

単結晶ブロックの任意方位切り出し方法

023年12月04日

HelperTex Office

概要

単結晶の方位測定は、ラウエカメラ、RASC0、極点測定で行われている。

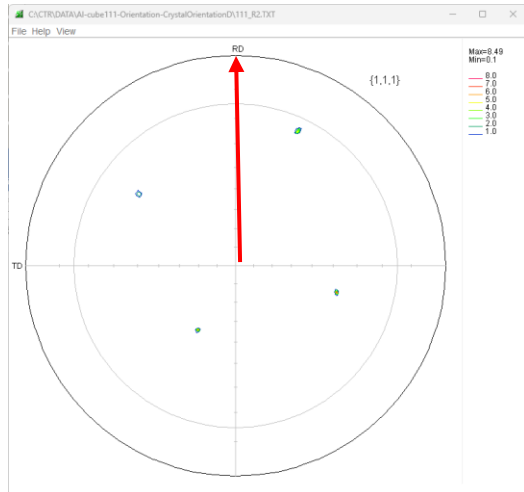
この測定結果から取り付け方位を計算し、所望の方位極点図から法線方向に近い反射を計算しブロックの切り出しをCrystalOrientationDソフトウェアでサポートします。

基準方位 (X軸) が異なります。CrystalOrientationDソフトウェアでは極点測定ではNorth方向、ラウエカメラとRASC0ではSouth方向とし、

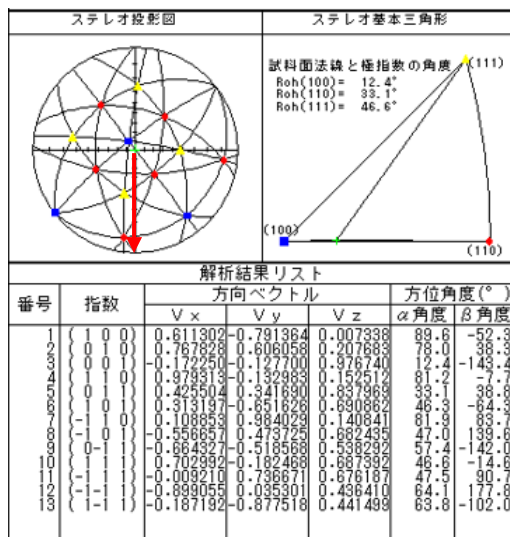
East方向の場合、入力後South方向に変換が行われ、取り付け方位の計算が行われる。

測定例

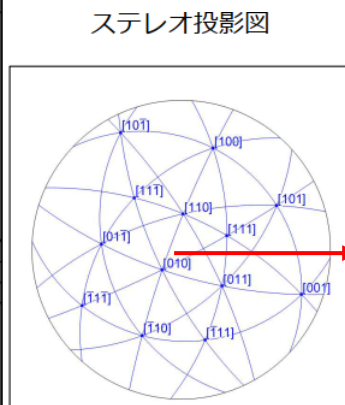
極点図 (North)



RASC0 (South)



ラウエカメラ (East)



方位解析結果

[hkl]	α (°)	β (°)
[100]	71.0	72.6
[010]	21.0	226.5
[001]	81.4	339.6
[110]	27.1	86.9
[101]	70.4	24.8
[011]	40.0	318.4
[-110]	64.6	245.5
[10-1]	82.8	117.4
[01-1]	56.3	175.9
[111]	35.6	17.2
[-111]	64.1	284.8
[11-1]	50.1	132.1
[-11-1]	74.7	209.3

