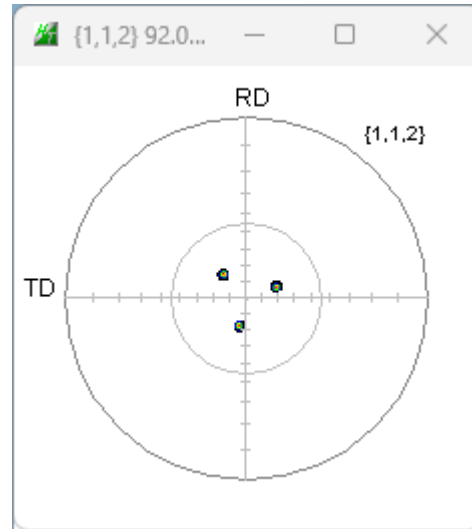


# 最新CTRソフトウェアによるBCC単結晶のSchmid因子解析①



この極点図からND,RTD,TD方向のSchmid因子を計算

測定極点図{112}から{001},{011},{112}極点図作成  
LaboTexによる方位解析で{hkl}<uvw>を求める  
BCCSchmidFactorCalc3でND,TD,RD方向のSchmid解析

# 測定極点図から完全極点図作成

Crystal orientation determination by two refraction method T.Kikuchi V1.12

File Help Blind-15 CreatePFStep:1.0 hkldisp=true a0->90

PoleFigure

112  Center of gravity PoleFigure(TXT2) C:\tmp\TEST\112\_TEST\_2.TXT

Alpha(center=0) 19.963 Beta(RD=180) 35.001 hkl 2 1 1

20.048 10.004 1 1 2

Calc PoleFigure

112

1 1 12 1 1  
1 1 2  
1 2 1  
2 1 -1  
1 1 -2  
1 2 -1  
2 -1 1

Clear Set Append All

calc U-matrix CalcPoleFigure FWHM 1 Max 100 Mini 0.1

C:\tmp\TEST\112\_TEST\_2.TXT peaksearch by center of gravity  
C:\tmp\TEST\112\_TEST\_2.TXT peaksearchCenter chiangle=0 phiangle=0 (RD=180)

chiangle	phiangle	Cente=90	
19.96	-135.0	70.04	44.999
20.05	110.0	69.95	290.004
18.08	-11.01	71.92	168.992

indexing(Center=0,RD=180->0)

19.96	-135.0	2 1 1
20.05	110.0	1 1 2
18.08	-11.01	1 2 1

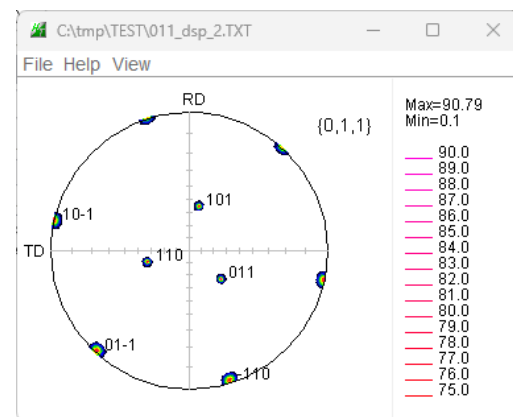
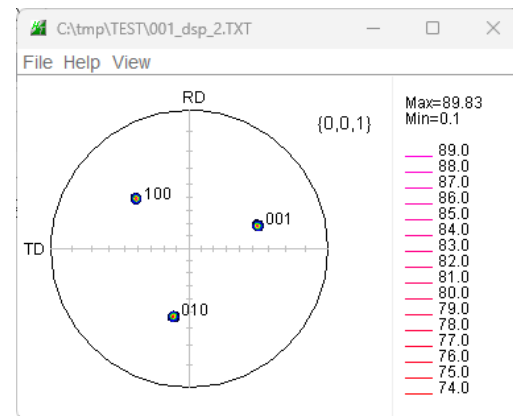
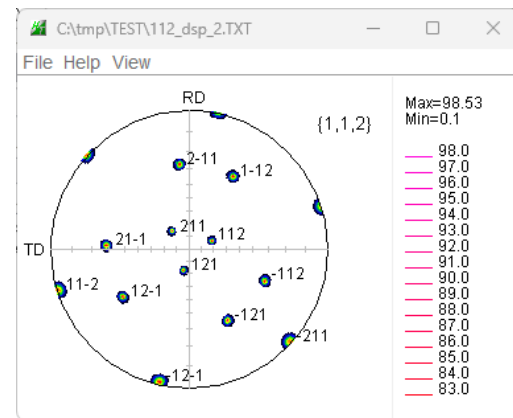
sqrtdelete: (2 1 1),(1 1 2) --> (1 2 1) 1.29

