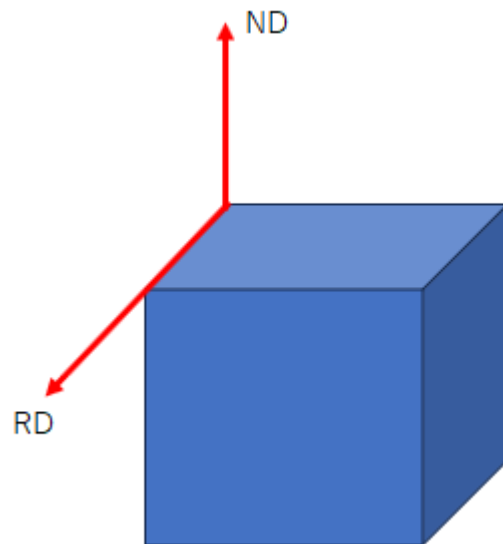


アルミニウム単結晶ブロックの極点測定から任意方位の切り出し

(Schmid 因子最大方向とする)

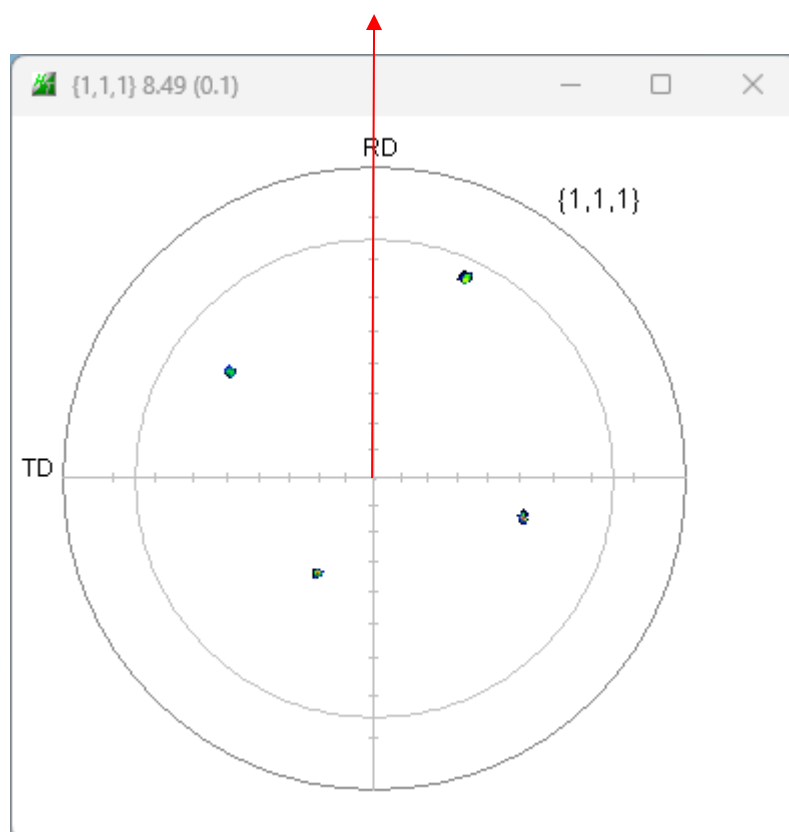


2023年12月04日

HelperTex Office

概要

単結晶ブロックから最大Schmid因子方位の切り出しを行う場合、ブロックの極点図測定から測定面方位を決定し、最大Schmid因子方位を求める事があります。この手順を以下の極点図から説明します。



極点図からU-matrixの計算

極点図の確認

結晶方位 $\{hkl\} \langle uvw \rangle$ の確認

FCC Schmid因子最大方向 $[9220]$ の極点図確認

ND方向に近い方位の決定

方位計算

CrystalOrientationD 2.021 by CTR PDuser HelperTex CTR

File Help Blind-40 CreatePFStep:1.0 hklisp=true α0->90 X-Axis:South

PoleFigure
 111 Center of gravity PoleFigure(TXT2) RD input mode is South.
 C:\tmp\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
 -1 -1 -1
 -1 -1 1
 -1 1 -1
 -1 1 1
 1 -1 -1
 1 -1 1
 1 1 -1

calc U-matrix CalcPoleFigure FWHM 0.1 Max 5.0 Mini 0.1

calc{hkl}<uvw> maxIndex 15 extentAngle 1.5 calcTD Other{h,k,l} 1,1,1

C:\tmp\AI-cube111-Orientation-CrystalOrientationD\111_R2.TXT peaksearch by center of gravity
 C:\tmp\AI-cube111-Orientation-CrystalOrientationD\111_R2.TXT peaksearchCenter chiangle=0 phiangle=0(RD=180)

chiangle	phiangle	Center=90		
52.99	75.07	37.01	255.073	
70.23	155.04	19.77	335.043	
59.22	-126.21	30.78	53.786	

indexing(Center=0,RD=180->0)
 52.99 75.07 1 1 1
 70.23 155.04 1 - 1 1
 59.22 -126.21 1 - 1 - 1