CrystalOrientationDソフトウェア

デモデータ

ピークサーチ除外範囲

極点図入力

作成極点図ステップ

East<->South切り替え

CrystalOrientationD 2.03 by CTR PDuser HaperTex CTR

File Help Blind-40 CreatePFStep:1.0 hkl disp=true alpha->90 X-Axis:East

PoleFigure

001 Center of gravity PoleFigure(TXT2) RD input mode is South.

Alpha(center=0) 0 Beta(RD=180) 0 hkl 0 0 1

90 180 -1 0 0

calc U-matrix CalcPoleFigure FWHM 0.1 Max 5.0 Mini 0.1

calc{hkl}<uvw> maxIndex 15 extentAngle 1.0 calcTD

CalcPoleFigure

001

0 0 -1

0 -1 0

-1 0 0

0 0 1

0 1 0

1 0 0

Clear

Set

Append

All

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

方位計算

(hkl)[uvw]計算

極点図作成

手入力

計算方位指定

Initialize

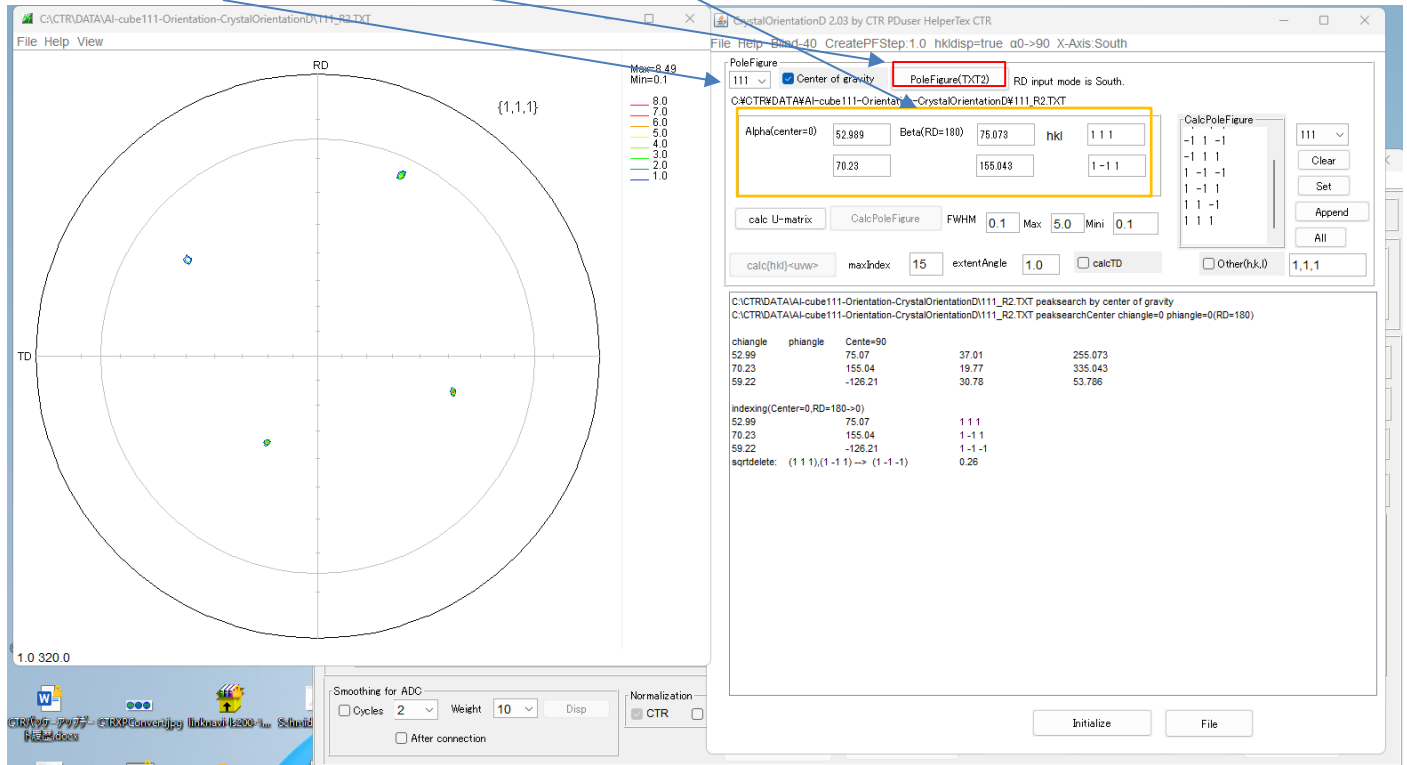
File

表示の初期化

表示データのファイル化

極点図の場合

極点図指数を指定し、極点ファイル選択と同時に主要ピークの指数付けが行われる。



方位計算

PoleFigure
 111 Center of gravity PoleFigure(TXT2) RD input mode is South.
 C:\CTR\DATA\AI-cube111-Orientation-CrystalOrientationD\111_R2.TXT

Alpha(center=0) 52.989 Beta(RD=180) 75.073 hkl 1 1 1
 70.23 155.043 1 -1 1

calc U-matrix CalcPoleFigure FWHM 0.1 Max 5.0 Mini 0.1

calc(hkl)<uvw> maxIndex 15 extentAngle 1.0 calcTD Other(h,k,l) 1,1,1

CalcPoleFigure
 111 Clear Set Append All

U-matrix

-0.2641746454146396	0.9175659592456563	-0.29712702191764423
0.06811334939072833	0.32505128735107974	0.9432402833987651
0.9620666964170552	0.22894185075036977	-0.1483687993486819
hkl	Alpha	Beta
1 1 1	52.99	75.07
1 1 -1	39.35	-30.06
1 -1 1	70.27	155.11
1 -1 -1	59.41	-126.39
		37.01
		50.65
		19.73
		30.59
		255.073
		335.105
		53.786

極点図を計算比較

PoleFigure
 111 Center of gravity PoleFigure(TXT2) RD input mode is South.
 C:\CTR\DATA\AI-cube111-Orientation-CrystalOrientationD\111_R2.TXT