C:\tmp\TEST\112\_TEST\_2.TXT

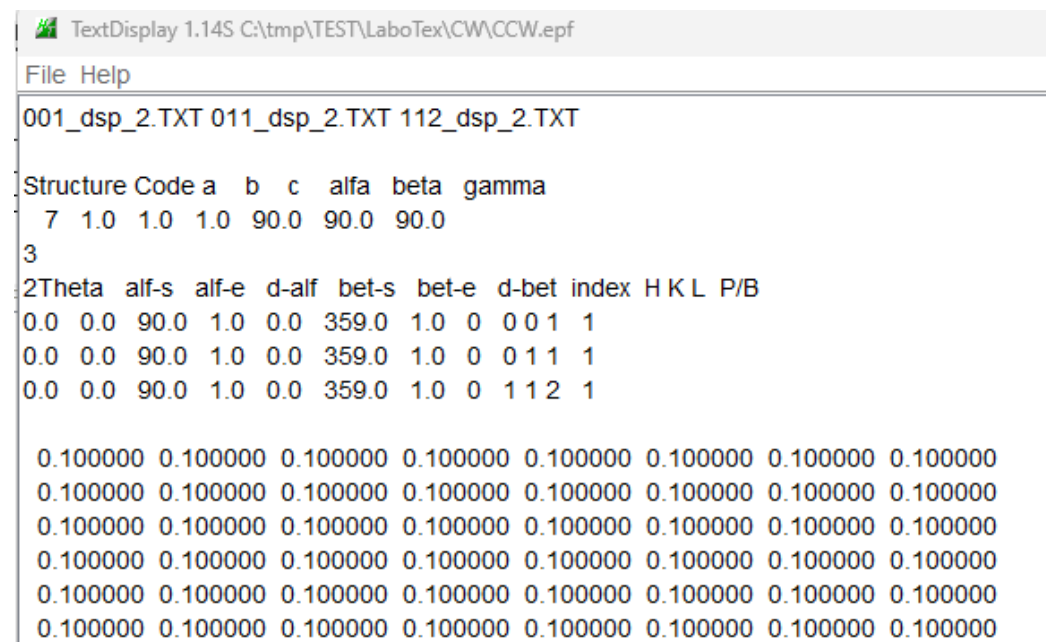
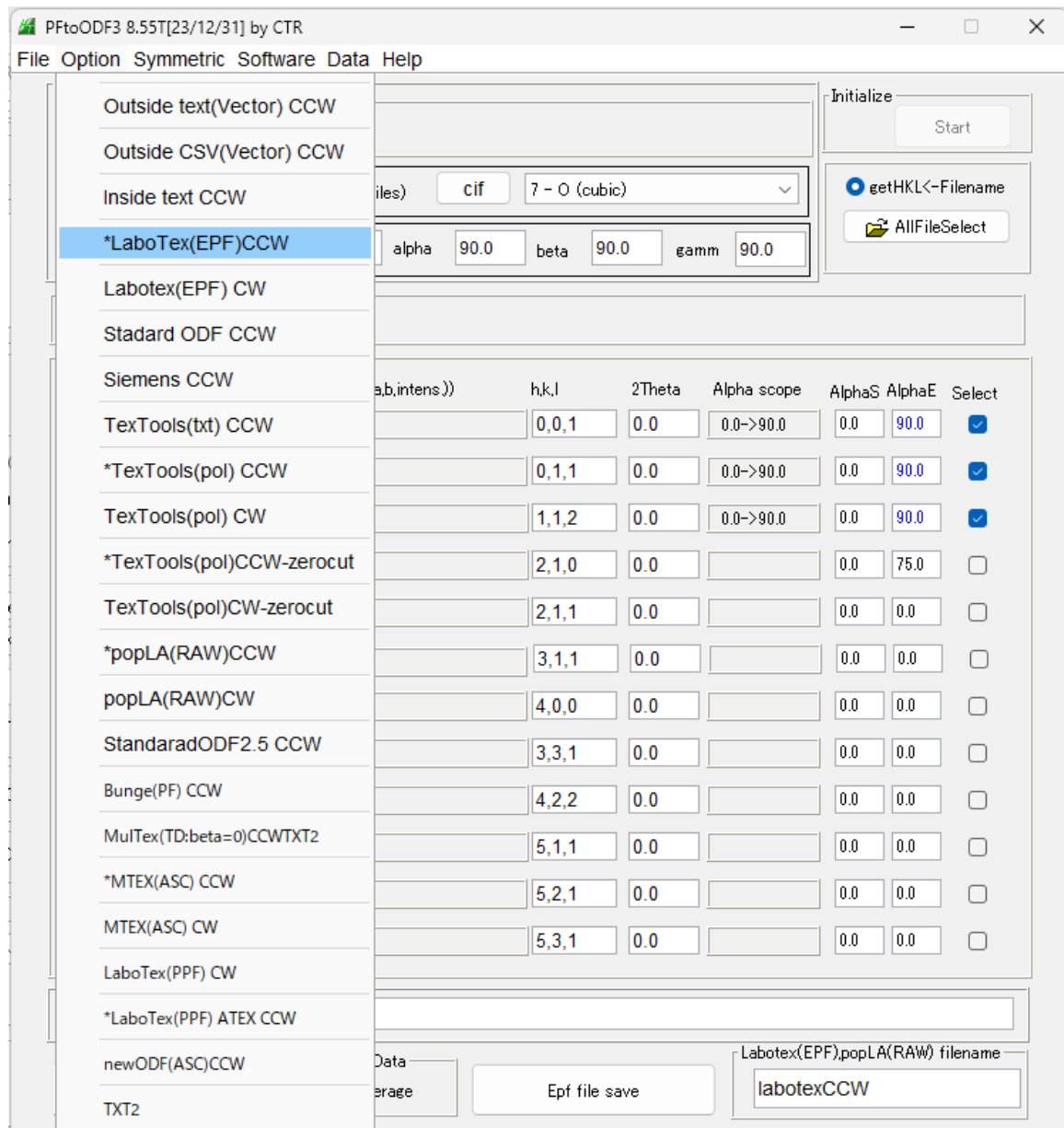
File Help View