sqrtdelete: (1 1 1),(1 - 1 1) -> (1 - 1 - 1) 0.26

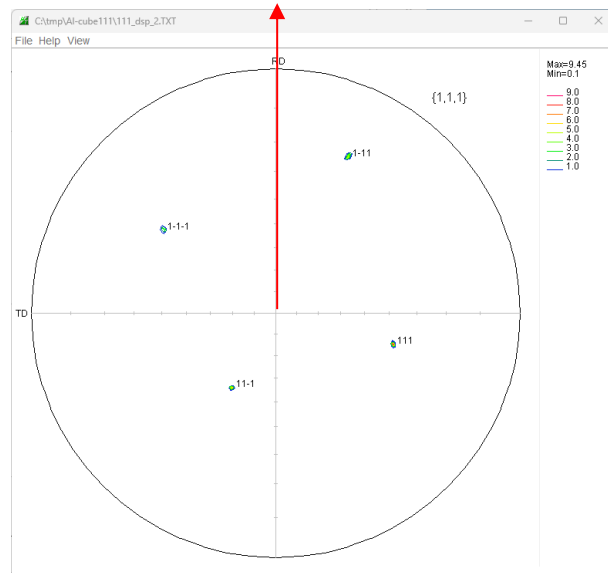
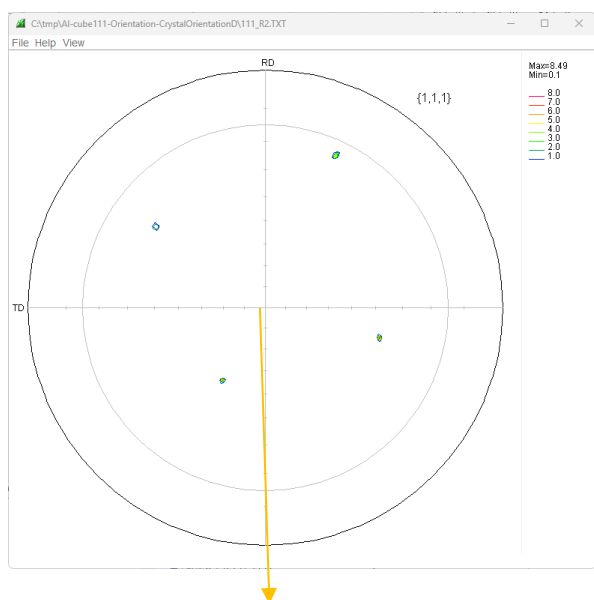
Alpha	Beta			
52.989	75.073	1 1 1		
70.23	155.043	1 - 1 1		

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	37.01	255.073
1 1 - 1	39.35	-30.06	50.65	149.942
1 - 1 1	70.27	155.11	19.73	335.105
1 - 1 - 1	59.41	-126.39	30.59	53.607

Initialize File

CalcPoleFigureにて入力極点図と異なる場合、別の極点図にて再計算してください。



方位計算 {h k l} < u v w >

CrystalOrientationD 2.021 by CTR PDuser HelperTex CTR

File Help Blind-40 CreatePFStep:1.0 hkldisp=true a0->90 X-Axis:South

PoleFigure
 111 Center of gravity PoleFigure(TXT2) RD input mode is South.
 C:\tmp\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
 -1 -1 -1
 -1 -1 1
 -1 1 -1
 -1 1 1
 1 -1 -1
 1 -1 1
 1 1 -1

calc U-matrix CalcPoleFigure FWHM 0.1 Max 5.0 Mini 0.1

calc{hkl}<uvw> maxIndex 15 extentAngle 1.5 calcTD Other(h,k,l) 1,1,1

```

52.989 75.073 1 1 1
70.23 155.043 1 -1 1
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 37.01 255.073
1 1 -1 39.35 -30.06 50.65 149.942
1 -1 1 70.27 155.11 19.73 335.105
1 -1 -1 59.41 -126.39 30.59 53.607
calchkl
chiangle phiangle calchkl
0.92 -27.98 12 3 -2
0.39 -163.51 13 3 -2
1.4 173.14 14 3 -2
calcuvw
chiangle phiangle calcuvw
90.8 1.14 -3 10 -3
89.2 -178.86 3 -10 3
91.13 0.73 -4 13 -4
88.87 -179.27 4 -13 4
88.85 -0.4 -4 15 -5
91.15 179.6 4 -15 5
{hkl}<uvw>(extentAngle=1.5)
{12 3 -2}<-3 10 -3> TD [-11 -42 -129]
{12 3 -2}<3 -10 3> TD [-11 -42 -129]
  
```

Initialize File

{ 1 2 3 -2 } < 3 -1 0 3 > と決定される。

CrystalRotation 1.10 by CTR PDuser HelperTex CTR

File Help RD(TDroate) {uvw}<hkl> {110}<1-12> RV:Integer Free

Material
 Material Cubic
 1.0 1.0 1.0 90.0 90.0 90.0

{hkl}<uvw>
 12 3 -2 3 -10 3 Disp

Rotation vector of crystal axis
 0 0 1 SET CTD

Rotation vector of machine axis(LaboTex,MTEX) Rotation angle
 0 1 0 SET -90 Calc Disp

```

{123-2}<3-103>
RD TD ND
3.0 -11.0 12.0
-10.0 -42.0 3.0
3.0 -129.0 -2.0
RDaxis [3 -10 3]
TDaxis [-11 -42 -129]
NDaxis [12 3 -2]
  
