

Schmid因子計算の確認 T o o l

単結晶測定反射極点図 1 面から複数の極点図生成

結晶方位回転確認

回転方位の e u l e r 角度計算

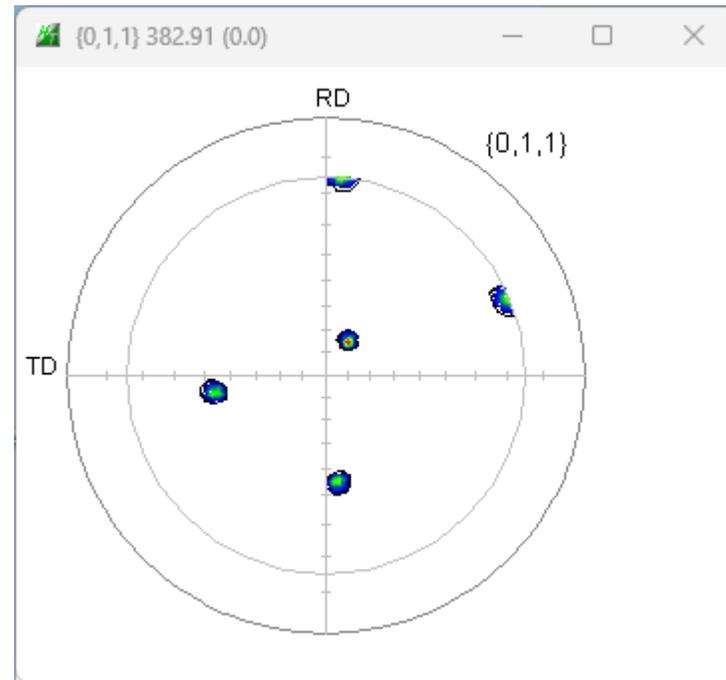
B C C, F C C, H C P シュミット因子計算

単結晶のSchmid因子

{220}面の極点測定 (step=2.5deg)

反射極点図{011}から{001},{011},{111}の完全極点図を作成

ODF解析により方位解析



{001},{011},{111}極点図作成

Crystal orientation determination by two refraction method T.Gikuchi V1.07

File Help beta-3 Step:2

PoleFigure

011 Center of gravity PoleFigure(TXT2) L:\DATA\#2023-04-27-rotationest\#Rotation\#TXT2\#011_2.TXT

Alpha(center=0) 45.187 Beta(RD=180) 7.258 hkl 1 1 0
 47.053 80.197 0 1 -1

CalcPoleFigure

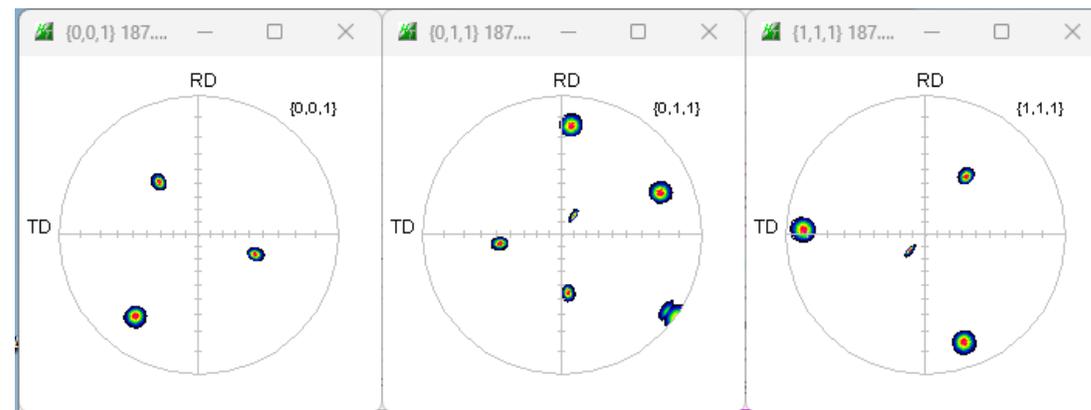
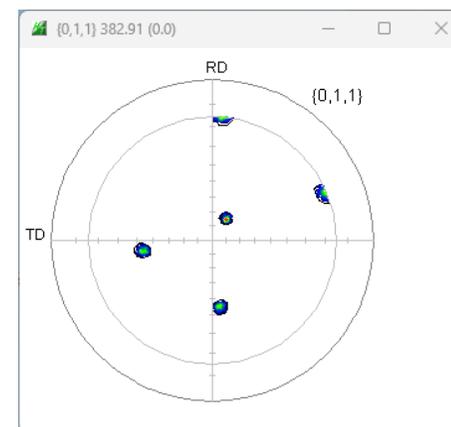
CalcPoleFigure
 -1 1 0
 -1 0 1
 0 -1 1
 1 -1 0
 1 0 -1
 -1 -1 0