{1,1,2} Max=92.0 Min=0.1

RD TD



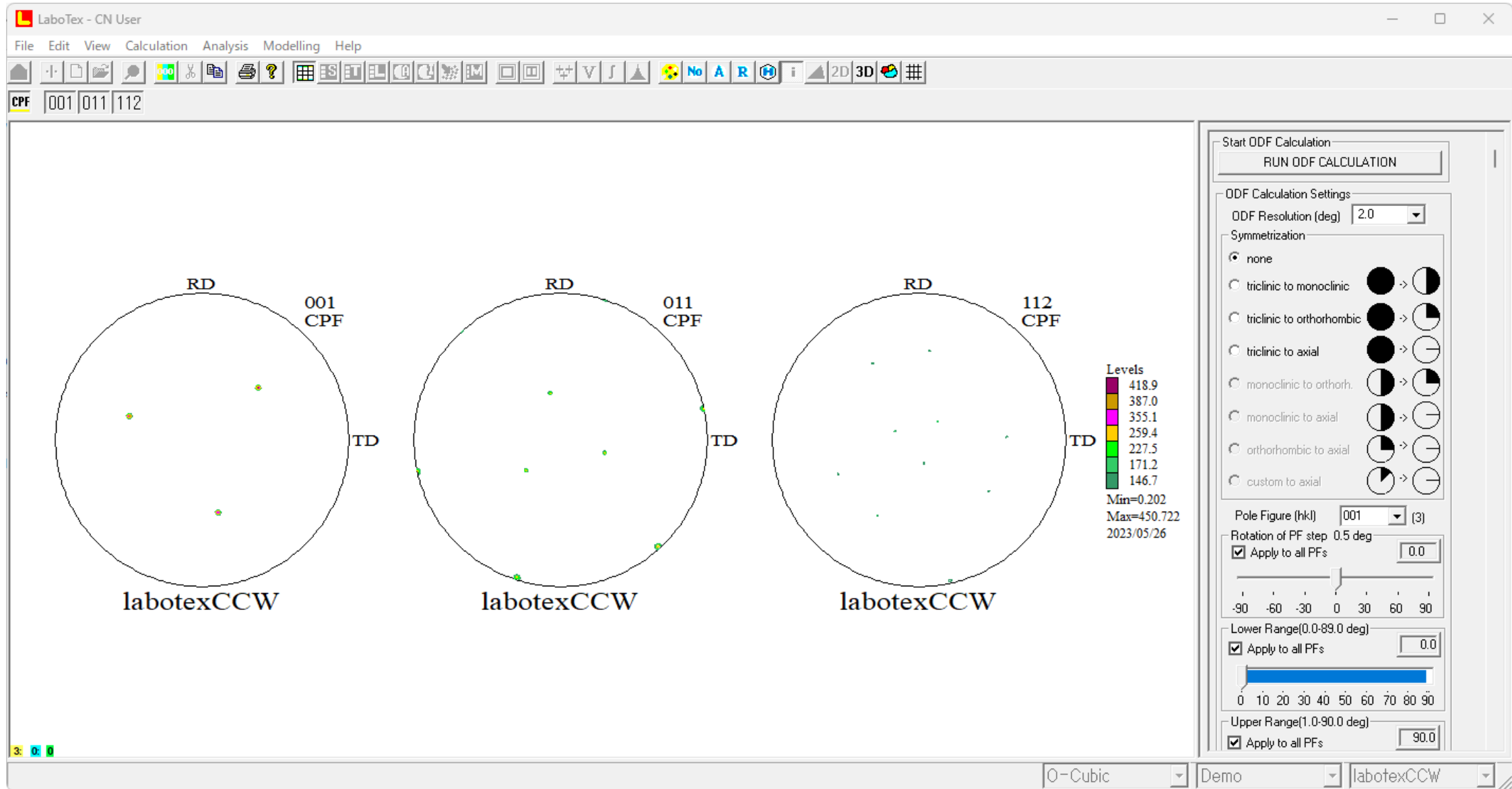
# LaboTex向けEPFファイルをCCWで作成



(C:) > tmp > TEST > LaboTex > CCW

名前	更新日時	種類	サイズ
labotexCCW.epf	2023/05/26 5:46	EPF ファイル	973 KB

# LaboTexによる方位解析(CCWで極点図はRD軸に反転)



# 方位の決定 {111}<-725>をDataBaseに登録しVF%

The screenshot displays the LaboTex software interface. The main window shows a large empty plot area with a red crosshair. To the right of the plot is a legend titled "labotexCCW Levels" with a color scale ranging from 19805.8 (dark purple) to 7922.3 (dark green). Below the legend, it indicates "Max=21126" and "Min=0.002".

The right-hand panel contains the "ODF Container's Info" settings. It includes a table for "Isolines/Levels for ODF" with 14 entries, each with a color number and a value. Below the table are controls for "Dec. Digit" (set to 1), "Adjustment of Isolines (Automatic Mode)" with a "Balance" slider, "Fill" settings (set to NORMAL), "Background Color" (set to Isoline), and "ODF Isolines Mode / Load ODF Isolines" with checkboxes for "Color", "Value" (checked), and "State". There is also a "Save ODF Isolines" button. At the bottom of the panel, "Global ODF values" are shown as Maximal: 21126 and Minimal: 0.002. The "ODF Properties" section shows "ODF Projection" as Phi 2 and "Sample" as labotexCCW.

The top status bar displays the HKL indices (1 1 1) and U VW indices [-7 2 5]. The bottom status bar shows navigation buttons (Sort, Auto, Prev, Next) and the current sample name "brass" with its HKL indices { 1 1 0 } and U VW indices < 1 -1 2 >.

Color No	Value	Color No	Value
1	1.0	8	11883.5
2	2640.8	9	13203.9
3	3961.2	10	14524.3
4	5281.5	11	15844.7
5	6601.9	12	17165.1
6	7922.3	13	18485.5
7	9242.7	14	19805.9

# VF%の決定

No	Texture Component	On	Distribution	FWHM $\phi_1$	FWHM $\phi_2$	FWHM $\phi_3$	Volume Fraction
1	{ 1 1 1 } < -7 2 5 >	<input checked="" type="checkbox"/>	Gauss	3.8	0.9	3.0	50
2	{ 0 1 3 } < 1 0 0 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10
3	{ 1 3 2 } < 6 -4 3 > S-1	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10
4	{ 5 2 5 } < 1 -5 1 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10
5	{ 1 1 1 } < -1 -1 2 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10
6	{ 2 3 3 } < 0 1 -1 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10
7	{ 3 2 3 } < 1 -3 1 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10
8	{ 2 3 1 } < -3 4 -6 > S-4	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10
9	{ 0 0 1 } < 1 0 0 > cube	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10
10	{ 1 1 0 } < 0 0 1 > goss	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10

Backgroundが高いのは  
完全極点図作成時最小値を0.1としたため

```
TextDisplay 1.14S C:\tmp\TEST\LaboTex\CW\CCW.epf
File Help
001_dsp_2.TXT 011_dsp_2.TXT 112_dsp_2.TXT

Structure Code a b c alfa beta gamma
7 1.0 1.0 1.0 90.0 90.0 90.0
3
2Theta alf-s alf-e d-alf bet-s bet-e d-bet index H K L P/B
0.0 0.0 90.0 1.0 0.0 359.0 1.0 0 0 0 1 1
0.0 0.0 90.0 1.0 0.0 359.0 1.0 0 0 1 1 1
0.0 0.0 90.0 1.0 0.0 359.0 1.0 0 1 1 2 1

0.100000 0.100000 0.100000 0.100000 0.100000 0.100000 0.100000 0.100000
0.100000 0.100000 0.100000 0.100000 0.100000 0.100000 0.100000 0.100000
0.100000 0.100000 0.100000 0.100000 0.100000 0.100000 0.100000 0.100000
0.100000 0.100000 0.100000 0.100000 0.100000 0.100000 0.100000 0.100000
0.100000 0.100000 0.100000 0.100000 0.100000 0.100000 0.100000 0.100000
0.100000 0.100000 0.100000 0.100000 0.100000 0.100000 0.100000 0.100000
```

