

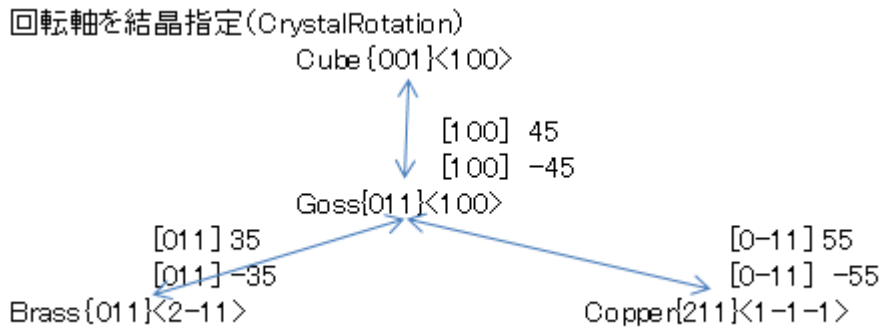
結晶方位の回転と極点図の回転

2023年11月27日

HelperTex Office

概要

極点図の回転(PFRotation)はTD軸、RD軸、ND軸の材料軸回転であり、
 結晶方位の回転(CrystalOrientation)は、TD方位、RD方位、ND方位の結晶軸回転で表現される。



では、cubeをRD軸[100](Crystal:[100])を軸に45度回転でGossが得られる。

File Help **TD(RDrotate)** TD<uvw> {001}<100> RV:Integer Orthorhombic

Material
 Material Cubic
 1.0 1.0 1.0 90.0 90.0 90.0

{hkl}<uvw>
 0 0 1 1 0 0 Disp

Rotation vector of crystal axis
 1 0 0 SET CTD

Rotation vector of machine axis(LaboTex,MTEX) Rotation angle
 1 0 0 SET 45 Calc Disp

(0 1 1)[1 0 0] (0.0 45.0 0.0)

GossのTD軸 [01-1] (Crystal:[01-1])を軸に55度回転でCopperが得られる

File Help **RD(TDrotate)** {uvw}<hkl> {001}<100> RV:Integer Orthorhombic

Material
 Material Cubic
 1.0 1.0 1.0 90.0 90.0 90.0

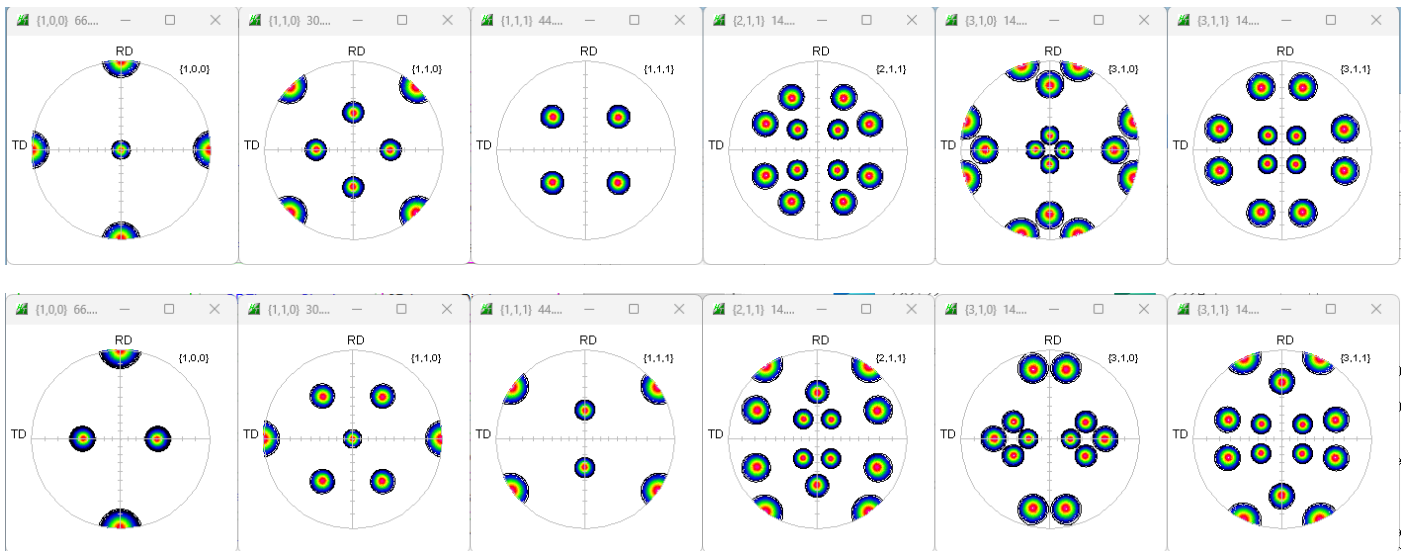
{hkl}<uvw>
 0 1 1 1 0 0 Disp

Rotation vector of crystal axis
 0 1 -1 SET CTD

Rotation vector of machine axis(LaboTex,MTEX) Rotation angle
 0 1 0 SET 55 Calc Disp

