

結晶方位の回転

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HelperTex Office

1. 概要

結晶方位 $(hkl)[uvw]$ は整数で表現され、結晶軸回転も整数で表現されている。

しかし、回転された方位は実数であり、整数化すると誤差が発生する。

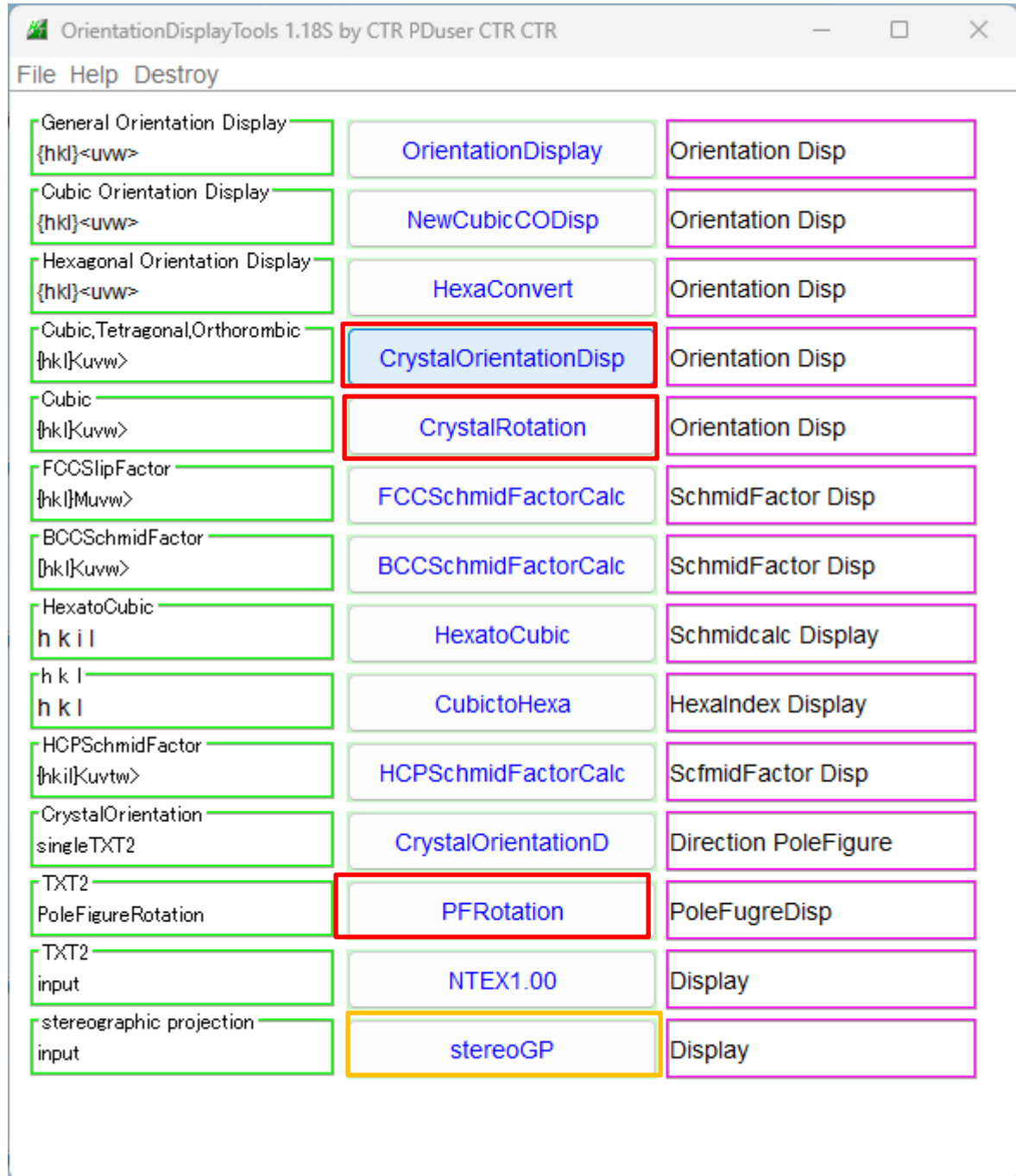
この確認を行うには、結晶軸回転し整数化した方位を逆回転すれば確認出来ます。

あるいは結晶軸回転後の結晶方位から極点図を作成し、回転前の極点図を軸回転し比較すれば誤差が確認出来ます。

極点図の回転では誤差は発生していません。

以上の確認を行ってみます。

簡単に確認出来るようにソフトウェアの変更を行いました。



2. 結晶方位の回転

copper(112)[-1-11]をTD軸 [1-10] で-35度回転

The screenshot shows the CrystalRotation 2.01 software interface. The title bar reads "CrystalRotation 2.01 by CTR PDuser CTR CTR". The menu bar includes "File Help RD(TDroate) {uvw}<hkl> (112)[-1-11] RV:Integer Orthorhombic".

The "Material" section is set to "Cubic" with lattice parameters "1.0 1.0 1.0 90.0 90.0 90.0".

The "{hkl}|{uvw}" input fields are set to "1 | 1 | 2 | -1 | -1 | 1".