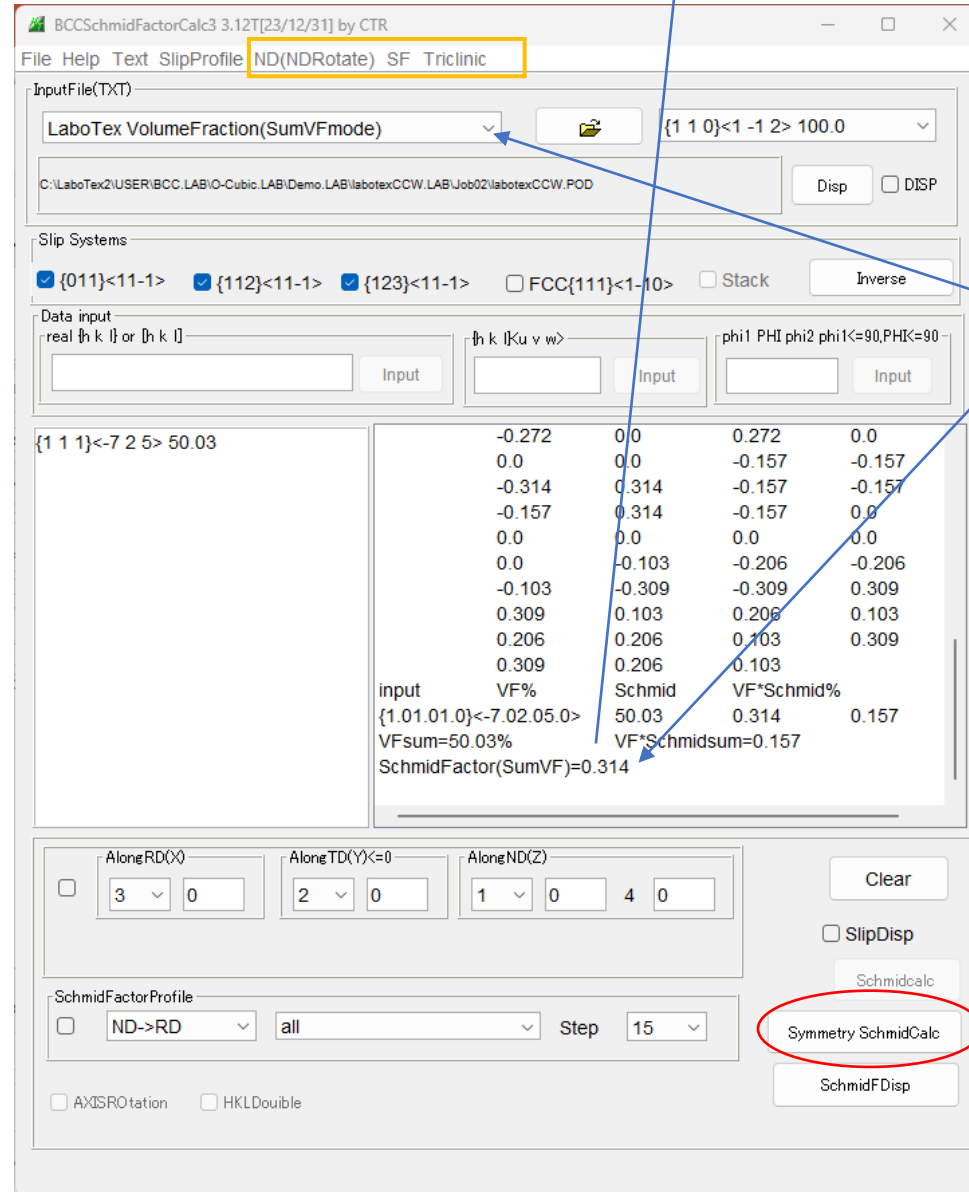
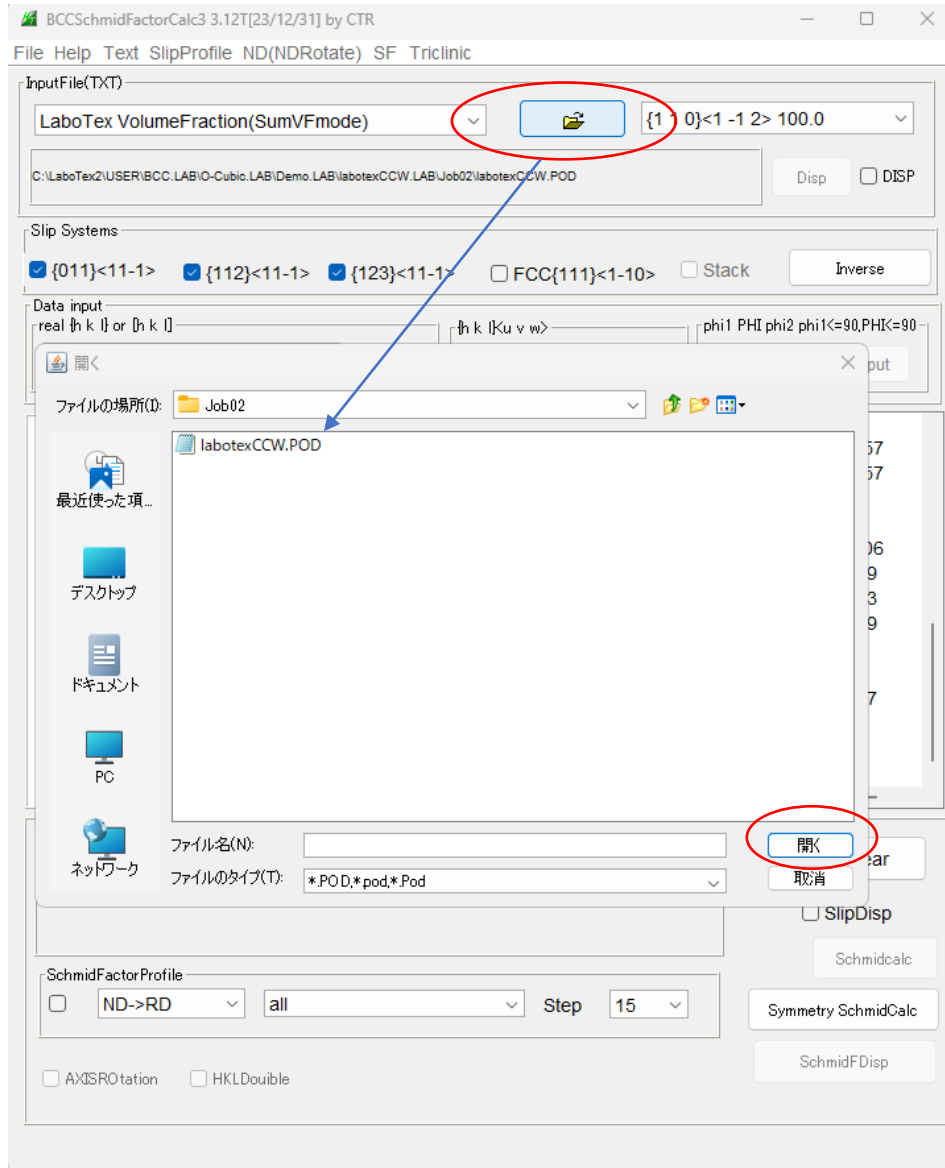
{111}<-725>のVF%が登録されている

C:\ > LaboTex2 > USER > BCC.LAB > O-Cubic.LAB > Demo.LAB > labotexCCW.LAB > Job02

名前	更新日時	種類	サイズ
labotexCCW.ODF	2023/05/26 6:26	ODF ファイル	1,496 KB
labotexCCW.POD	2023/05/26 6:27	POD ファイル	1 KB

# BCCSchmidFactorCalc3で計算

ND方向引っ張り (SF) = 0.314



VF%=50.03%を  
100%として計算

# TD方向引っ張り(SF)=0.4985

BCCSchmidFactorCalc3 3.12T[23/12/31] by CTR

File Help Text SlipProfile **TD(RDRotate) SF Triclinic**

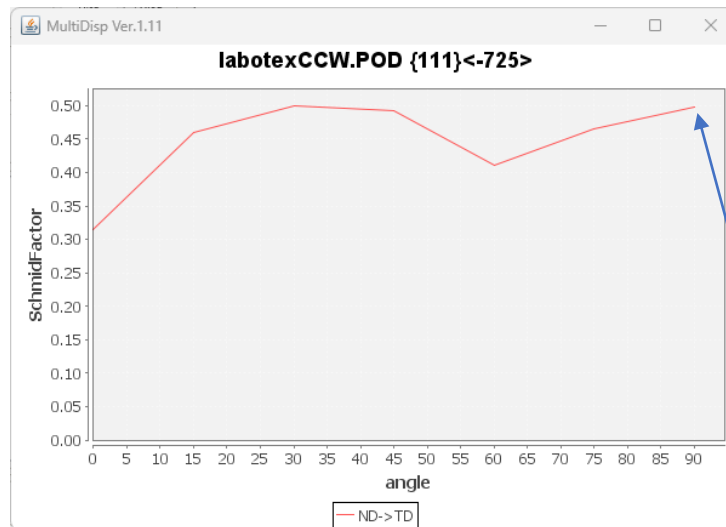
InputFile(TXT)  
 LaboTex VolumeFraction(SumVFmode) {1 1 0}<-1 -1 2> 100.0  
 C:\LaboTex2\USER\BCC.LAB\O-Cubic.LAB\Demo.LAB\labotexCCW.LAB\Job02\labotexCCW.POD Disp  DISP