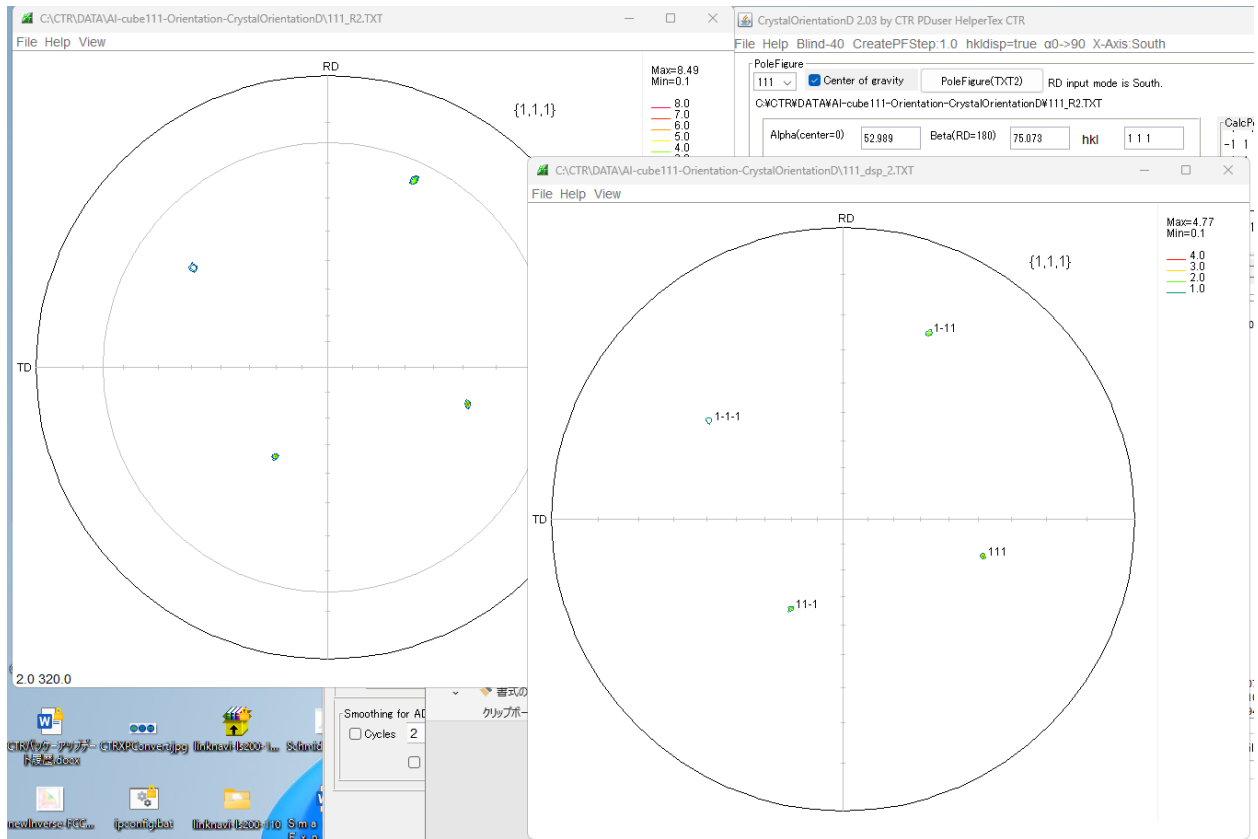
Alpha(center=0) 52.989 Beta(RD=180) 75.073 hkl 1 1 1
 70.23 155.043 1 -1 1

calc U-matrix **CalcPoleFigure** FWHM 0.1 Max 5.0 Mini 0.1

calc{hkl}<uvw> maxIndex 15 extentAngle 1.0 calcTD Other(h,k,l) 1,1,1

CalcPoleFigure
 111
 -1 1 -1
 -1 1 1
 1 -1 -1
 1 -1 1
 1 1 -1
 1 1 1

111
 Clear
 Set
 Append
 All



同一極点図が表示されれば、計算は正常である。

方位計算

calc{hkl}<uvw> maxIndex 15 extentAngle 1.5 calcTD

[hkl]<uvw>(extentAngle=1.5)

(12 3 -2)[-3 10 -3]
 (12 3 -2)[3 -10 3]