```

CrystalOrientationD 2.00 by CTR PDuser HelperTex CTR

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

PoleFigure

111 Center of gravity PoleFigure(TXT2) C:\tmp\AI-cube111\111_R2.TXT

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

39.08 -30.046 1 1 -1

CalcPoleFigure

calc U-matrix CalcPoleFigure FWHM 1 Max 10 Mini 0.1

calc[hkl]Muwv> maxIndex 15 extentAngle 2 Other(hk,l) -11,-42,-129

Direction	Alpha	Beta	Center=90
11 42 129	89.6	91.0	0.4
11 129 42	75.48	38.53	14.52
42 129 11	59.74	27.88	30.26
42 11 129	80.03	108.96	9.97
129 11 42	27.95	125.14	82.05
129 42 11	14.0	88.5	76.0
11 42 -129	73.06	-55.59	16.94
11 129 -42	69.92	1.25	20.08
42 129 -11	58.12	17.22	31.88
42 11 -129	62.77	-72.27	27.23
129 11 -42	12.58	-113.84	77.42
129 42 -11	5.99	58.88	84.01
42 -129 11	86.27	-167.94	3.73
42 -11 129	82.2	116.08	7.8
129 -11 42	32.22	141.62	57.78
129 -42 11	34.17	175.06	55.83
11 -42 -129	81.46	-91.49	8.54
42 -129 -11	84.88	-158.75	5.12
42 -11 -129	65.16	-82.24	24.84
129 -11 -42	20.19	-133.23	69.81
129 -42 -11	31.61	-167.88	58.39
-11 129 42	84.52	36.48	5.48
-11 42 -129	82.18	-53.9	7.82
-11 129 -42	79.16	0.54	10.84