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

Data input  
 real {h k l} or {h k l} {h k l}Ku v w> phi1 PHI phi2 phi1<=90,PHI<=90  
 Input Input Input

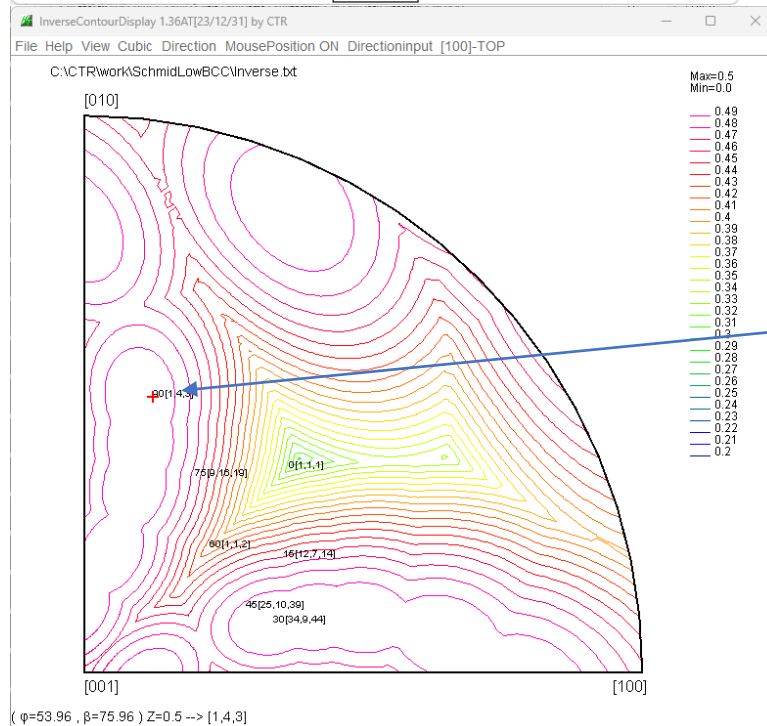
{1 1 1}<-7 2 5> 50.03

AlongRD(X) 3 90 AlongTD(Y)<=0 2 0 AlongND(Z) 1 0 4 0 Clear  
 SlipDisp Schmidcalc  
 Symmetry SchmidCalc SchmidFDisp  
 SchmidFactorProfile  ND->TD all Step 15  
 AXISRotation  HKLDouble



OBJFILE=C:\LaboTex2\U  
 COMMENT  
 AXIS=angle ND->TD  
 DATA-NUMBER=7  
 0.0 0.3143  
 15.0 0.4605  
 30.0 0.5  
 45.0 0.4934  
 60.0 0.4115  
 75.0 0.4656  
 90.0 0.4985

ND->TD



0	54.73561	45.0	1,1,1
15	44.77906	30.25644	12,7,14
30	38.63678	14.82648	34,9,44
45	34.62142	21.80141	25,10,39
60	35.26439	45.0	1,1,2
75	44.01478	60.64225	9,16,19
90	53.96011	75.96376	1,4,3

+ 90[1,4,3]



# RD方向引っ張り (SF)=0.4946

BCCSchmidFactorCalc3 3.12T[23/12/31] by CTR

File Help Text SlipProfile **RD(TDRotate) SF Triclinic**

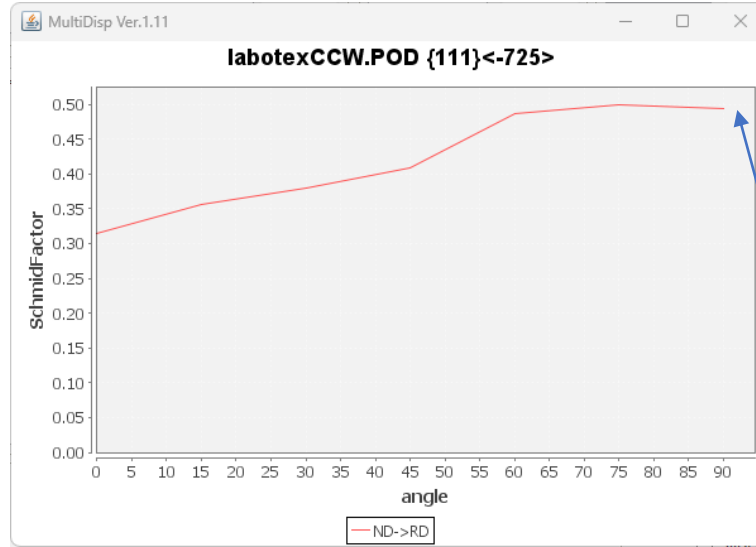
InputFile(TXT)  
 LaboTex VolumeFraction(SumVFmode) [1 1 0]<-1 -1 2> 100.0  
 C:\LaboTex2\USER\BCC.LAB\IO-Cubic.LAB\Demo.LAB\labotexCCW.LAB\Job02\labotexCCW.POD Disp  DISP

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

Data input  
 real [h k l] or [h k l] [h k l] [k u v w] phi1 PHI phi2 phi1<=90,PHI<=90

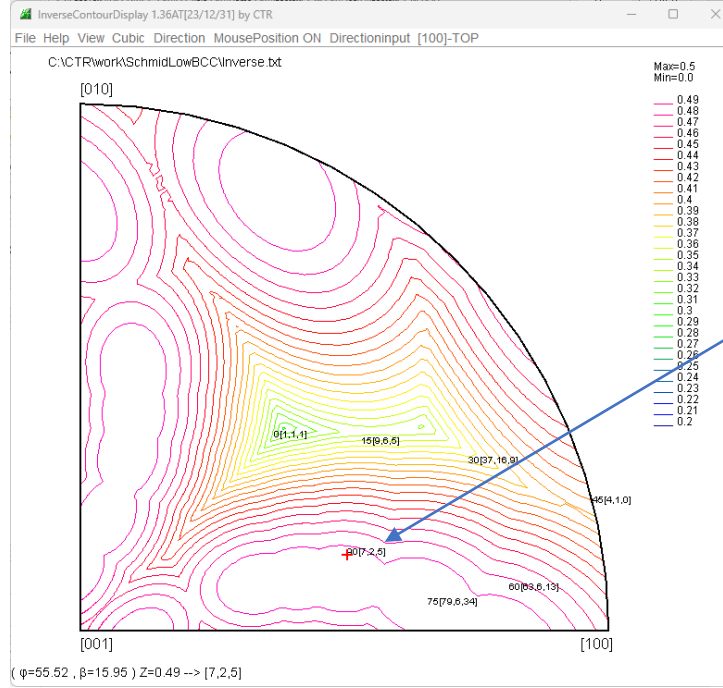
{1 1 1}<-7 2 5> 50.03

AlongRD(X) 3 0 AlongTD(Y)<=0 2 -90 AlongND(Z) 1 0 4 0 Clear  
 SlipDisp Schmidcalc  
 Symmetry SchmidCalc SchmidFDisp  
 SchmidFactorProfile  ND->RD all Step 15  
 AXISRotation  HKLDouble