(1 2 1)[1 -1 1] (39.23 65.91 26.57)

CubeからGossをPFRotationで確認 (RD軸を45度回転)



PFRotation 1.20 by CTR PDuser HelperTex CTR

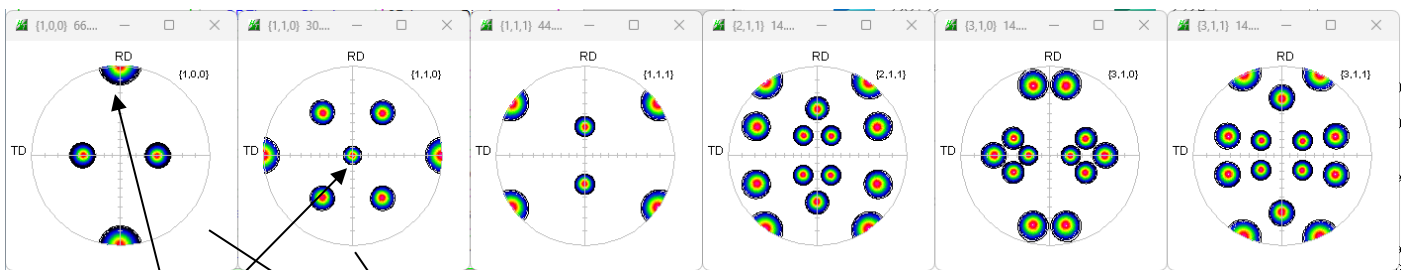
File Help Polefigure(Contour)

TXT2 files select
 Path: C:\CTR\work\PoleHKLUVWSearch\ORG\DATA\Euler10degStep1deg\001-100
 File: 100.TXT 110.TXT 111.TXT 211.TXT 310.TXT 311.TXT

Rotation(-360 <= degrees <= 360) of vector machine axis
 AlongRD(X) [1] [45] AlongTD(Y) [2] [0] AlongND(Z) [3] [0] [4] [0] toOrthorhombic Rotate PoleFigure
 MTEX

Check
 Previous Next 100R45T0N0.TXT Alfa angle check

Save
 Normalization TXT(Pole) ASC(Pole) Ras(Pole) TXT2(Pole) Save
 PoleFigureStepChenger



$$\{hkl\} \rightarrow \{110\}$$

$$\langle uvw \rangle \rightarrow \langle 100 \rangle$$

CubeからGossをCrystalRotationで確認（[100]軸を45度回転）

CrystalRotation 1.13 by CTR PDuser HelperTex CTR

File Help TD(RDrotate) {TD}<uvw> {001}<100> RV:Integer Orthorhombic

Material

Material **Cubic**
1.0 1.0 1.0 90.0 90.0 90.0

{hk}l{Kuvw}>

0 0 1 1 0 0 Disp

Rotation vector of crystal axis

1 0 0 SET CTD

Rotation vector of machine axis(LaboTex,MTEX)

1 0 0 SET

Rotation angle

45 Calc Disp

Result

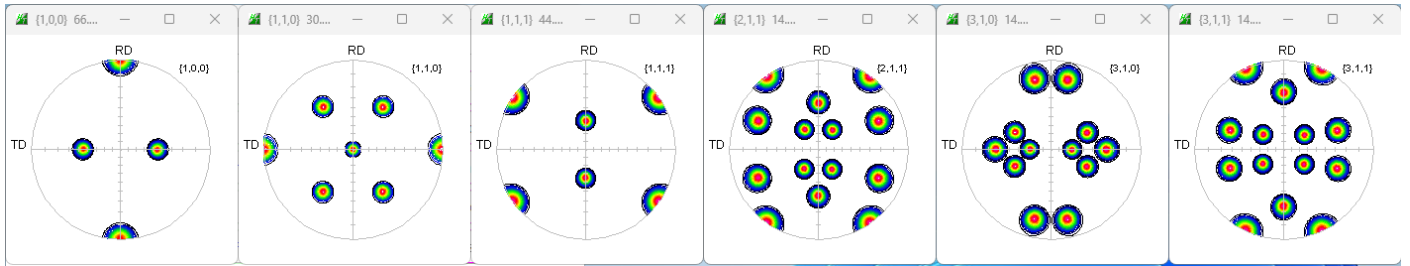
```

1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0
RDaxis [1 0 0]
TDaxis [0 1 0]
NDaxis [0 0 1]
1.0 0.0 0.0 (1 0 0)
{001}<100> eulerangle:(0.0,0.0,0.0)
Eulerangle g(φ1Φφ2)=
    1.0 0.0 0.0
    0.0 1.0 0.0
    0.0 0.0 1.0
Rotation [1,0,0] angle:45.0
Calc-d=(1.0,0.0,0.0)
a(1.0,0.0,0.0),45.0
Rotated Euulerangle
    1.0 0.0 0.0
    0.0 0.7071 0.7071
    0.0 -0.7071 0.7071
Rotated RD TD ND
    1.0 0.0 0.0
    0.0 0.7071 0.7071
    0.0 -0.7071 0.7071
Calc Miller indices ***** NewCalc *****
(0.0 1.0 1.0)[1.0 0.0 0.0]
(0 1 1)[1 0 0] (0.0 45.0 0.0)
INT/DOUBLE= (0.0 1.0 1.0)[1.0 0.0 0.0]