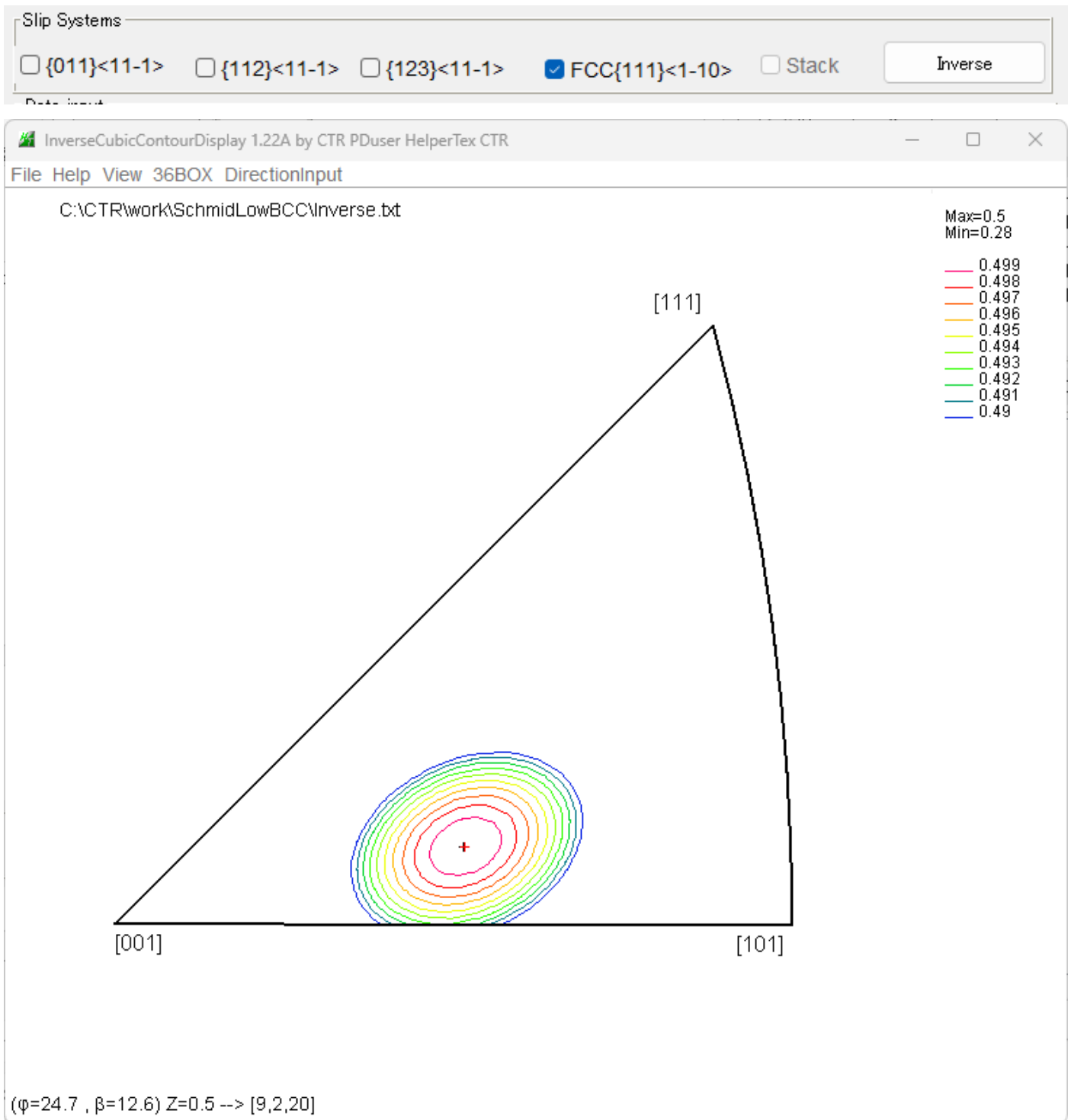
Initialize File



Direction 11 42 129 Alpha 89.6 Beta 91.0 Center=90 0.4 270.999

[-11 -42 -129]は Alpha が 90.0 より大きいため、計算結果が表示されていない

F C C S c h m i d 最大方位は



[9 2 2 0] と決定される。

[9 2 2 0] 方位の計算

CrystalOrientationD 2.00 by CTR PDuser HelperTex CTR

File Help Blind-10 CreatePFStep:1.0 hkldisp=true a0->90

PoleFigure

111 Center of gravity PoleFigure(TXT2) C:\tmp#Al-cube111#111_R2.TXT

Alpha(center=0) 52.989 Beta(RD=180) 75.073 hkl 1 1 1
 39.08 -30.046 1 1 -1

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 10 Mini 0.1

calc{hkl}Muvw> maxIndex 15 extentAngle 1.5

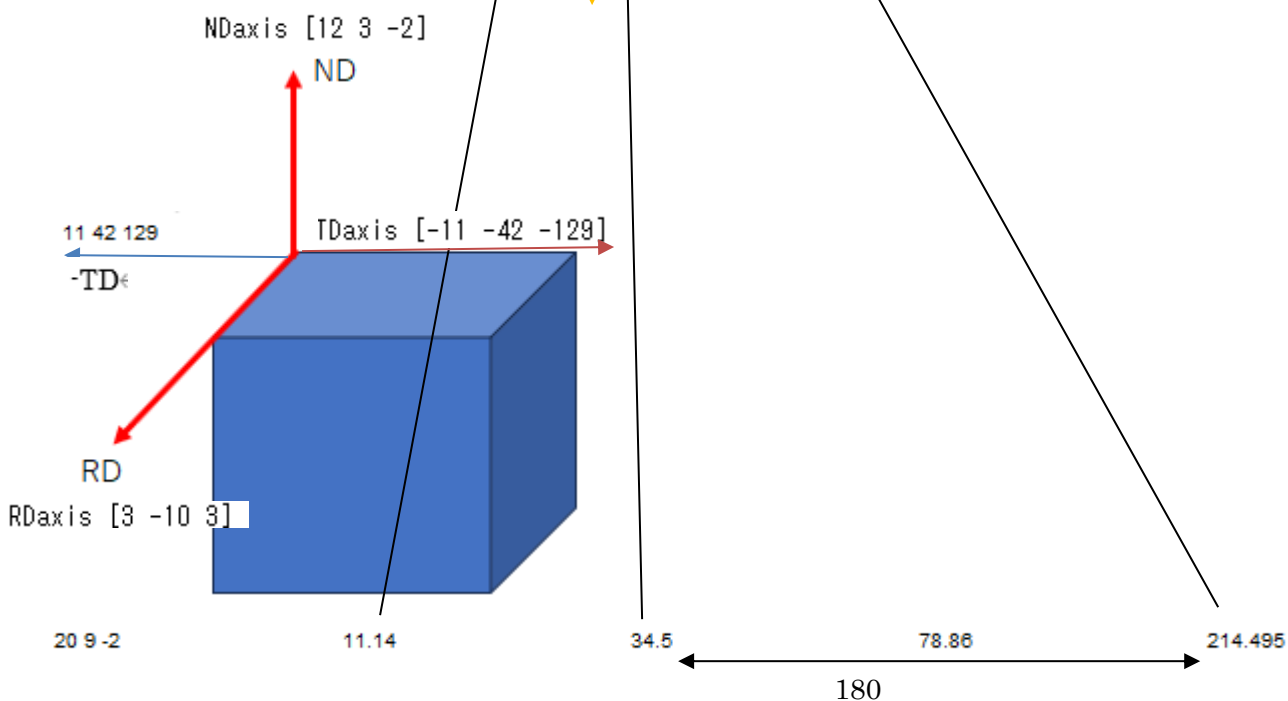
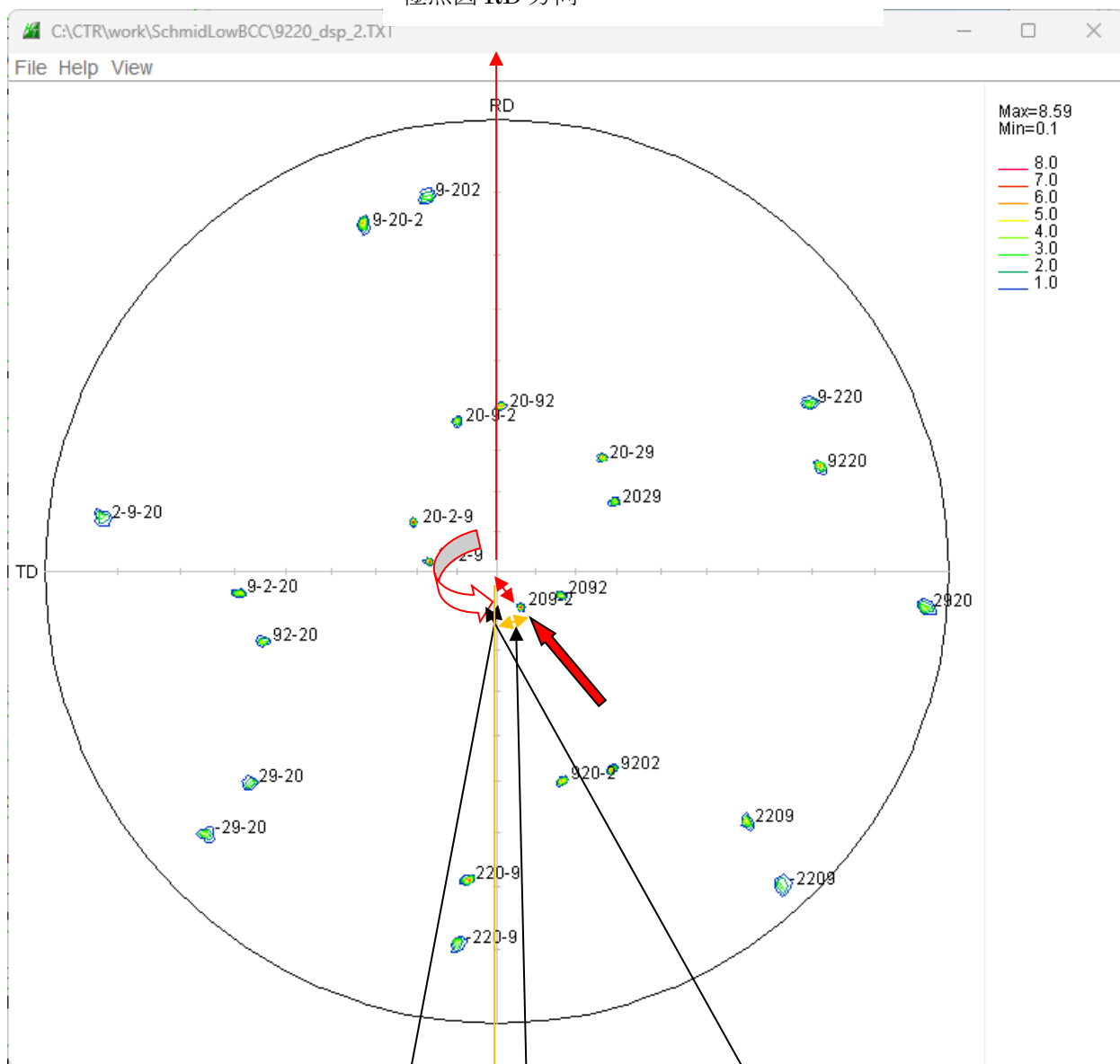
Other(h,k,l) 9,2,20