The "Rotation vector of crystal axis" is set to "1 | -1 | 0".

The "Rotation vector of machine axis(LaboTex,MTEx)" is set to "0 | 1 | 0".

The "Rotation angle" is set to "-35".

The "Result" section displays the following output:

```
-1.0 1.0 1.0
-1.0 -1.0 1.0
1.0 0.0 2.0
RDaxis [-1 -1 1]
TDaxis [1 -1 0]
NDaxis [1 1 2]
1.0 -1.0 0.0 (1 -1 0)
(112)[-1-11] eulerangle:(90.0,35.264,45.0)
Eulerangle g(φ1 Φφ2)=
-0.5774 0.7071 0.4082
-0.5774 -0.7071 0.4082
0.5774 0.0 0.8165
Rotation [1,-1,0] angle:-35.0
Calc-d=(0.7071,-0.7071,0.0)
a(1.0,-1.0,0.0),-35.0
Rotated Eulerangle
0.9096 -0.0904 -0.4056
-0.0904 0.9096 -0.4056
0.4056 0.4056 0.8192
Rotated RD TD ND
-0.7071 0.7071 0.0033
-0.7071 -0.7071 0.0033
0.0046 0.0 1.0
Calc Miller indices ***** NewCalc *****
(0.0 0.0 1.0)[-1.0 -1.0 0.0]
(0 0 1)[-1 -1 0] (45.0 0.0 90.0)
INT/DOUBLE= (0.0 0.0 1.0)[1.0 1.0 0.0]
```

The output "(0 0 1)[-1 -1 0]" is circled in yellow.

The bottom of the interface shows buttons for "ODF", "set{hkl}|{uvw}", "OrientationDisp", and "ResultCreat".

(001)[-1-10]を得る。

3. 結晶方位の逆回転で確認

[1 1 2] [-1 -1 1]

ODF

set{hkl}<uvw>

OrientationDisp

ResultCreat

Set{hkl}<uvw>で回転した方位をセットし、-35度回転

The screenshot shows the CrystalRotation 2.01 software interface. The title bar reads "CrystalRotation 2.01 by CTR PDuser CTR CTR". The menu bar includes "File", "Help", "RD(TDroate) {uvw}<hkl> (112)[-1-11] RV:Integer Orthorhombic".

The "Material" section is set to "Cubic" with lattice parameters "1.0 1.0 1.0 90.0 90.0 90.0".

The "{hkl}<uvw>" section has input fields for h, k, l, u, v, w set to 0, 0, 1, -1, -1, 0. Buttons for "ODF" and "OrientationDisp" are visible.

The "Rotation vector of crystal axis" section has input fields for rotation angles set to 1, -1, 0, with "SET" and "CTD" buttons.

The "Rotation vector of machine axis(LaboTex,MTEX)" section has input fields for rotation angles set to 0, 1, 0, with "SET" and "Calc" buttons. The "Rotation angle" field is set to 35.

The "Result" section displays the following output:

```

-1.0  1.0  0.0
-1.0 -1.0  0.0
 0.0  0.0  1.0
RDaxis [-1 -1 0]
TDaxis [1 -1 0]
NDaxis [0 0 1]
1.0 -1.0  0.0      (1 -1 0 )
(001)[-1-10]  eulerangle:(45.0,0.0,90.0)
Eulerangle g(φ1 φ2)=
  -0.7071  0.7071  0.0
  -0.7071 -0.7071  0.0
   0.0     0.0     1.0
Rotation [1,-1,0]      angle:35.0
Calc-d=(0.7071,-0.7071,0.0)
a(1.0,-1.0,0.0),35.0
Rotated Eulerangle
  0.9096 -0.0904  0.4056
 -0.0904  0.9096  0.4056
 -0.4056 -0.4056  0.8192
Rotated RD    TD    ND
 -0.5792  0.7071  0.4056
 -0.5792 -0.7071  0.4056
  0.5736  0.0     0.8192
Calc Miller indices ***** NewCalc *****
(1.0 1.0 2.0197)[-1.0099 -1.01 1.0]
(1 1 2)[-1 -1 1]      (90.0 35.26 45.0)
INT/DOUBLE= (1.0 1.0 0.9902)[0.9902 0.9902 1.0]

```

At the bottom of the window, the input fields and buttons are repeated: "[1 1 2] [-1 -1 1]", "ODF", "set{hkl}<uvw>", "OrientationDisp", and "ResultCreat".