OBJFILE=C:\LaboTex2\ COMMENT  
 AXIS=angle ND->RD  
 DATA-NUMBER=7

0.0	0.3143
15.0	0.3564
30.0	0.3805
45.0	0.4085
60.0	0.4865
75.0	0.4995
90.0	0.4946



ND->RD

0	54.73561	45.0	1,1,1
15	65.19125	33.69007	9,6,5
30	77.4144	23.38522	37,16,9
45	90.0	14.03624	4,1,0
60	78.3918	5.44033	63,6,13
75	66.77371	4.34324	79,6,34
90	55.51861	15.9454	7,2,5



# 方位{111}<-725>の回転検証 ND[111],RD[-725],TD[-14-3]

TD方向回転

CrystalRotation 1.09T[23/12/31] by CTR

File Help **TD(RDrotate) {TD}<uvw> <110><-1-12> RV:Integer Triclinic**

Material Cubic  
1.0 1.0 1.0 90.0 90.0 90.0

hkl{Kuvw}>  
1 1 1 -7 2 5 Disp

Rotation vector of crystal axis  
 -7 2 5 SET CTD

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

Result

RD	TD	ND
-7.0	-1.0	1.0
2.0	4.0	1.0
5.0	2.0	1.0

RDaxis [-7 2 5]  
TDaxis [-1 4 -3]  
NDaxis [1 1 1]

-7.0 2.0 5.0 (-7 2 5)  
{111}<-725> eulerangle:(136.102,54.736,45.0)  
Eulerangle  $\varphi(\psi_1 \Phi \psi_2)=$   
-0.7926 0.1961 0.5774  
0.2265 0.2154 0.5774  
0.5661 0.5883 0.5774  
Rotation [-7,2,5] angle:90.0  
Calc-d=(-0.7926,0.2265,0.5661)  
a(-7.0,2.0,5.0),90.0  
Rotated Eulerangle  
0.6282 0.3867 -0.6752  
-0.7456 0.0513 -0.6644  
-0.2223 0.9208 0.3205  
Rotated RD TD ND  
-0.7926 -0.1908 0.1961  
0.2265 -0.5261 -0.7845  
0.5661 0.3433 0.5883  
Calc Miller indices  
{1 0 1 0 0 0}<-3 1 1 0 2.5>  
{1 4 3}<-7 -2 5> (135.56 53.96 14.04)

{1 4 3}<-7 -2 5> sethkl{Kuvw> ResultCreat

Result: {1-43}<-725> toTriclinic {143}<-7-25> (135.56 53.96 14.04)

TD方向への回転は  
RD軸[-725]に90度回転

Euler角度  
{360,90,90}範囲内の  
{143}<-7-25>を得る

RD方向回転

CrystalRotation 1.09T[23/12/31] by CTR

File Help **RD(TDrotate) {uvw}<hkl> <110><-1-12> RV:Integer Triclinic**

Material Cubic  
1.0 1.0 1.0 90.0 90.0 90.0

hkl{Kuvw}>  
1 1 1 -7 2 5 Disp

Rotation vector of crystal axis  
 -1 4 -3 SET CTD

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

Result

RD	TD	ND
-7.0	-1.0	1.0
2.0	4.0	1.0
5.0	-3.0	1.0

RDaxis [-7 2 5]  
TDaxis [-1 4 -3]  
NDaxis [1 1 1]

-1.0 4.0 -3.0 (-1 4 -3)  
{111}<-725> eulerangle:(136.102,54.736,45.0)  
Eulerangle  $\varphi(\psi_1 \Phi \psi_2)=$   
-0.7926 0.1961 0.5774  
0.2265 0.2154 0.5774  
0.5661 0.5883 0.5774  
Rotation [-1,4,-3] angle:-90.0  
Calc-d=(-0.1961,0.7845,-0.5883)  
a(-1.0,4.0,-3.0),-90.0  
Rotated Eulerangle  
0.0385 0.4345 0.8998  
-0.7422 0.6154 -0.2654  
-0.6691 -0.6577 0.3462  
Rotated RD TD ND  
0.5774 0.6305 0.7926  
0.5774 -0.1692 -0.2265  
0.5774 -0.0692 -0.5661  
Calc Miller indices  
{3 5 -1 0 -2 5}<1 0 1.0 1.0>  
{7 2 5}<-1 -1 -1> (315.54 55.52 74.05)

{7 2 5}<-1 -1 -1> sethkl{Kuvw> ResultCreat

Result: {7-25}<111> toTriclinic {725}<-1-1-1> (315.54 55.52 74.05)

RD方向への回転は  
TD軸[-14-3]に-90度回転

Euler角度  
{360,90,90}範囲内の  
{725}<-1-1-1>を得る

# 最小値を0.001の場合

Crystal orientation determination by two refraction method T.Kikuchi V1.12

File Help Blind-15 CreatePFStep:1.0 hkdsp=true a0->90

PoleFigure

112  Center of gravity PoleFigure(TXT2) C:\tmp\TEST\112\_TEST\_2.TXT

Alpha(center=0) 19.963 Beta(RD=180) 35.001 hkl 2 1 1

20.048 10.004 1 1 2

CalcPoleFigure

112

Clear Set Append All

calc U-matrix CalcPoleFigure FWHM 1 Max 100 Mini 0.001

Alpha Beta

19.963 -135.001 2 1 1

20.048 110.004 1 1 2

U-matrix

-0.5609185495484192 0.7870956954248873 -0.256614003936087

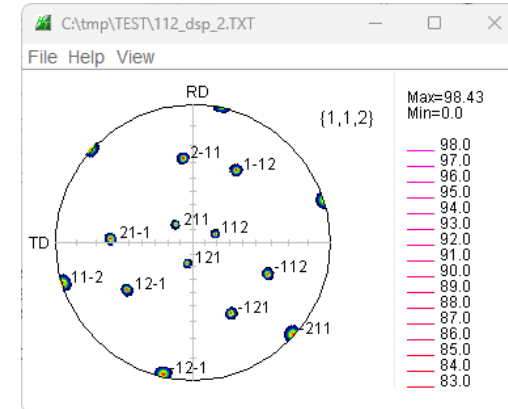
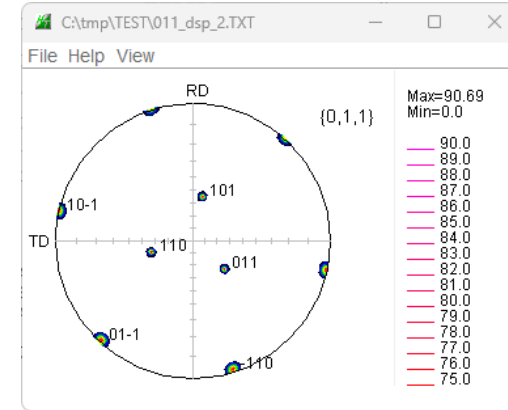
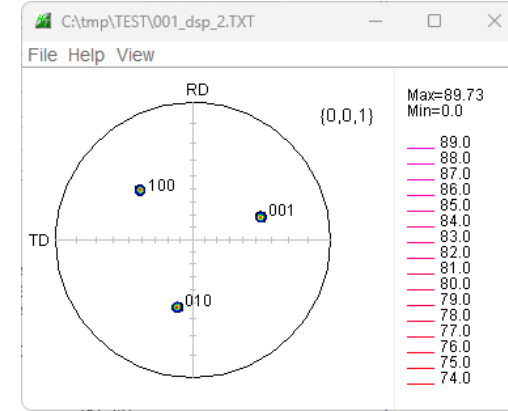
-0.5998733457752577 -0.17280002937460293 0.7812119551546393