90.62	1.0	-3	10	-3
89.38	-179.0	3	-10	3
CalcPoleFigure				
Direction	Alpha	Beta	Center=90	
-2 20 -9	79.38	-5.76	10.62	174.238
-2 9 -20	81.74	-47.66	8.26	132.345
-2 20 9	86.47	42.38	3.53	222.38
9 -2 -20	59.47	-85.01	30.53	94.99
9 -20 -2	78.69	-159.05	11.31	20.953
2 -9 -20	82.59	-97.64	7.41	82.356
20 -9 -2	37.63	-165.34	52.37	14.663
20 -2 -9	24.05	-120.28	65.95	59.718
9 -2 20	76.38	118.24	13.62	298.236
9 -20 2	80.27	-169.52	9.73	10.477
20 -9 2	40.12	178.5	49.88	358.501
20 -2 9	37.76	136.76	52.24	316.758
9 2 -20	56.63	-73.18	33.37	106.815
9 20 -2	51.93	17.45	38.07	197.45
2 20 -9	68.97	-5.29	21.03	174.711
2 9 -20	71.45	-49.31	18.55	130.693
20 9 -2	11.14	34.5	78.86	214.495
20 2 -9	17.2	-97.54	72.8	82.46
9 2 20	73.89	107.76	16.11	287.765
9 20 2	53.88	30.29	36.12	210.294
2 20 9	76.34	44.86	13.66	224.858
2 9 20	87.38	85.21	2.62	265.21
20 9 2	17.47	69.36	72.53	249.357
20 2 9	33.63	120.3	56.37	300.299