chiangle	phiangle	calcuvw		
90.8	1.14	-3	10	-3
89.2	-178.86	3	-10	3

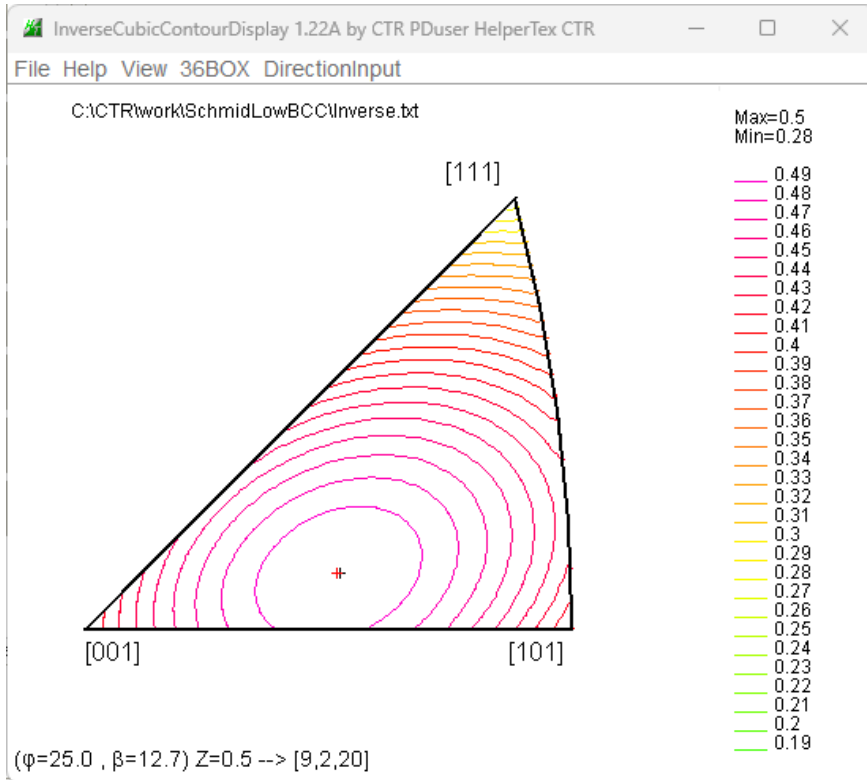
極点図の場合 Nouth で判断する

S C h m i d 因子最大方位

Slip Systems

{011}<11-1>
 {112}<11-1>
 {123}<11-1>
 FCC{111}<1-10>
 Stack

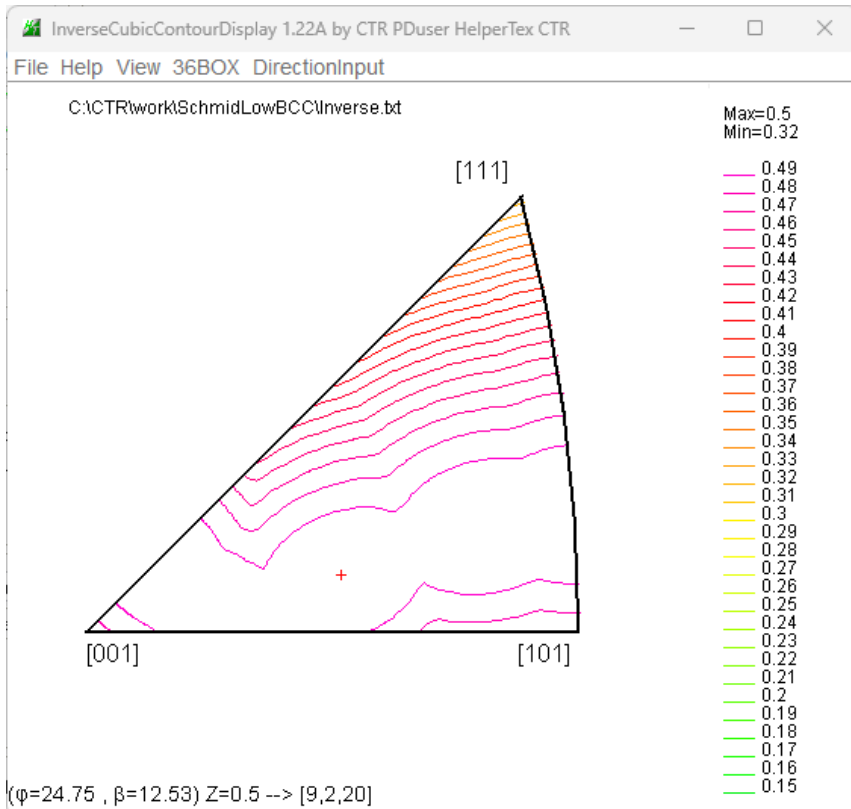
F C C



Slip Systems

{011}<11-1>
 {112}<11-1>
 {123}<11-1>
 FCC{111}<1-10>
 Stack

B C C



Schmid因子最大方位 {9, 2, 20} の描画

PoleFigure
 111 Center of gravity PoleFigure(TXT2) RD input mode is South.
 C:\CTR\DATA\AI-cube111-Orientation-CrystalOrientationD\111_R2.TXT