(1 1 2) [-1 -1 1] が得られる。

4. 極点図による確認

結晶方位を回転し、得られた結晶方位から極点図を作成
回転前の結晶方位から極点図を作成し、極点図を回転する。
極点図の回転は整数化していないため、誤差はありません。

4. 1 回転前の結晶方位から極点図作成

The screenshot displays the CrystalRotation 2.01 software interface. The main window is titled "CrystalRotation 2.01 by CTR PDuser CTR CTR" and shows the material "Cubic" with lattice parameters "1.0 1.0 1.0 90.0 90.0 90.0". The Miller indices are set to $\{111\}$ with hkl values of 1, 1, 2, -1, -1, 1. The "OrientationDisp" button is highlighted with a yellow circle. A secondary window titled "CrystalOrientationDisp 2.11S by CTR PDuser CTR CTR" is open, showing the same material and Miller indices. The "Calc" button in this window is also highlighted with a yellow circle. A third window titled "C:\CTR\work\NewC..." displays a pole figure plot. The plot shows intensity contours on a circular grid with axes labeled "RD" (vertical) and "TD" (horizontal). The plot is labeled "RD_{-11}" and "TD_{-11}" at the top and bottom respectively. A legend on the right indicates intensity values from 19.0 to 32.0, with "Max=32.81" and "Min=0.0". The "Disp" button in the main window is highlighted with a yellow circle, and the "PFRotation" button is highlighted with a red circle. Arrows indicate the flow of data from the main window to the secondary window, and from the secondary window to the pole figure plot.

TD 軸を -35 度回転

The screenshot displays the PFRotation 1.21 software interface. At the top, two windows show the initial pole figure with RD and TD axes. The main window shows the following settings:

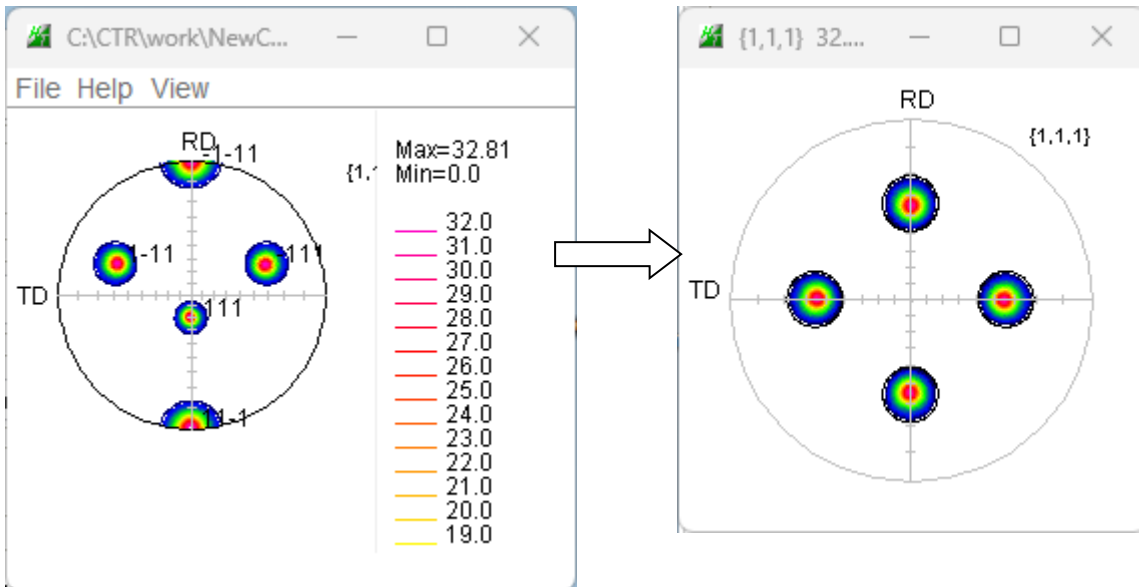
- Path: C:\CTR\work\NewCubicCODisp
- File: 111_dsp_2.TXT
- Rotation(-360 <= degrees <= 360) of vector machine axis:
 - AlongRD(X): 1, 0
 - AlongTD(Y): 2, -35 (highlighted with a yellow circle)
 - AlongND(Z): 3, 0
 - 4, 0
- toOrthorhombic
- Rotate PoleFigure** (highlighted with a red circle)
- MTEX