```

(0 1 1)[1 0 0] set{hk}l{Kuvw}> ResultCreat

GossからCopperをPFRotationで確認 (TD軸を55度回転)



PFRotation 1.20 by CTR PDuser HelperTex CTR

File Help Polefigure(Contour)

TXT2 files select

Path: C:\CTR\work\PoleHKLUVWSearch\ORG\DATA\Euler10degStep1deg\001-100\tmp

File: 100R45T0N0.TXT 110R45T0N0.TXT 111R45T0N0.TXT 211R45T0N0.TXT 310R45T0N0.TXT 311R45T0N0.TXT

Rotation(-360 <= degrees <= 360) of vector machine axis

AlongRD(X) [1] [0] AlongTD(Y) [2] [55] AlongND(Z) [3] [0] [4] [0] toOrthorhombic

Rotate PoleFigure

MTEX

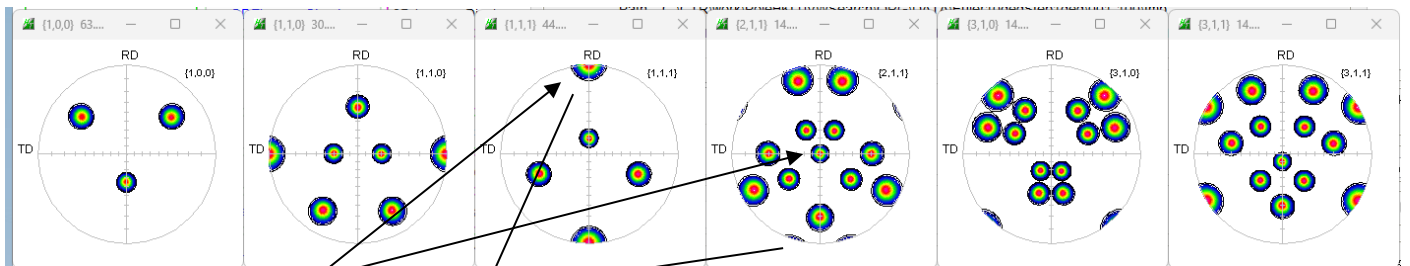
Check

Previous Next 100R45T0N0R0T55N0.TXT Alfa angle check

Save

Normalization TXT(Pole) ASC(Pole) Ras(Pole) TXT2(Pole) Save

PoleFigureStepChenger



$$\{h k l\} \rightarrow \{2 1 1\}$$

$$\langle u v w \rangle \rightarrow [1 1 1]$$

CubeからGossをCrystalRotationで確認（[0 1 -1] 軸を55度回転）

CrystalRotation 1.13 by CTR PDuser HelperTex CTR

File Help RD(TDroate) {uvw}<hkl> {001}<100> RV:Integer Orthorhombic

Material
 Cubic
 1.0 1.0 1.0 90.0 90.0 90.0

{hkl|Kuvw}>

Rotation vector of crystal axis

Rotation vector of machine axis(LaboTex,MTEX) Rotation angle

Result

```

0.0  1.0  1.0
0.0 -1.0  1.0
RDaxis [1 0 0]
TDaxis [0 1 -1]
NDaxis [0 1 1]
0.0  1.0  -1.0  (0 1 -1 )
      {011}<100>  eulerangle:(0.0,45.0,0.0)
Eulerangle g(ψ1Φψ2)=
          1.0  0.0  0.0
          0.0  0.7071  0.7071
          0.0 -0.7071  0.7071
Rotation [0,1,-1]  angle:55.0
Calc-d=(0.0,0.7071,-0.7071)