Alpha(center=0) 52.989 Beta(RD=180) 75.073 hkl 1 1 1
 70.23 155.043 1 -1 1

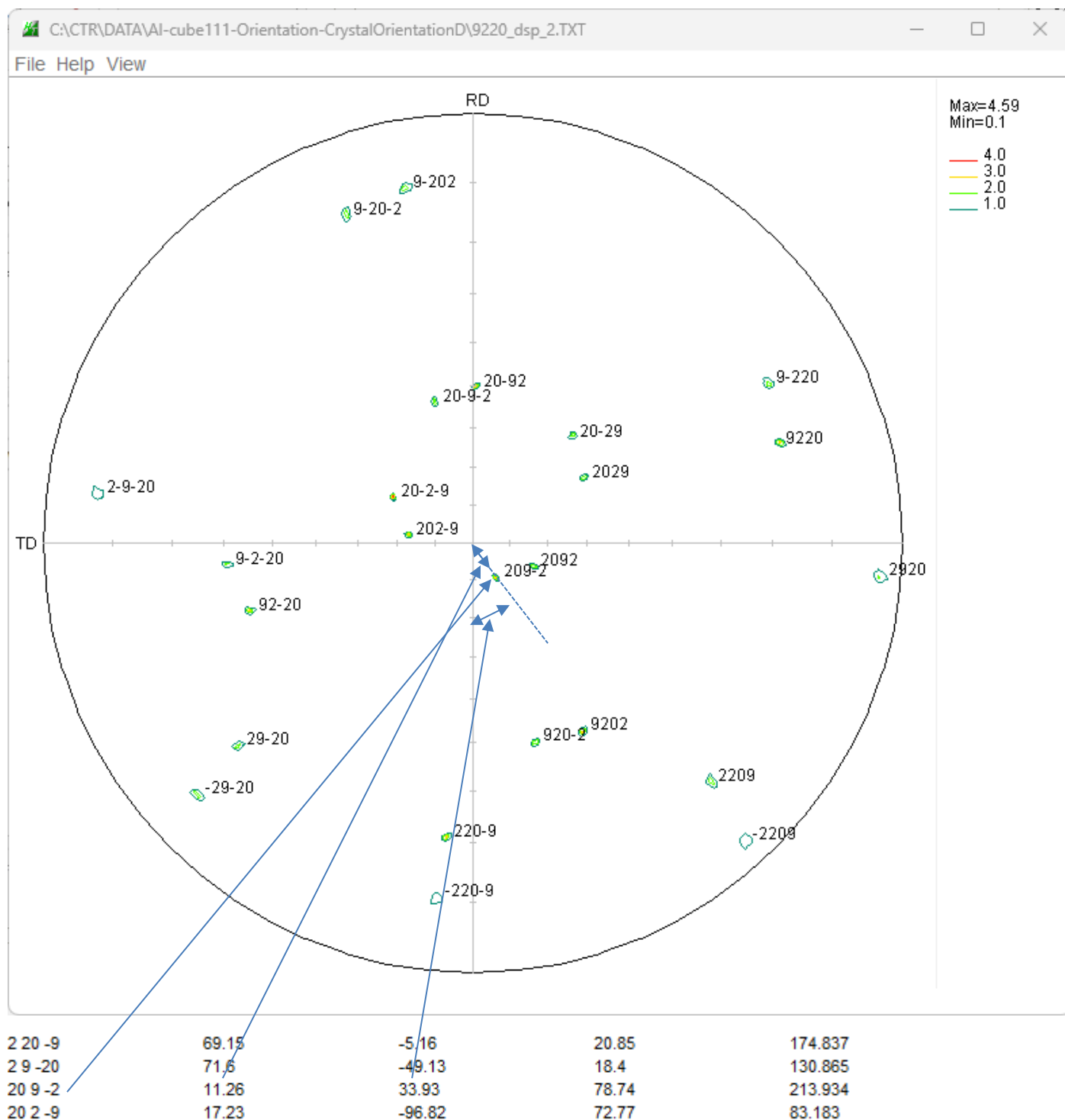
Calc PoleFigure
 9 2 20
 9 20 2
 2 20 9
 2 9 20
 20 9 2
 20 2 9

111

FWHM 0.1 Max 5.0 Mini 0.1

maxIndex 15 extentAngle 1.5 calcTD

Other(h,k,l) 9,2,20



-RDから (11.26, 33.93) が切り出しデータである。

検証 (入力は回転順位1: 転-33.93, 転順位2: TD回転11.26, 回転順位3: RD回転0.0)

File Help Polefigure(Contour)