Check section:
Previous Next 111_dsp_2.TXT Alfa angle check

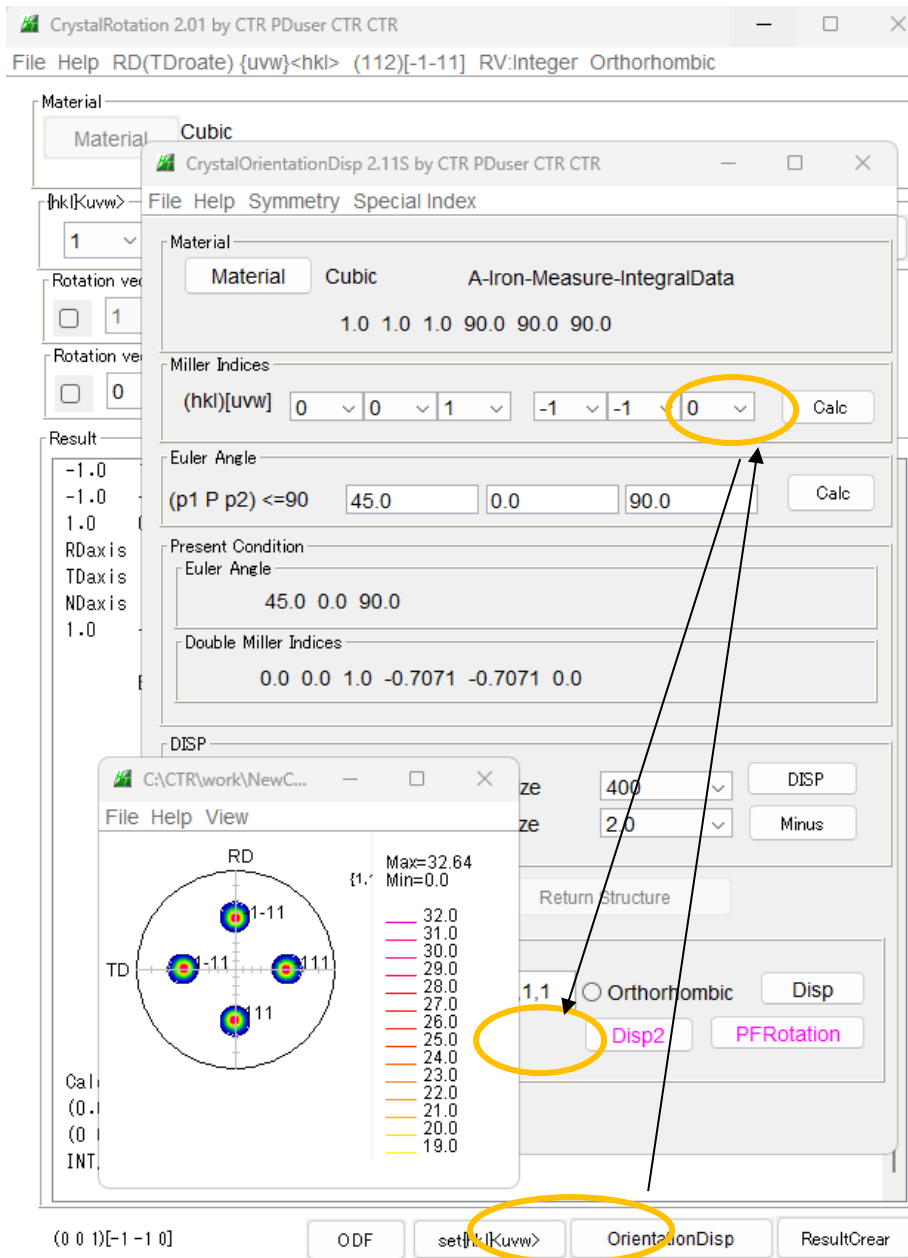
Save section:
 Normalization TXT(Pole) ASC(Pole) Ras(Pole) TXT2(Pole) Save

PoleFigureStepChenger

極点図を TD 軸 -35 度回転で得られる極点図

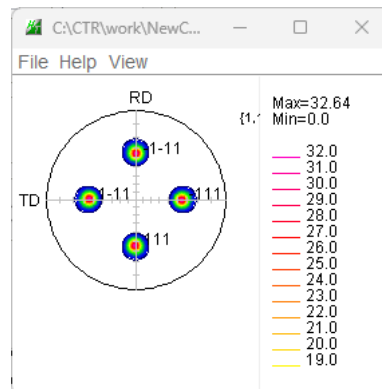
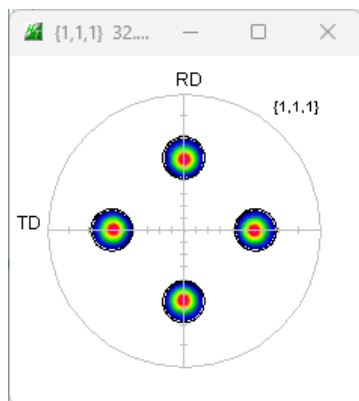