a(0.0,1.0,-1.0),55.0
Rotated Eulerangle
          0.5736 -0.5792 -0.5792
          0.5792  0.7868 -0.2132
          0.5792 -0.2132  0.7868
Rotated RD  TD  ND
          0.5736  0.0  -0.8192
          0.5792  0.7071  0.4056
          0.5792 -0.7071  0.4056
Calc Miller indices ***** NewCalc *****
          (-2.0197 1.0 1.0)[1.0 1.01 1.0099]
          (1 2 1)[1 -1 1]  (39.23 65.91 26.57)
INT/DOUBLE= (0.9902 1.0 1.0)[1.0 0.9902 0.9902
    
```

(1 2 1)[1 -1 1]

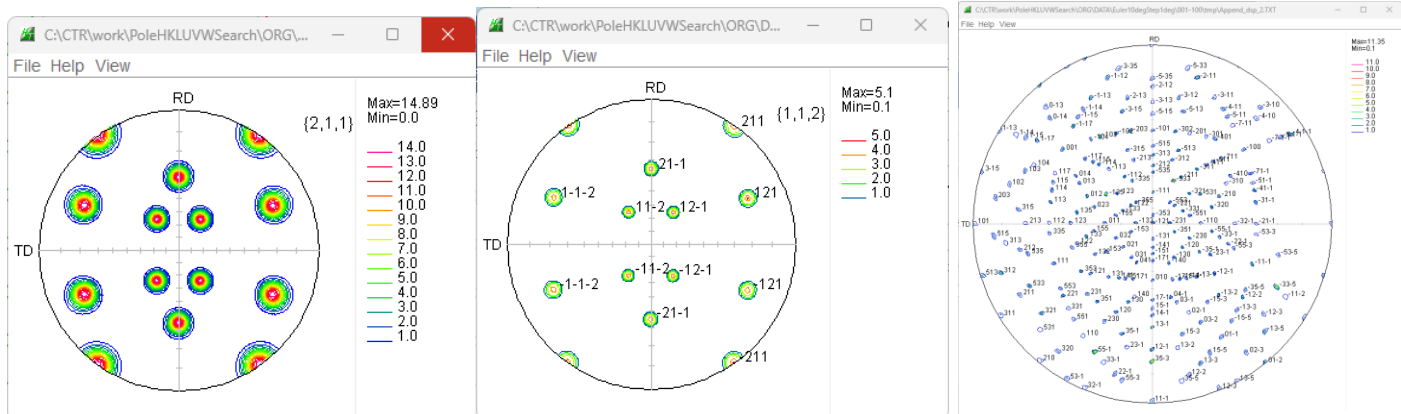
Result (-211)[111] toOrthorhombic (121)[1-11] (39.23 65.91 26.57)

おまけ

単結晶であれば、CubeからGossをPFRotationで確認 (RD軸を45度回転) した
 $\{112\}$ 極点図から方位の決定 (代表2点から)

入力極点図

計算された極点図



CrystalOrientationD 2.00 by CTR PDuser HelperTex CTR

File Help Blind-4 CreatePFStep:1.0 hkdisp=true a0->90

PoleFigure

112 Center of gravity PoleFigure(TXT2) C:\CTR\work\PoleHKLUVWSearch\ORG#DATA#Euler 10degStep 1de...

Alpha(center=0) 73.003 Beta(RD=180) 115.003 hkl 1 2 1
 73.003 64.997 -1 2 1

calc U-matrix CalcPoleFigure FWHM 0.1 Max 5.0 Mini 0.1

calc{hkl}Muw> maxIndex 15 extentAngle 1.5

CalcPoleFigure

112

1 1 -2
 1 2 -1
 2 1 -1
 1 1 2
 1 2 1
 2 1 1

Clear Set Append All

Other(h,k,l) 1,1,1

73.003	115.003	1 2 1
73.003	64.997	-1 2 1

U-matrix

-0.9999902041425026	0.003958951278936862	0.0019794756394685142
0.004194107726656626	0.7045843862211045	0.7096078157361336
0.0014145951411775742	0.7096091666531659	-0.7045940884810107