TXT2 files select

Path: C:\CTR\DATA\AI-cube111-Orientation-CrystalOrientationD

File: 9220_dsp_2.TXT

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

AlongRD(X) 3 0

AlongTD(Y) 2 11.2

AlongND(Z) 1 -33.93 4 0

toOrthorhombic

Rotate PoleFigure

MTEX

Check

Previous Next 9220_dspN-33N0T11R0.TXT

Alfa angle check

Save

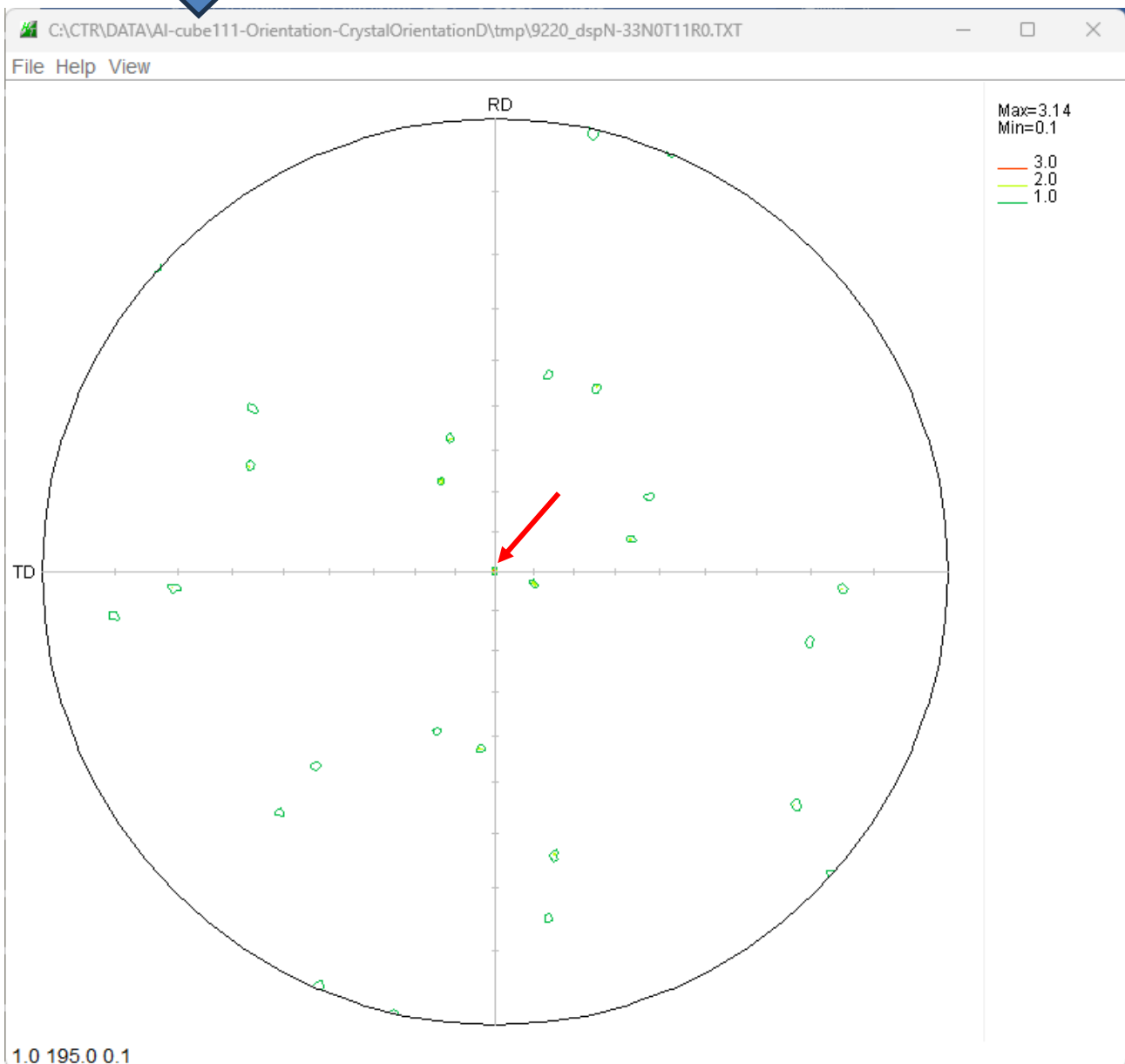
Normalization TXT(Pole) ASC(Pole) Ras(Pole) TXT2(Pole)

Save

PoleFigureStepChenger

> ぼかし

> 3-D 書式



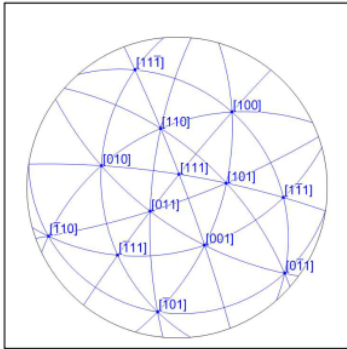
ラウエカメラの場合 (East入力)

East入力をcalcU-matrix操作でSouthに変換して計算される。

RASCOの場合、Southを選択し入力する。

ステレオ投影図

方位解析結果



[hkl]	$\alpha(^{\circ})$	$\beta(^{\circ})$
[100]	63.7	54.0
[010]	55.4	163.9
[001]	46.1	295.5
[110]	44.3	105.5
[101]	36.5	5.1
[011]	26.9	221.3
[-110]	85.0	200.7
[-101]	79.8	261.1
[0-11]	84.9	321.4
[111]	10.2	81.2
[-111]	61.8	228.7
[1-11]	70.8	354.6
[11-1]	79.4	109.7

CrystalOrientationD 2.03 by CTR PDuser HelperTex CTR

File Help Blind-40 CreatePFStep:1.0 hkl disp=true $\alpha_0 \rightarrow 90$ X-Axis:East

PoleFigure
 Center of gravity PoleFigure(TXT2) RD input mode is East.

Alpha(center=0) 63.70 Beta(RD=180) 54 hkl 1 0 0
 55.4 163.9 0 1 0

calc U-matrix CalcPoleFigure FWHM 0.1 Max 5.0 Mini 0.1

calc{hkl}<uvw> maxIndex 15 extentAngle 1.0 calcTD Other(h,k,l) 1,1,1

CalcPoleFigure
 0 0 -1
 0 -1 0
 -1 0 0
 0 0 1
 0 1 0
 1 0 0

CalcU-matrix で角度が返還される

CrystalOrientationD 2.03 by CTR PDuser HelperTex CTR

File Help Blind-40 CreatePFStep:1.0 hkl disp=true $\alpha_0 \rightarrow 90$ X-Axis:East

PoleFigure
 Center of gravity PoleFigure(TXT2) RD input mode is East.