4. 2 回転後の結晶方位から極点図作成



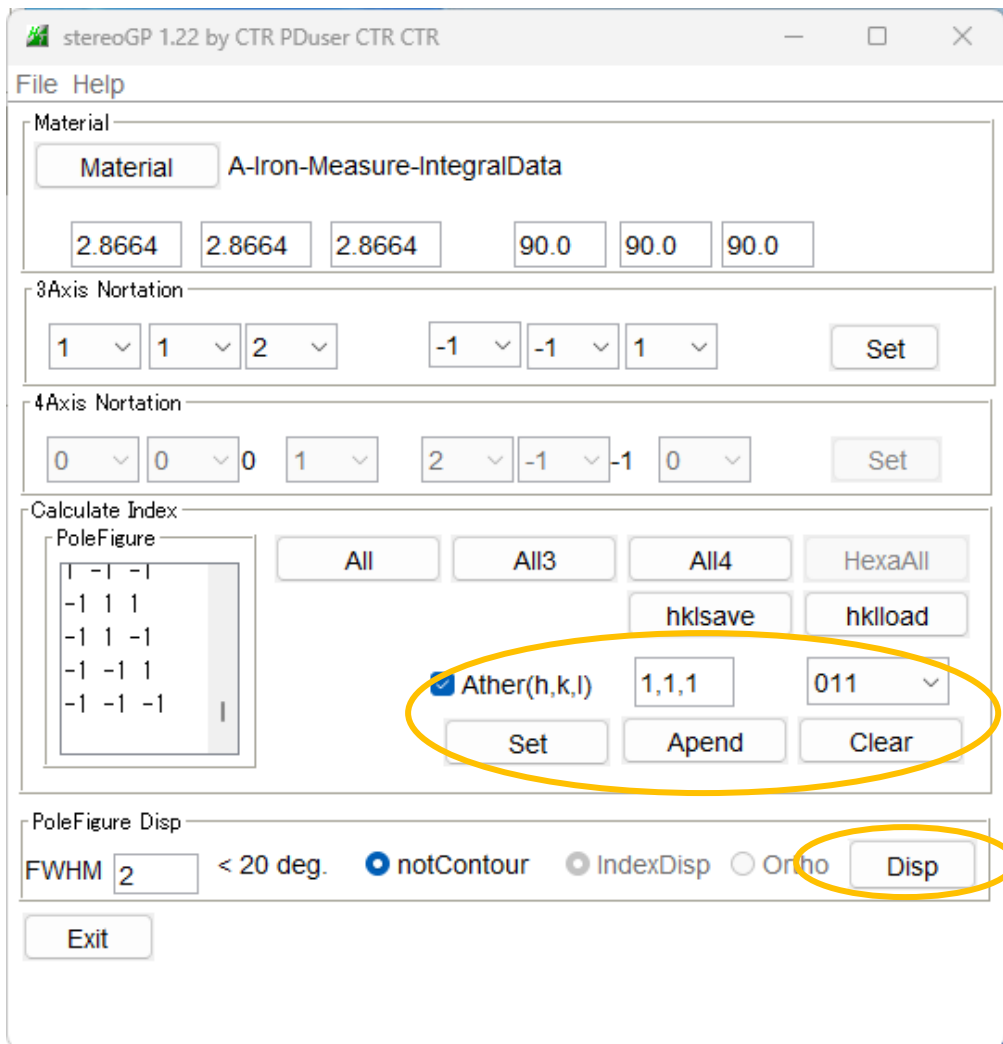
回転前の極点図を回転

結晶方位回転後の極点図

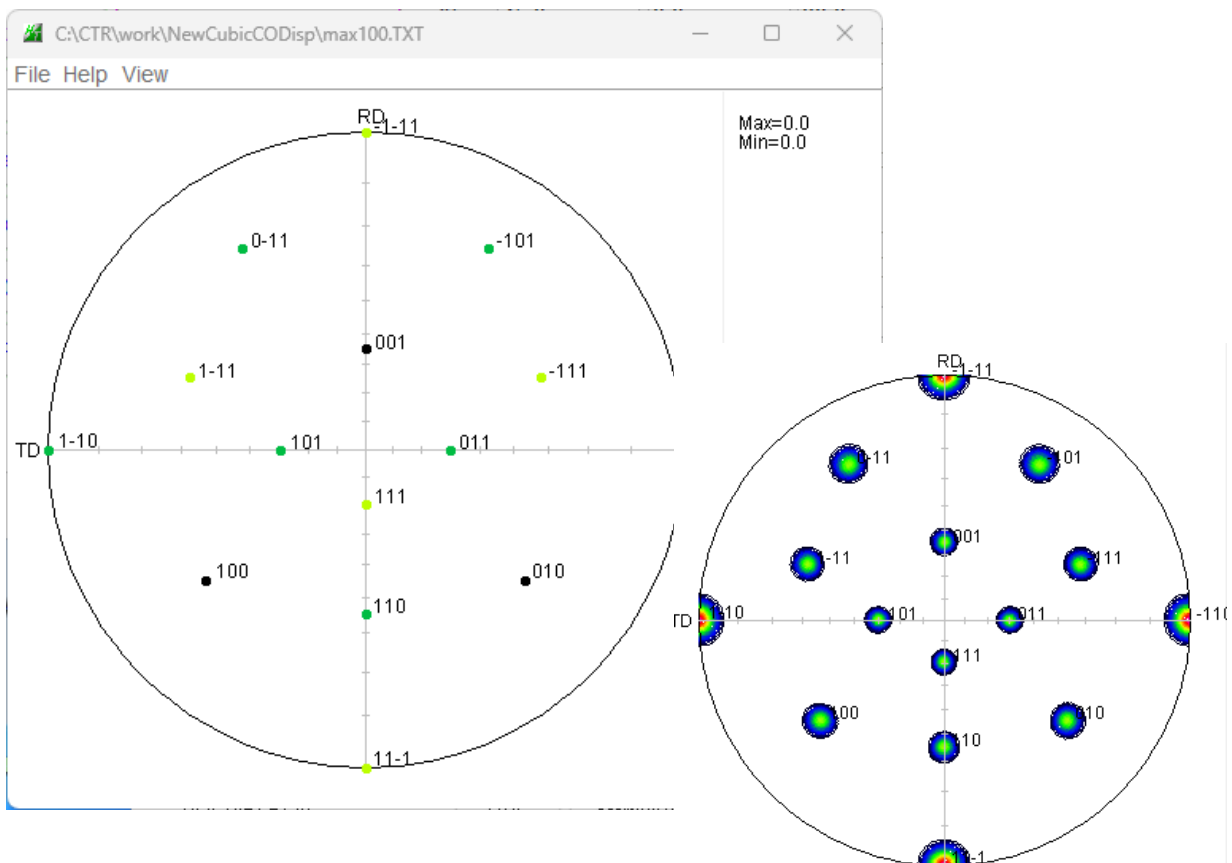


一致が確認出来ます。

5. 結晶方位から複数の極点図を重ね合わせた確認



極点図を S e t し、次の極点図を A p e n d し、 D i s p



6. 誤差が発生する場合

(1.0 1.0 4.8474)[-2.4237 -2.424 1.0]
 (6 6 29)[-12 -17 6] (80.6 16.31 45.0)
 INT/DOUBLE= (6.0 6.0 5.9826)[4.9511 7.0141 6.0]