0.5705456596985866 0.5921321778891507 0.5690844700985571

CalcPoleFigure

Direction	Alpha	Beta	Center=90	
2 1 1	19.96	-135.0	70.04	44.999
1 1 2	20.06	109.97	69.84	289.975
1 2 1	18.43	-12.25	71.57	167.752
2 1 -1	61.62	-92.08	28.38	87.923
1 1 -2	89.43	-72.43	0.57	107.57
1 2 -1	61.05	-53.67	28.95	126.333
2 -1 1	62.84	-173.53	27.16	6.474
1 -1 2	62.88	148.62	27.12	328.617
-2 1 1	89.53	47.58	0.47	227.579
-1 1 2	61.74	67.24	28.26	247.237
-1 2 1	61.13	28.86	28.87	208.865
-1 2 -1	88.96	-12.42	1.04	167.575

Initialize File



最小値を0.001で{111}<-725>が99%を得られます。

```
TextDisplay 1.14S C:\tmp\TEST\LaboTex\CCW\CCW0.001.epf
File Help
001_dsp_2.TXT 011_dsp_2.TXT 112_dsp_2.TXT
Structure Code a b c alfa beta gamma
7 1.0 1.0 1.0 90.0 90.0 90.0
3
2Theta alf-s alf-e d-alf bet-s bet-e d-bet index H K L R/B
0.0 0.0 90.0 1.0 0.0 359.0 1.0 0 0 1 1
0.0 0.0 90.0 1.0 0.0 359.0 1.0 0 0 1 1
0.0 0.0 90.0 1.0 0.0 359.0 1.0 0 1 1 2 1
0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000
0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000
0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000
0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000
0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000
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0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000
0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000
0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000
0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000
0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000
0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000
0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000 0.001000
```

The screenshot displays the 'Quantitative Analysis - Model Functions Method - Project: Demo Sample:CCW0.001 Job:1' window. It features several panels for crystallographic data and texture analysis.

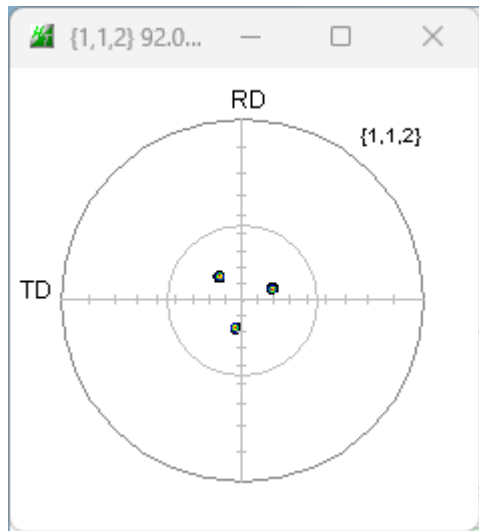
- Crystal Symmetry:** (Cubic)
- Sample Symmetry:** Triclinic
- Grid Cells for Output ODF:** 2.0\*2.0
- Step:** 0.50
- Diagram Range +/-:** 45.0

Three texture component plots are shown, each with a 'Misfit', 'Good', and 'Backgr.' legend. The x-axis for each plot ranges from -45.0 to 45.0.

No	Texture Component	On	Distribution	FWHM $\phi$	FWHM $\Phi$	FWHM $\varphi$	Volume Fraction
1	{ 1 1 1 } < -7 2 5 >	<input checked="" type="checkbox"/>	Gauss	4.0	1.7	3.1	99%
2	{ 1 2 3 } < 4 1 -2 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10%
3	{ 1 2 3 } < 4 1 -2 > R	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10%
4	{ 0 0 1 } < 1 1 0 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10%
5	{ 1 3 2 } < 6 -4 3 > S-1	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10%
6	{ 0 0 1 } < 1 0 0 > cube	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10%
7	{ 5 2 5 } < 1 -5 1 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10%
8	{ 2 3 1 } < -3 4 -6 > S-4	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10%
9	{ 2 1 3 } < -3 -6 4 > S-3	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10%
10	{ 0 1 3 } < 1 0 0 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10%

Calculation Mode:  Automatic  Manual  
Max. Iteration Number: 1,000  
Max. Fit Error % (\*1000): 100  
Iteration: 132  
Fit Error% (\*1000): 107390  
Fit Calculation Progress: [Progress Bar]

Buttons: Change Initial Parameters, Fix Angles, Fix Fractions, Start Volume Fraction Calculation, View Report, Exit and Show, Exit



左極点図が{111}<-725>であるか？  
 {111}の極点図の中心に極がある。  
 {725}の極点図RDに極がある

Crystal orientation determination by two refraction method T.Kikuchi V1.12

File Help Blind-15 CreatePFStep:1.0 hkdsp=true a0->90

PoleFigure  
 112  Center of gravity PoleFigure(TXT2) C:\tmp\TEST#112\_TEST\_2.TXT