Alpha(center=0) 63.70 Beta(RD=180) 144.0 hkl 1 0 0
 55.4 -106.1 0 1 0

calc U-matrix CalcPoleFigure FWHM 0.1 Max 5.0 Mini 0.1

calc{hkl}<uvw> maxIndex 15 extentAngle 1.0 calcTD Other(h,k,l) 1,1,1

CalcPoleFigure
 0 0 -1
 0 -1 0
 -1 0 0
 0 0 1
 0 1 0
 1 0 0

Alpha	Beta	
63.7	144.0	1 0 0
55.4	-106.1	0 1 0

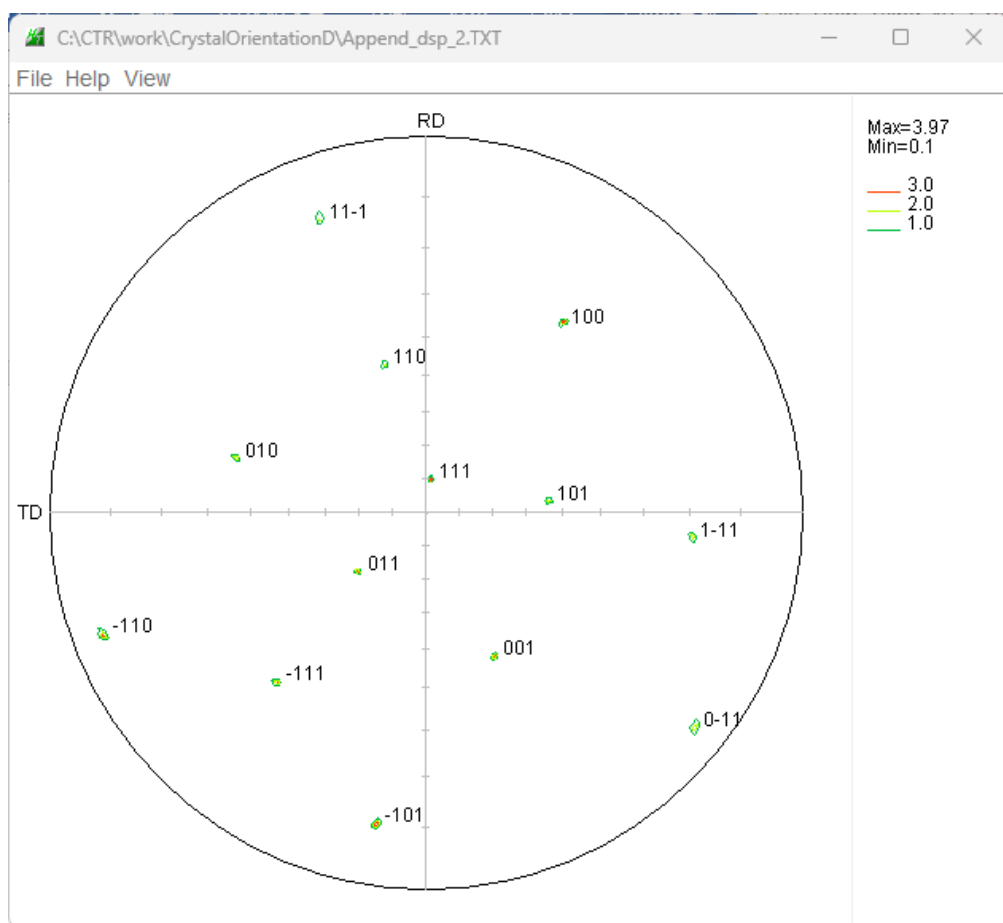
U-matrix
 -0.7252727574067366 -0.2279641076813063 0.6496243475830435
 0.5269415026597094 -0.7910729762136492 0.3107027503566821
 0.4430711908241796 0.5676582703647901 0.6938674282224944

(0 0 1), (0 1 1), (1 1 1) の指定し極点図作成

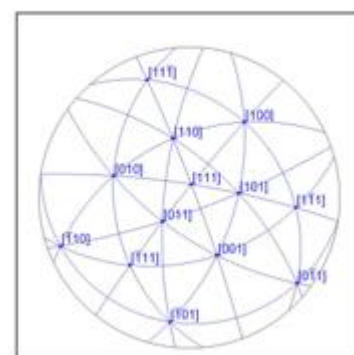
Three CalcPoleFigure dialog boxes are shown. The first dialog is set to '001' and has the 'Set' button circled. The second dialog is set to '011' and has the 'Append' button circled. The third dialog is set to '111' and has the 'Append' button circled. Each dialog contains a list of hkl values, buttons for 'Clear', 'Set', 'Append', and 'All', and a checkbox for 'Other(h,k,l)' with a value of '1,1,1'.

calc U-matrix CalcPoleFigure FWHM 0.1 Max 5.0 Mini 0.1

calc{hkl}<uvw> maxIndex 15 extentAngle 1.0 calcTD



ステレオ投影図



ラウエカメラのステレオ投影図が表示されれば、計算結果は正常です。

必要な極点図は、極点図の場合と同様の操作が可能になります。

ND方向に [9, 2, 2 0] を向ける軸回転

CrystalOrientationD 2.03 by CTR PDuser HelperTex CTR

File Help Blind-40 CreatePFStep:1.0 hkldisp=true $\alpha_0 \rightarrow 90$ X-Axis:East