整数化部分

6. 1 逆回転

CrystalRotation 2.02 by CTR PDuser CTR CTR

File Help RD(TDroate) {uvw}<hkl> (112)[-1-11] RV:integer Free calcNew

Material

Material Cubic

1.0 1.0 1.0 90.0 90.0 90.0

hkl|Kuvw>

6 6 29 -12 -17 6 ODF OrientationDisp

Rotation vector of crystal axis

51 -37 -3 SET CTD

Rotation vector of machine axis(LaboTex,MTEX)

0 1 0 SET

Rotation angle

19 Calc

Result

```

-12.0 51.0 6.0
-17.0 -37.0 6.0
6.0 -3.0 29.0
RDaxis [-12 -17 6]
TDaxis [51 -37 -3]
NDaxis [6 6 29]
51.0 -37.0 -3.0 (51 -37 -3)
(6629)[-12-176] eulerangle:(80.604,16.309,45.0)
Eulerangle g(phi1 phi2)=
-0.5541 0.8084 0.1986
-0.785 -0.5868 0.1986
0.2771 -0.0458 0.9598
Rotation [51,-37,-3] angle:19.0
Calc-d=(0.8085,-0.5868,-0.0476)
a(51.0,-37.0,-3.0),19.0
Rotated Eulerangle
0.9811 -0.0413 0.1889
-0.0104 0.9643 0.2647
-0.1931 -0.2617 0.9456
Rotated RD TD ND
-0.4589 0.8088 0.3679
-0.6778 -0.5864 0.4435
0.5744 -0.0459 0.8173
Calc Miller indices
(1.0 1.2055 2.2215)[-1.0 -1.477 1.2517]
(5 6 11)[-1 -1 1] (94.24 35.38 39.81)
INT/DOUBLE= (5.0 4.977 4.9515)[1.0 0.677 0.7989]

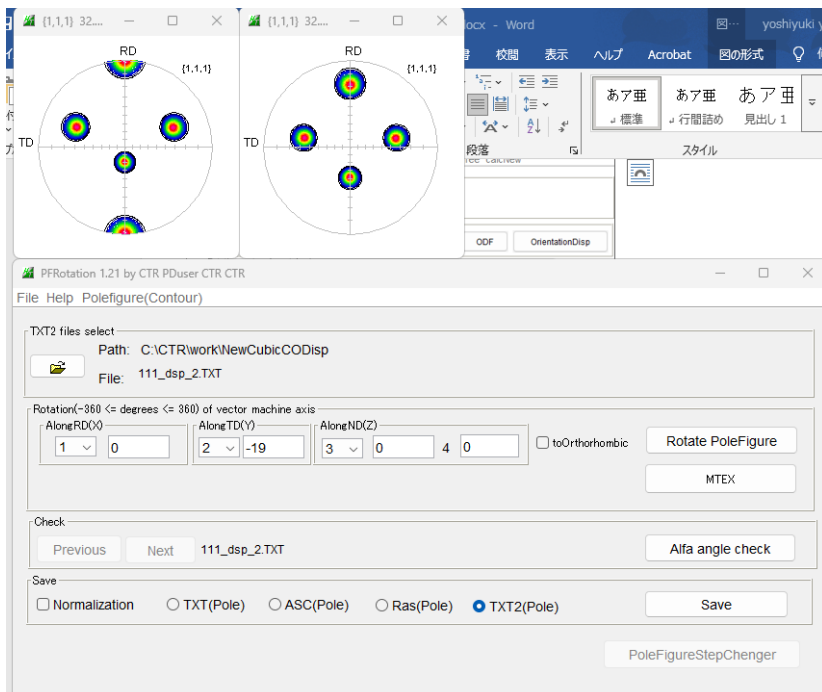
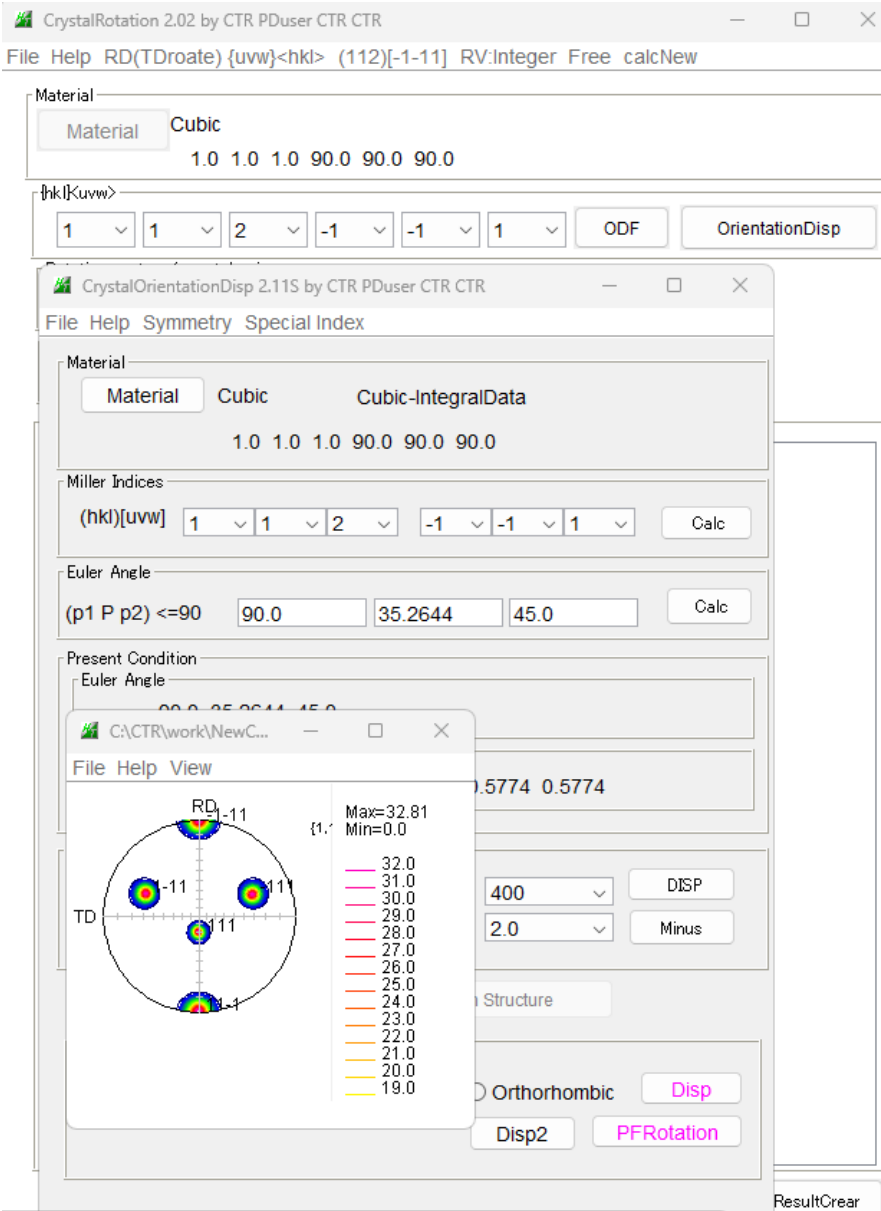
```