011
 Clear
 Set
 Append
 All

calc U-matrix CalcPoleFigure FWHM 5 Max 1000 Mini 0.1

0.6871009020637029	-0.560351761826078	0.46249135494802074		
0.6906510989863125	0.3060798150282693	-0.6552222571778672		
Direction	Alpha	Beta	center=90	
1 1 0	45.19	7.26	44.81	187.258
1 0 1	88.56	54.4	1.44	234.404
0 1 -1	47.18	-80.44	42.82	99.562
1 -1 0	74.22	113.56	15.78	293.563
1 0 -1	17.88	148.86	72.12	328.858
CalcPoleFigure				
Direction	Alpha	Beta	Center=90	
1 1 0	45.19	7.26	44.81	187.258
0 1 1	75.71	175.91	14.29	355.905
1 0 1	88.56	54.4	1.44	234.404
0 1 -1	47.18	-80.44	42.82	99.562
-1 1 0	74.22	113.56	15.78	293.563
-1 0 1	17.88	148.86	72.12	328.858
0 -1 1	47.18	-80.44	42.82	99.562
1 -1 0	74.22	113.56	15.78	293.563
1 0 -1	17.88	148.86	72.12	328.858
-1 -1 0	45.19	7.26	44.81	187.258

Initialize File



ODFにより方位解析
 反射極点図 1 面から方位解析が可能

回転

CrystalRotation 1.08T[23/12/31] by CTR

File Help **RD(TDroate) {uvw}<hkl>** {312}<4-6-3> RV:Integer **Orthorhombic**

Material: Cubic
1.0 1.0 1.0 90.0 90.0 90.0

{hkl|Kuvw}>: 2 1 3 -3 -6 4 Disp

Rotation vector of crystal axis: -22 17 9 SET CTD

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

Result:

```

RD   TD   ND
-3.0 -22.0 2.0
-6.0 17.0 1.0
4.0  9.0  3.0
RDaxis [-3 -6 4]
TDaxis [-22 17 9]
NDaxis [2 1 3]
-22.0 17.0 9.0      (-22 17 9 )
{213}<-3-64>      eulerangle:(58.98,36.699,63.435)
Eulerangle g(φ1 φφ2)=
      -0.3841 0.7528 0.5345
      -0.7682 -0.2761 0.2673
      0.5121 -0.308 0.8018
Rotation [-22,17,9]      angle:-90.0
Calc-d=(-0.7528,0.5817,0.308)
a(-22.0,17.0,9.0),-90.0
Rotated Eulerangle
      0.5867 -0.7459 0.3499
      -0.13 0.3384 0.932
      -0.8136 -0.5737 0.0948
Rotated RD   TD   ND
      0.5345 0.5249 0.3841
      0.2673 -0.4783 0.7682
      0.8018 -0.4833 -0.5121
Calc Miller indices
      {1.0 2.0 -1.3333}<2.0 1.0 3.0>
      {3 4 6}<2 -3 1>
    
```

{3 4 6}<2 -3 1> set{hkl|Kuvw}>

{312}<4-6-3> toOrthorhombic {213}<-3-64>
Result: {36-4}<213> toOrthorhombic {346}<-2-31>

入力方位{312}<4-6-3>に対しOrthorhombic変換{213}<-3-64>
TD軸[-22 17 9]90度回転、{36-4}<213>を得て、Orthorhombic変換で{346}<-2-31>を得る

NewCubicCODisp 1.18ST[23/12/31] by CTR

File Help Symmetry Special Index

Miller Indices
(hkl)[uvw] 3 1 2 4 -6 -3 Calc

Euler Angle
(p1 P p2) <=90 332.9681 57.6885 71.5651 Calc

DISP
Position 10 Disp size 400 DISP
BG color Black Line size 2.0 Minus

NewCubicCODisp 1.18ST[23/12/31] by CTR

File Help Symmetry Special Index

Miller Indices
(hkl)[uvw] 2 1 3 -3 -6 4 Calc

Euler Angle
(p1 P p2) <=90 58.9799 36.6992 63.4349 Calc

DISP
Position 10 Disp size 400 DISP
BG color Black Line size 2.0 Minus

NewCubicCODisp 1.18ST[23/12/31] by CTR

File Help Symmetry Special Index

Miller Indices
(hkl)[uvw] 3 6 -4 2 1 3 Calc

Euler Angle
(p1 P p2) <=90 68.9877 120.807 26.5651 Calc

DISP
Position 10 Disp size 400 DISP
BG color Black Line size 2.0 Minus

NewCubicCODisp 1.18ST[23/12/31] by CTR

File Help Symmetry Special Index

Miller Indices
(hkl)[uvw] 3 4 6 2 -3 1 Calc

Euler Angle
(p1 P p2) <=90 24.6753 39.8056 36.8699 Calc

DISP
Position 10 Disp size 400 DISP
BG color Black Line size 2.0 Minus

{hkl}<uvw>をTD軸回転で{uvw}<hkl>を得る

回転方向を選択し方位入力

方向によりSchmid因子は異なるが絶対値で一致する

BCCSchmidFactorCalc3 3.10T[23/12/31] by CTR

File Help Text SlipProfile ND(NDRotate) SF Orthorhombic

InputFile(TXT): Data input {1 1 0}<-1 -1 2> 100.0

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

Data input: real {h k l} or {h k l} {h k l} {u v w} phi1 PHI phi2 phi1<=90,PHI<=90