CalcPoleFigure

Direction	Alpha	Beta	Center=90	
-1 -1 -2	73.44	-85.01	16.56	114.995
-1 1 -2	30.18	-35.71	59.82	144.29
-1 2 -1	29.95	34.65	60.05	214.655
-2 1 -1	54.82	-0.38	35.18	179.618
-1 2 1	73.07	64.47	16.93	244.472
-2 1 1	89.95	35.02	0.05	215.024
1 -1 -2	73.37	-115.43	16.63	64.568
1 1 -2	30.05	-144.61	59.95	35.392
1 2 -1	29.82	144.7	60.18	324.703
2 1 -1	54.65	179.9	35.35	359.904
1 2 1	73.0	115.0	17.0	295.003
2 1 1	89.82	144.5	0.18	324.495

calchkl	phiangle	calchkl		
0.22	-68.49	0	1	-1

calcuw	phiangle	calcuw		
90.08	-0.24	-1	0	0

Initialize File

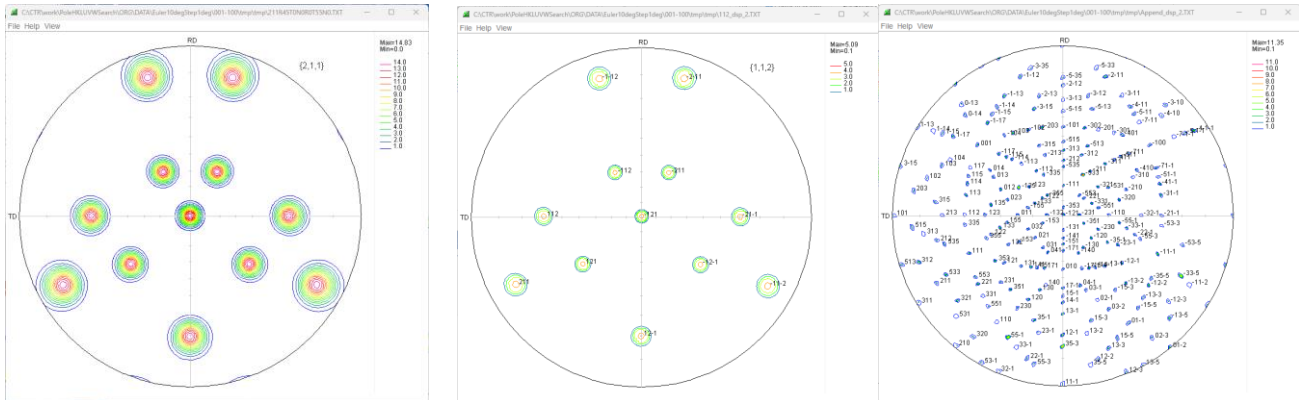
$\{011\} \langle 100 \rangle$ が求められる。

単結晶であればG o s sからC o p p e rをP F R o t a t i o nで確認 (TD軸を55度回転)

{ 1 1 2 } 極点図から方位の決定

入力された極点図

計算された極点図



CrystalOrientationD 2.00 by CTR PDuser HelperTex CTR

File Help Blind-4 CreatePFStep:1.0 hkl disp=true a0->90

PoleFigure

112 Center of gravity PoleFigure(TXT2) C:#CTR#work#PoleHKLUVWSearch#ORG#DATA#Euler10degStep1de...

Alpha(center=0) 70.005 Beta(RD=180) 0.0 hkl 1 2 -1

33.997 148.004 -2 1 1

calc U-matrix CalcPoleFigure FWHM 2 Max 5.0 Mini 0.1

calc{hkl}Muvw> maxIndex 15 extentAngle 0.7

CalcPoleFigure

112 Other(h,k,l) 1,1,1

1 1 -2
1 2 -1
2 1 -1
1 1 2
1 2 1
2 1 1

Clear Set Append All

Alpha	Beta	Direction	Center=90
70.005	0.0	1 2 -1	9.22
33.997	148.004	-2 1 1	16.78
			342.784
			241.399
			231.219
			270.148
			30.383
			321.064
			328.24
			180.0
			89.543
			128.953
			118.364

Direction	Alpha	Beta	Center=90
-1 -1 2	80.78	-163.22	9.22
-2 -1 1	81.03	162.78	8.97
-1 1 -2	80.53	61.4	9.47
-1 2 -1	48.19	51.22	41.81
-2 1 -1	60.42	90.15	29.58
-1 1 2	33.79	-149.62	56.21
-1 2 1	0.67	141.06	89.33
-2 1 1	34.22	148.24	55.78
1 2 -1	70.01	0.0	20.0
1 1 2	59.58	-90.46	30.42
1 2 1	47.53	-51.05	42.47
2 1 1	78.75	31.81	16.21

calchkl	chiangle	calchkl	chiangle
0.67	141.06	-1 2 1	179.85

calcuw	chiangle	calcuw	chiangle
90.52	179.85	-1 -1 1	179.85

Initialize File

{ 1 2 1 } < 1 - 1 1 >が決定される。