Alpha(center=0) 19.963 Beta(RD=180) 35.001 hkl 2 1 1  
 20.048 10.004 1 1 2

Calc PoleFigure  
 7 2 5  
 7 5 2  
 2 5 7  
 2 7 5  
 5 7 2  
 5 2 7

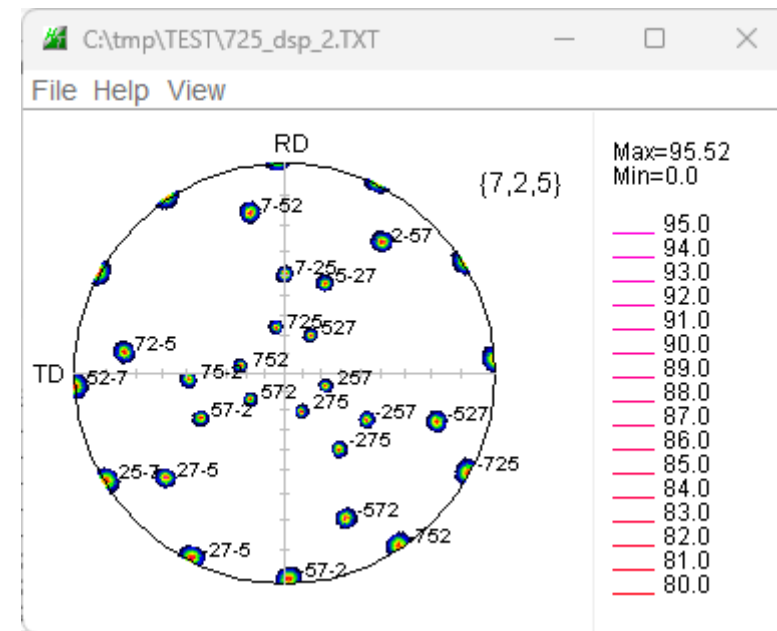
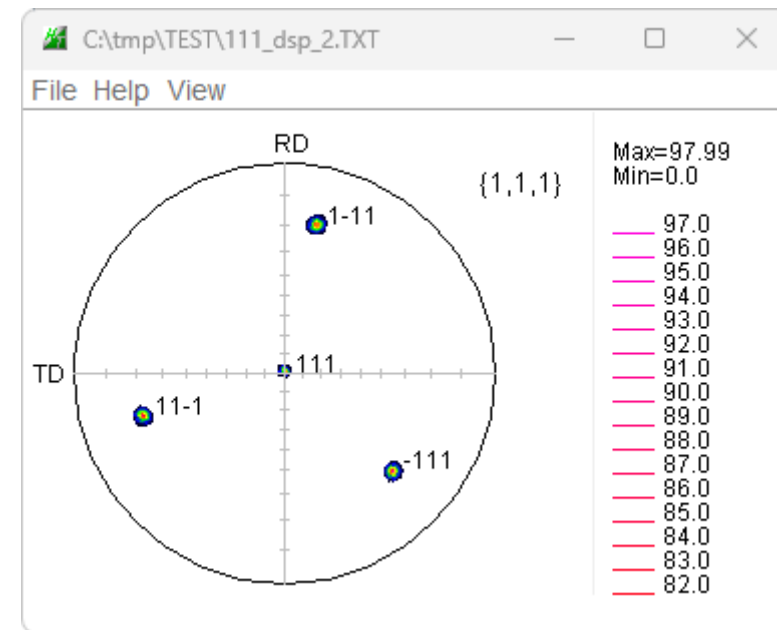
Other(h,k,l) 7,2,5

calc U-matrix CalcPoleFigure FWHM 1 Max 100 Mini 0.001

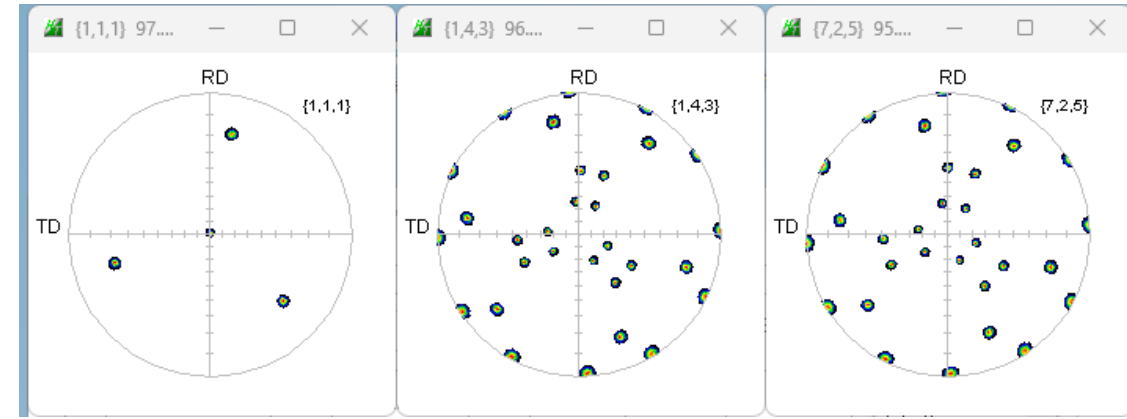
-7 2 5	89.77	81.47	0.23	241.475
-7 5 2	89.32	33.68	0.68	213.682
-2 5 7	48.92	60.67	41.08	240.671
-2 7 5	48.52	36.07	41.48	216.072
-5 7 2	74.03	23.25	15.97	203.254
-5 2 7	74.8	72.36	15.2	252.362
7 -2 5	50.19	179.56	39.81	359.556
7 -5 2	75.77	-168.05	14.23	11.951
2 -5 7	75.82	143.17	14.18	323.17
5 -2 7	50.21	155.5	39.79	335.496
7 2 -5	74.69	-97.21	15.31	82.789
7 5 -2	48.81	-85.49	41.19	94.507
2 5 -7	89.23	-58.53	0.77	121.468
2 7 -5	73.96	-48.08	16.04	131.922
5 7 -2	48.44	-60.85	41.56	119.145
5 2 -7	89.85	-86.33	0.35	93.874
7 2 5	24.7	-170.04	65.3	9.964
7 5 2	23.61	-98.2	66.39	81.804
2 5 7	23.73	73.36	66.27	253.364
2 7 5	22.97	25.74	67.03	205.737
5 7 2	22.9	-50.37	67.1	129.631
5 2 7	24.75	144.95	65.25	324.947

Initialize File

CrystalOrientationDを  
 改造し、手入力による  
 極点図生成を追加



# 極点図回転



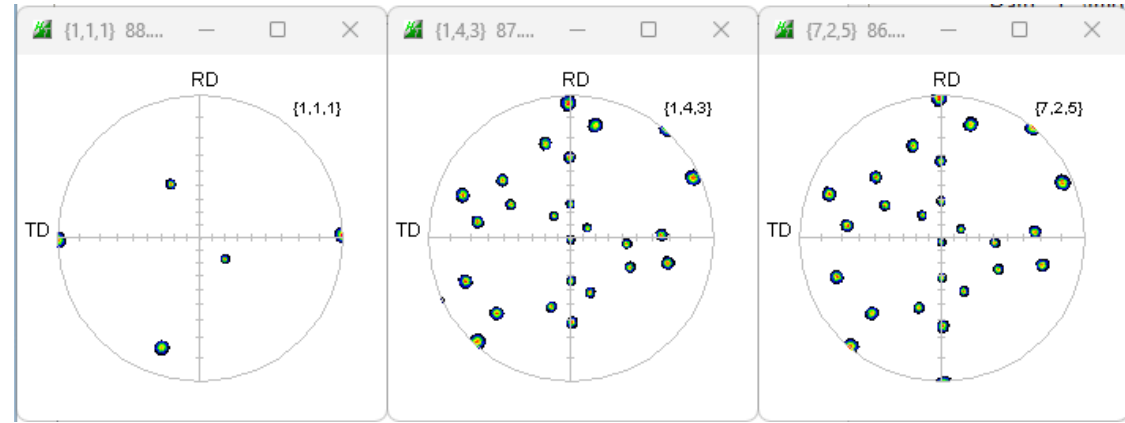
TD方向回転で[143]  
RD方向回転で[725]が計算されたが  
{143},{725}極点図はほぼ同一である。

回転で{143},{725}の中心に極が現れる

TD方向

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

AlongRD(X)	AlongTD(Y)	AlongND(Z)
1 90	2 0	3 0 4 0



RD方向

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

AlongRD(X)	AlongTD(Y)	AlongND(Z)
1 0	2 -90	3 0 4 0