PoleFigure

001 Center of gravity PoleFigure(TXT2) RD input mode is South.

Alpha(center=0) 63.70 Beta(RD=180) 144.0 hkl 1 0 0
 55.4 -106.1 0 1 0

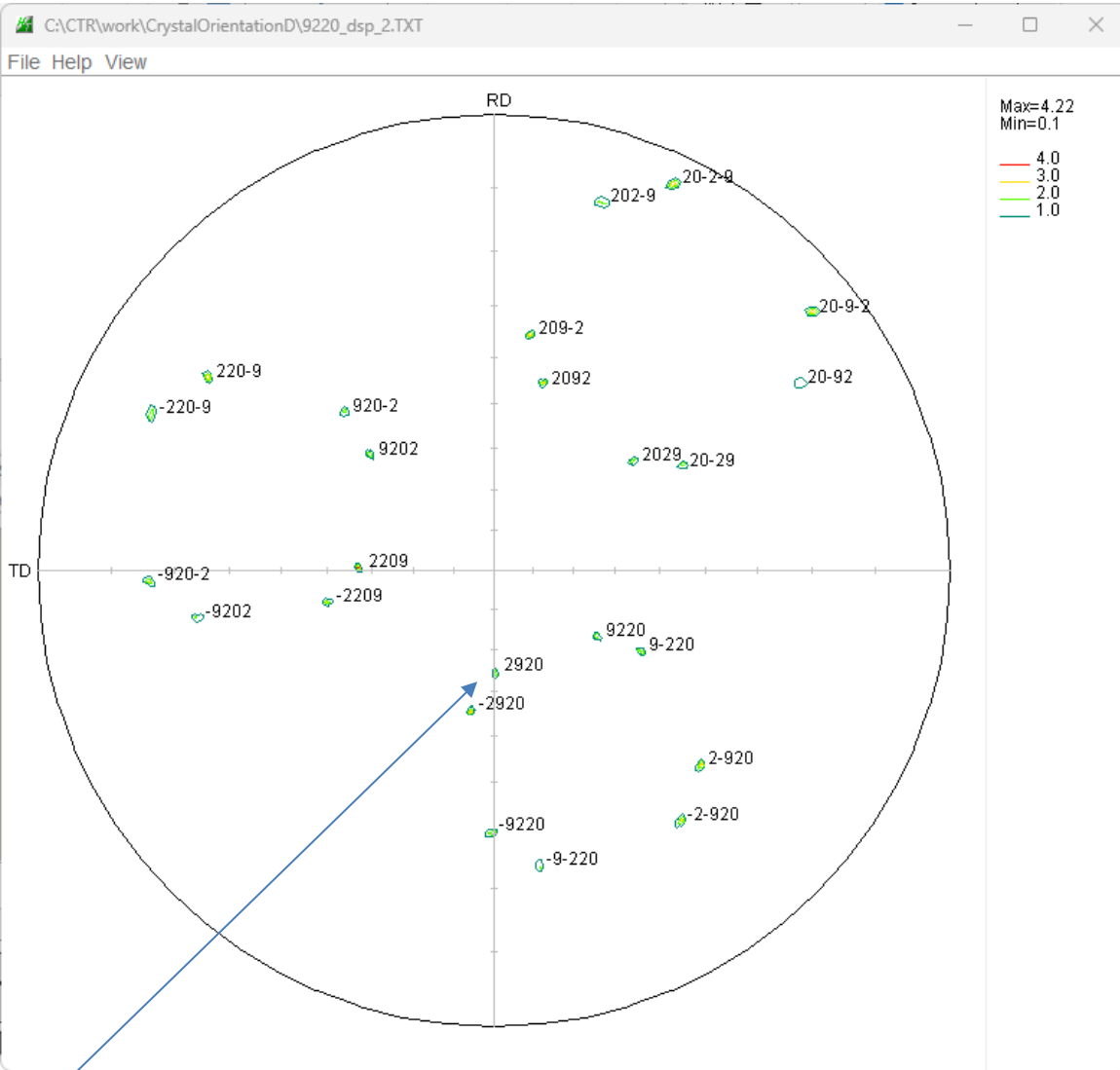
Calc PoleFigure

9 2 20
 9 20 2
 2 20 9
 2 9 20
 20 9 2
 20 2 9

111
 Clear
 Set
 Append
 All

calc U-matrix CalcPoleFigure FWHM 0.1 Max 5.0 Mini 0.1

calc{hkl}<uvw> maxIndex 15 extentAngle 1.0 calcTD Other(h,k,l) 9,2,20



2 20 9	32.93	-90.78	57.07	89.219
2 9 20	25.53	0.9	64.47	180.895
20 9 2	45.78	165.17	44.22	345.167

検証

2 9 20 25.53 0.9 64.47 180.895

File Help Polefigure(Contour)

TXT2 files select
Path: C:\CTR\work\CrystalOrientationD
File: 9220_dsp_2.TXT

Rotation(-360 <= degrees <= 360) of vector machine axis
Along RD(x) 3 0 Along TD(y) 2 25.53 Along ND(z) 1 -0.9 4 0 toOrthorhombic

Check
Previous Next 9220_dspN0N0T25R0.TXT Alfa angle check

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

PoleFigureStepChenger

[001]
[110]