Initialize File

極点図上では

極点図 RD 方向

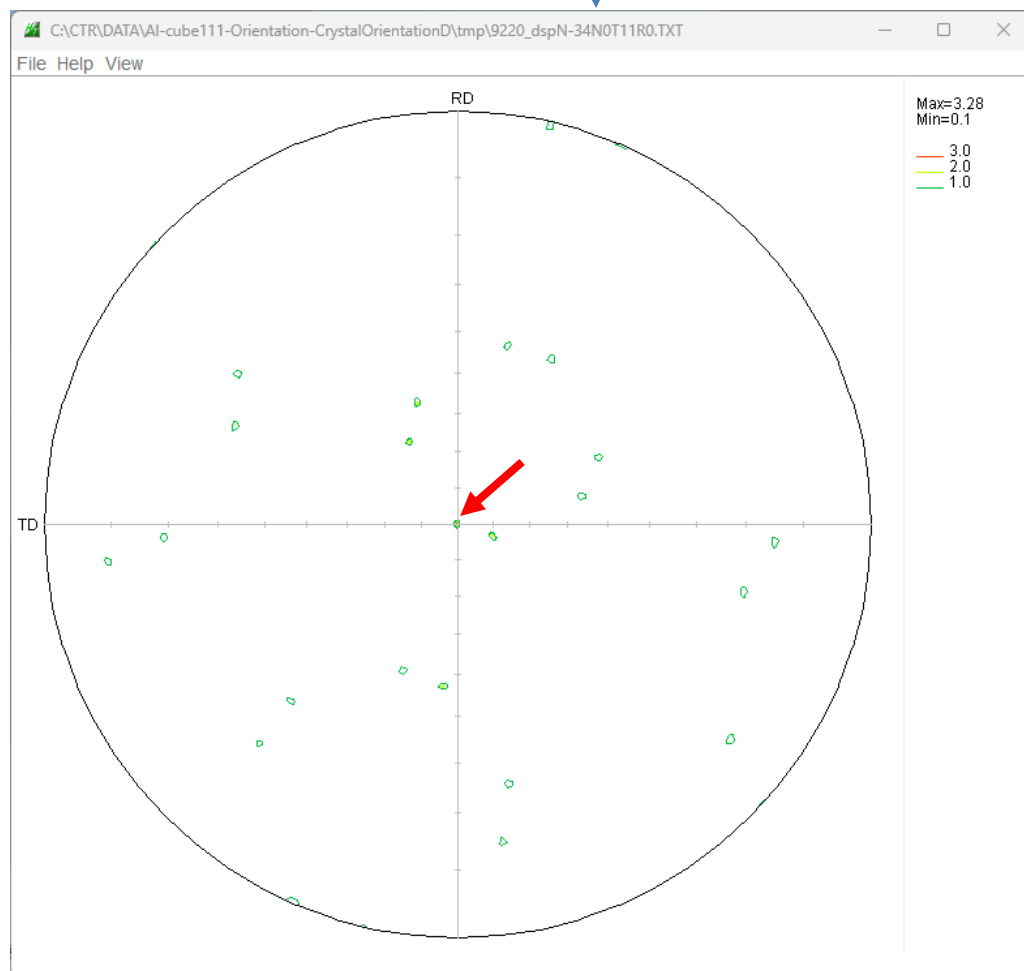
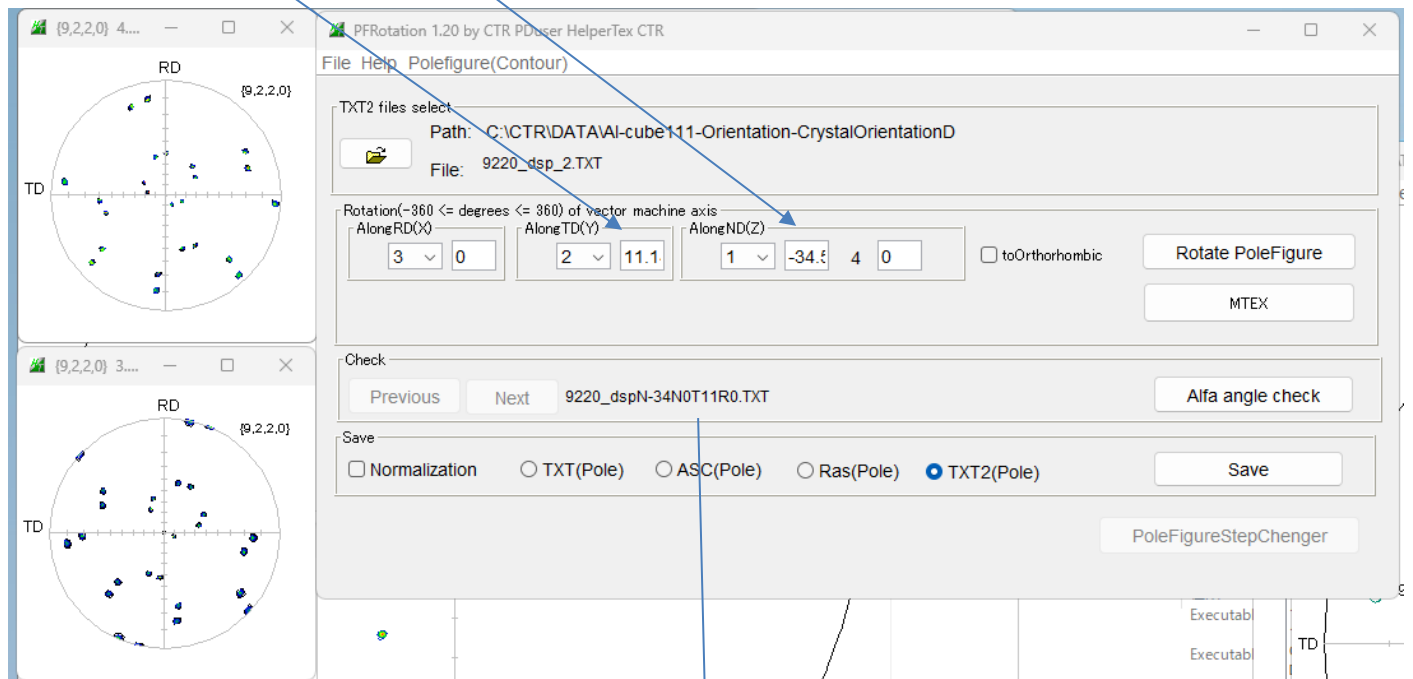