(5 6 11)[-1 -1 1] ODF set|hkl|Kuvw> OrientationDisp ResultClear

Result: (5611)[-1-11] (94.24 35.38 39.81)

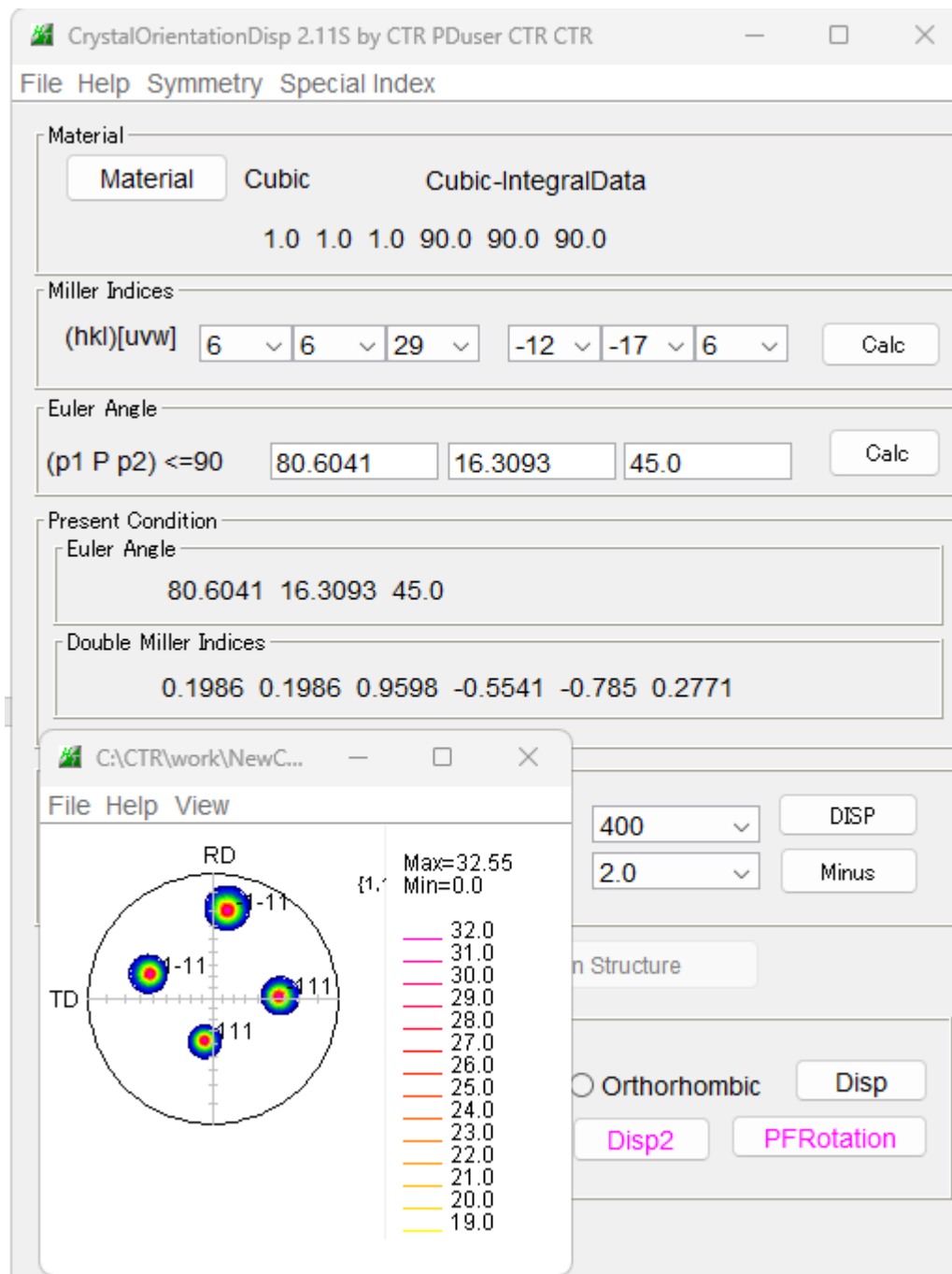
(1 1 2) [-1 -1 1] TD 軸-19度回転で (6 6 29) [-1 2 -1 7 6] 逆回転で (6 5 1 1) [-1 -1 1] でずれている。

