] eulerangle:(27.032,57.689,18.435)
Eulerangle g(ψ1 φψ2)=
0.7682 0.5817 0.2673
-0.5121 0.308 0.8018
0.3841 -0.7528 0.5345
Rotation [6,-4,3] angle:30.0
Calc-d=(0.7682,-0.5121,0.3841)
a(6.0,-4.0,3.0),30.0
Rotated Eulerangle
0.9451 0.1393 0.2956
-0.2448 0.9012 0.3578
-0.2165 -0.4105 0.8858
Rotated RD TD ND
0.7682 0.3702 0.5223
-0.5121 -0.1342 0.8484
0.3841 -0.9192 0.0865
Calc Miller indices
(6.0386 9.8079 1.0)[2.0 -1.333 1.0]
(15 24 2)[6 -4 3] (22.65 85.96 32.01)
INT/DOUBLE= (2.484 2.447 2.0)[3.0 3.0 3.0]
```

(15 24 2)[6 -4 3] ODF set|hkl|Kuvw> NewCubicCODisp ResultCreat

Result (15242)[6-43] (22.65 85.96 32.01)

計算した方位の読み込み

CrystalRotation 2.04T[25/12/31] by CTR

File Help RD(TDroate){uvw}<hkl> (132)[6-43] RV:Integer Free calcNew NewCubicCODisp

Material

Material Cubic

1.0 1.0 1.0 90.0 90.0 90.0

{hkl}<uvw>

15 24 2 6 -4 3 ODF NewCubicCODisp

Rotation vector of crystal axis

☐ 5 -2 -13 SET CTD

Rotation vector of machine axis(LaboTex,MTEX)

☒ 0 1 0 SET

Rotation angle

50 Calc

Result

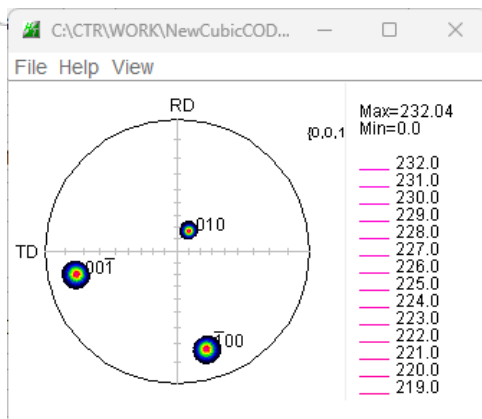
```

6.0 5.0 15.0
-4.0 -2.0 24.0
3.0 -13.0 2.0
RDaxis [6 -4 3]
TDaxis [5 -2 -13]
NDaxis [15 24 2]
5.0 -2.0 -13.0 (5 -2 -13 )
(15242)[6-43] eulerangle:(22.648,85.958,32.005)
Eulerangle g(ψ1Φψ2)=
0.7682 0.361 0.5287
-0.5121 -0.1489 0.8459
0.3841 -0.9206 0.0705
Rotation [5,-2,-13] angle:50.0
Calc-d=(0.3553,-0.1421,-0.9239)
a(5.0,-2.0,-13.0),50.0
Rotated Eulerangle
0.6879 -0.7258 -0.0084
0.6897 0.65 0.3191
-0.2261 -0.2253 0.9477
Rotated RD TD ND
0.8969 0.3641 -0.2508
0.3195 -0.1416 0.9369
0.3057 -0.9205 -0.2433
Calc Miller indices
(-1.0308 3.8505 -1.0)[2.9343 1.045 1.0]
(-6 23 -6)[37 12 9] (13.44 104.17 345.38)
INT/DOUBLE= (5.8205 5.9732 6.0)[12.6093 11.4803 9.0]

```

(-6 23 -6)[37 12 9] ODF set{hkl}<uvw> NewCubicCODisp ResultCreat

Result (-623-6)[37129] (13.44 104.17 345.38)



計算された方位を NewCubicCODisp で表示

PFRotationで計算した極点図と一致します。


まとめ

単結晶極点図の場合、Crystal Rotationによる結晶軸の回転が可能であるが、複数の結晶方位が含まれている場合、ODF解析によるeuler角度回転が必要になります。例えばLaboTexの場合

ODF Transformation (Rotation)

Project: Demo

Sample: copper-T

Crystal Symmetry:  (Cubic)

Sample Symmetry: Triclinic

☒ Sample Frame Rotation

☐ Crystallites/Planes Rotations

Build Rotations Model

Choose Rotation Model

Euler Angles

ϕ_1	Φ	ϕ_2
(-360 - 360)	(-180 - 180)	(-360 - 360)
0	0	0

Options

☐ Draft ☒ Medium Quality ☐ High Quality

☐ Reversed Spin ☒ Triclinic s.s. (Output ODF)

START Cancel

Transformation Progress: 0.00 %