RD 方向は極点図測定から計算のため 2 1 4 . 4 9 5 を採用

極点図の回転の検証

TD 軸に -34.5 回転で -RD 軸上に移動

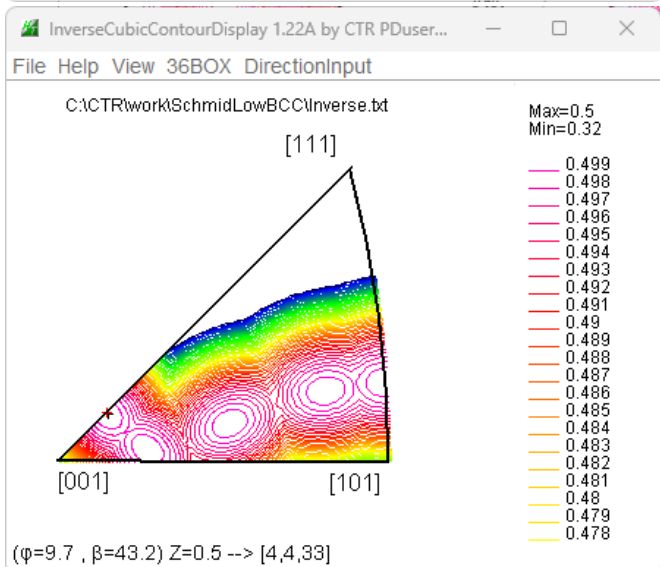
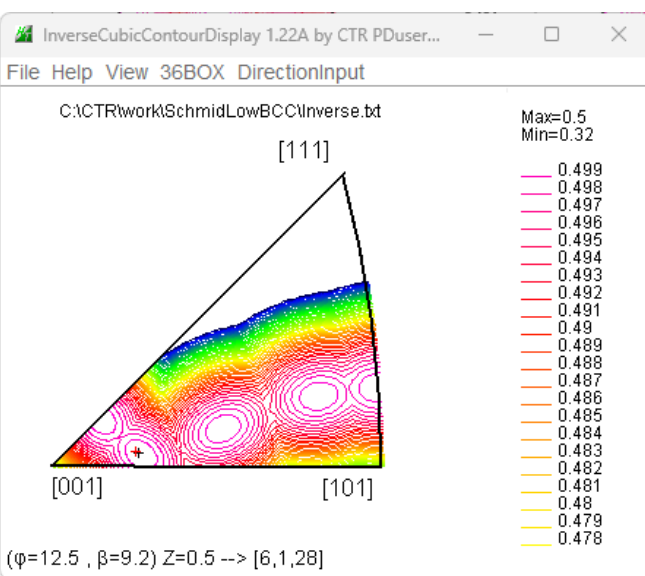
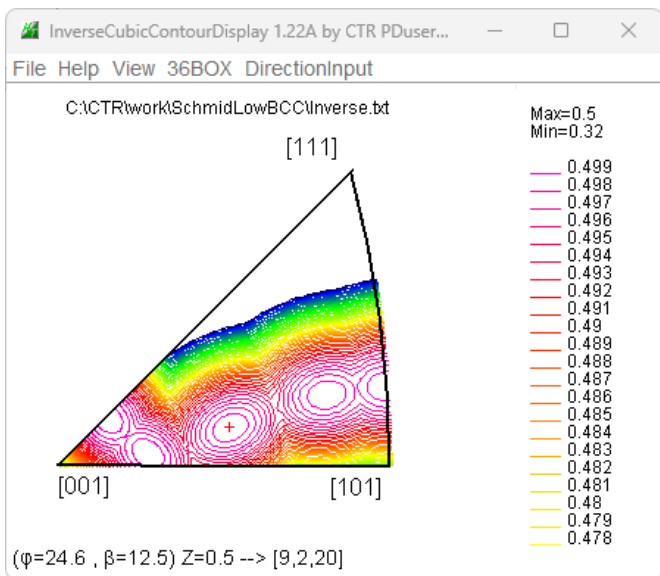
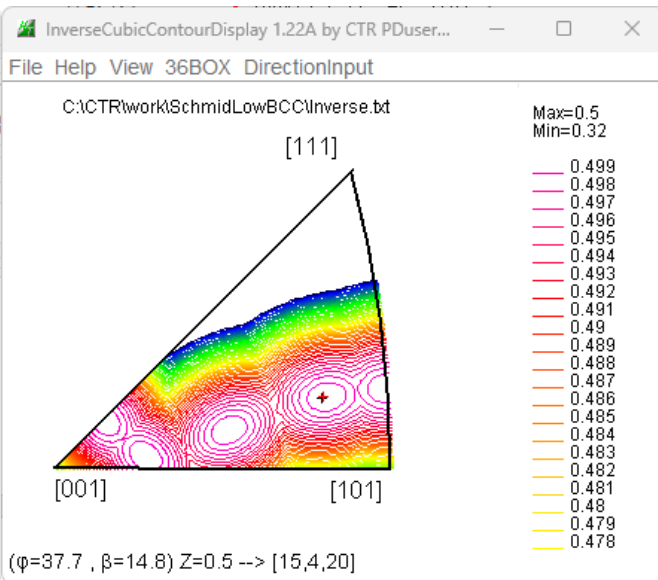
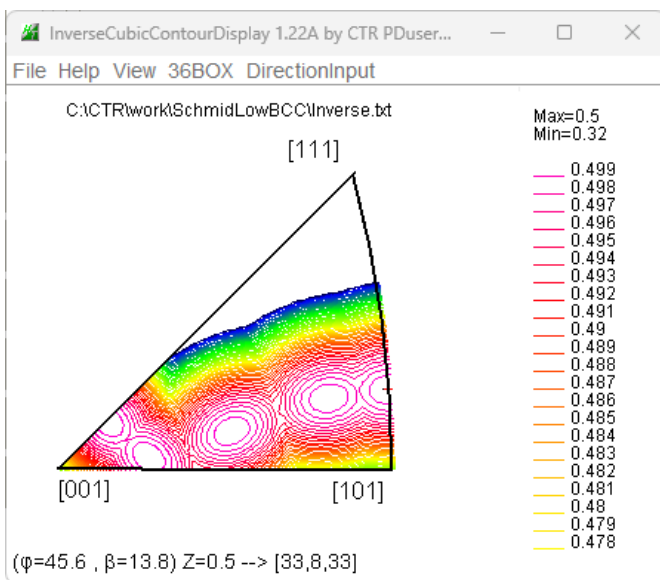
TD 軸に 11.1 度回転