6. 2 極点図で確認 ((112)[-1-11]を PFRotation で TD-19 度回転



回転後の極点図

CrystalRotation で TD- 1 9 度回転の極点図



TD 軸回転で ND 方向の回転が含まれている。

結晶方位の回転にずれが発生する。

整数化の問題である。

6. 3 極点図回転から方位を決定し方位の逆回転
 極点図の指数付けから結晶方位を求める

The screenshot shows the CrystalOrientationD 2.15 software interface. The main window is titled "PoleFigure" and contains several input fields and buttons. A yellow circle highlights the "PoleFigure(TXT2)" dropdown menu. Another yellow circle highlights the output list containing the entry $(5\ 1\ 1)[2\ -5\ -5]$ with coordinates $(316.1\ 78.9\ 78.69)$. A blue arrow points from this entry to the left pole figure plot. The left plot shows a circular pole figure with a color scale from 19.0 to 32.0. The right plot shows a circular pole figure with a color scale from 87.0 to 99.0. Below the plots, a list of $\{hkl\}\langle uvw \rangle$ pairs is displayed, including $(5\ 1\ 1)[2\ -5\ -5]$. At the bottom of the window, there are "Initialize" and "File" buttons.

$(5\ 1\ 1)[2\ -5\ -5]$ が得られる。

この方位を逆回転すると copper が得られる。

Material

Material

Cubic

1.0 1.0 1.0 90.0 90.0 90.0

{hkl|Kuvw>

5

1

1

2

-5

-5

ODF

OrientationDisp

Rotation vector of crystal axis

0

1

-1

SET

CTD

Rotation vector of machine axis(LaboTex,MTEX)

0

1

0

SET

Rotation angle

19

Calc

Result

```

2.0  0.0  5.0
-5.0  1.0  1.0
-5.0 -1.0  1.0
RDaxis [2 -5 -5]
TDaxis [0 1 -1]
NDaxis [5 1 1]
0.0  1.0  -1.0  (0 1 -1 )
(511)[2-5-5]  eulerangle:(316.102,78.904,78.69)
Eulerangle g( $\psi_1 \Phi \psi_2$ )=
      0.2722  0.0  0.9623
      -0.6804  0.7071  0.1924
      -0.6804 -0.7071  0.1925
Rotation [0,1,-1]  angle:19.0
Calc-d=(0.0,0.7071,-0.7071)
a(0.0,1.0,-1.0),19.0
Rotated Eulerangle
      0.9455 -0.2302 -0.2302
      0.2302  0.9728 -0.0272
      0.2302 -0.0272  0.9728
Rotated RD  TD  ND
      0.5706  0.0  0.8212
      -0.5807  0.7071  0.4035
      -0.5807 -0.7071  0.4035
Calc Miller indices
(2.0353 1.0 1.0)[1.0 -1.018 -1.0177]
(2 1 1)[1 -1 -1]  (320.77 65.91 63.43)
INT/DOUBLE= (0.9827 1.0 1.0)[1.0 0.9827 0.9827]

```

(2 1 1)[1 -1 -1]

ODF

set{hkl|Kuvw>

OrientationDisp

ResultCreat

Result (211)[1-1-1] (320.77 65.91 63.43)