BCCの場合5方向が考えられる

Slip Systems

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



5方向をAppendし、極点図作成

CrystalOrientationD 2.03 by CTR PDuser HelperTex CTR

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

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

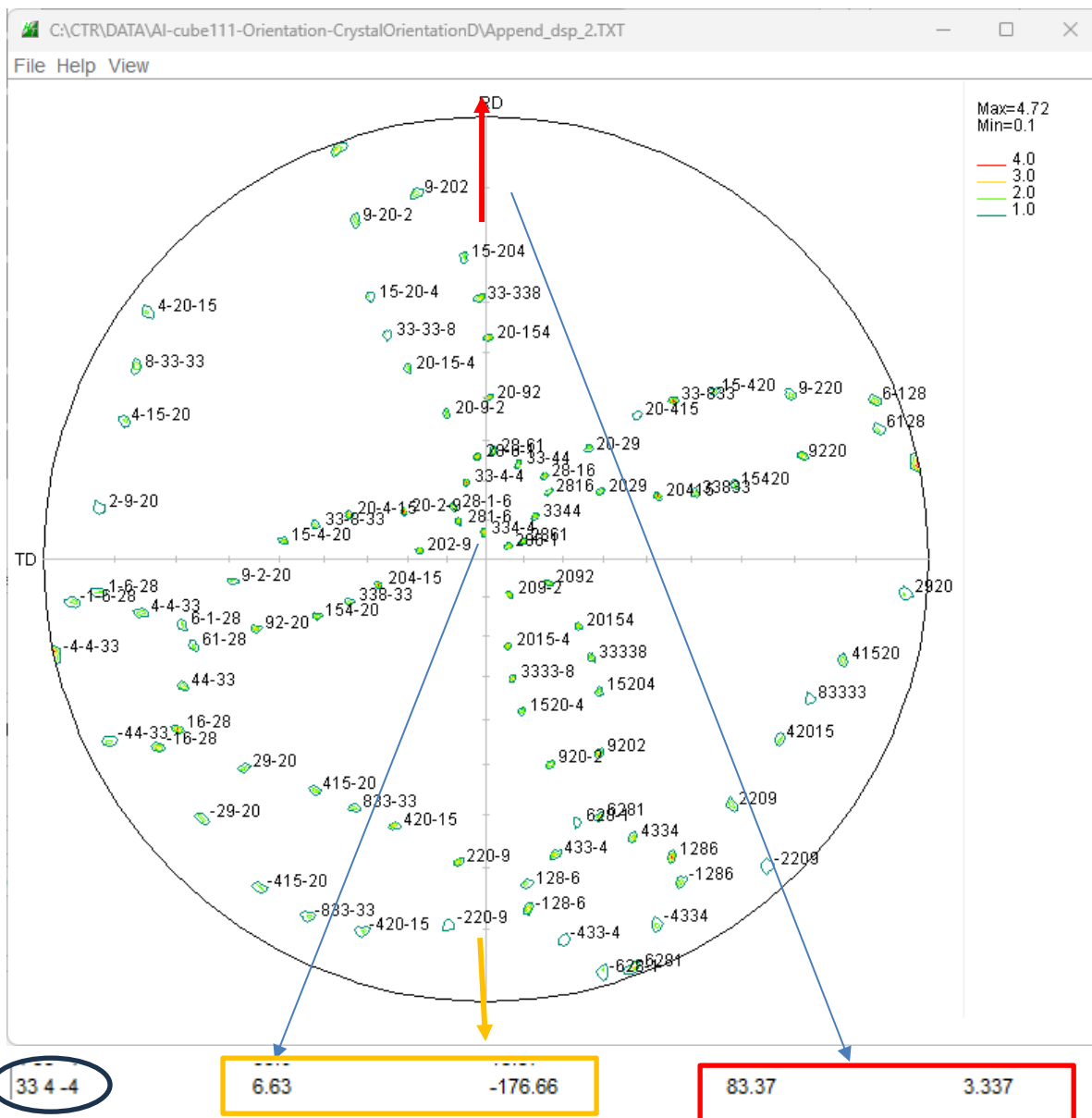
Calc PoleFigure

4 4 -33
4 33 -4
33 4 -4
4 4 33
4 33 4
33 4 4

111

FWHM 0.1 Max 5.0 Mini 0.1

maxIndex 15 extentAngle 1.0 calcTD Other(h,k,l) 4,4,33



まとめ

単結晶の極点図から取り付け方位を計算し、所定の極点図描画が行えます。

又、ラウエカメラ図から角度一指数を2点入力でも同一計算が行えます。

今回使用したソフトウェアの最新バージョンは、以下のソフトウェアを使用しています。

C r y s t a l O r i e n t a t i o n D (V e r . 2 . 0 3)

P o l e F i g u r e C o n t o u r D i s p l a y (V e r . 1 . 2 1)

P F R o t a t i o n (V e r . 1 . 2 0)

B C C S c h m i d F a c t o r C a l c 3 (V e r . 3 . 1 4)

関連ソフトウェア

C r y s t a l R o t a t i o n (V e r . 1 . 1 2)

旧ソフトウェアの場合、update致します。問い合わせください。