3 2 1 Input Input Input

{h k l}<u v w> phi1 PHI phi2	-0.303	0.0	0.303	-0.337
{1.0 2.0 3.0}	-0.135	-0.471	0.0	0.0
{2.0 3.0 1.0}	0.0	-0.236	0.269	-0.034
{3.0 2.0 1.0}	-0.265	-0.331	-0.066	0.066
	0.265	0.331	-0.265	-0.397
	-0.22	-0.044	-0.441	-0.485
	0.0	0.0	0.0	0.0
	0.0	0.0	0.265	0.198
	0.242	0.287	0.088	-0.022

Input	max	Slipsystem
[1.0 2.0 3.0]	0.485	(312)[-111]
[2.0 3.0 1.0]	0.467	(0-1-1)[-1-11]
[3.0 2.0 1.0]	0.35	(0-1-1)[-1-11]

AlongRD(X): 3 0 AlongTD(Y)<=0: 2 0 AlongND(Z): 1 0 4 0 Clear

SlipDisp Schmidcalc

SchmidFactorProfile: ND->RD Step 1 Symmetry SchmidCalc SchmidFDisp

AXISRotation HKLDouble

BCCSchmidFactorCalc3 3.10T[23/12/31] by CTR

File Help Text SlipProfile ND(NDRotate) abs(SF) Orthorhombic

InputFile(TXT): Data input {1 1 0}<-1 -1 2> 100.0

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

Data input: real {h k l} or {h k l} {h k l} {u v w} phi1 PHI phi2 phi1<=90,PHI<=90

3 2 1 Input Input Input

{h k l}<u v w> phi1 PHI phi2	-0.303	0.0	0.303	-0.337
{1.0 2.0 3.0}	-0.135	-0.471	0.0	0.0
{2.0 3.0 1.0}	0.0	-0.236	0.269	-0.034
{3.0 2.0 1.0}	-0.265	-0.331	-0.066	0.066
	0.265	0.331	-0.265	-0.397
	-0.22	-0.044	-0.441	-0.485
	0.0	0.0	0.0	0.0
	0.0	0.0	0.265	0.198
	0.242	0.287	0.088	-0.022

Input	max	Slipsystem
[1.0 2.0 3.0]	0.485	(312)[-111]
[2.0 3.0 1.0]	0.485	(123)[-1-11]
[3.0 2.0 1.0]	0.485	(213)[-1-11]

AlongRD(X): 3 0 AlongTD(Y)<=0: 2 0 AlongND(Z): 1 0 4 0 Clear

SlipDisp Schmidcalc

SchmidFactorProfile: ND->RD Step 1 Symmetry SchmidCalc SchmidFDisp

AXISRotation HKLDouble

絶対値は対称方位を含む絶対値シュミット因子最大値が計算される

回転

$$\{1\ 1\ 2\} \langle -1\ -1\ 1 \rangle 100.0$$

RDaxis [-1 -1 1]

TDaxis [-1 1 0]

NDaxis [1 1 2]

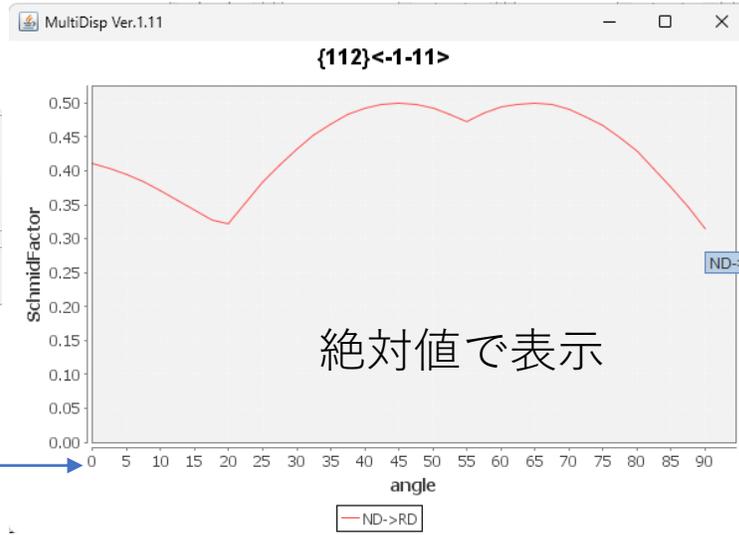
AlongRD(X) 3 0 AlongTD(Y)<=0 2 -90 AlongND(Z) 1 0 4 0

{1.0 1.0 -1.0}<1.0 1.0 2.0> {1 1 -1}<1 1 2>

SchmidFactorProfile
 ND->RD all Step 2.5

RD方向は{uvw}<hkl>

TD-axisで回転



絶対値で表示

ND->RD: (90, 0.314)

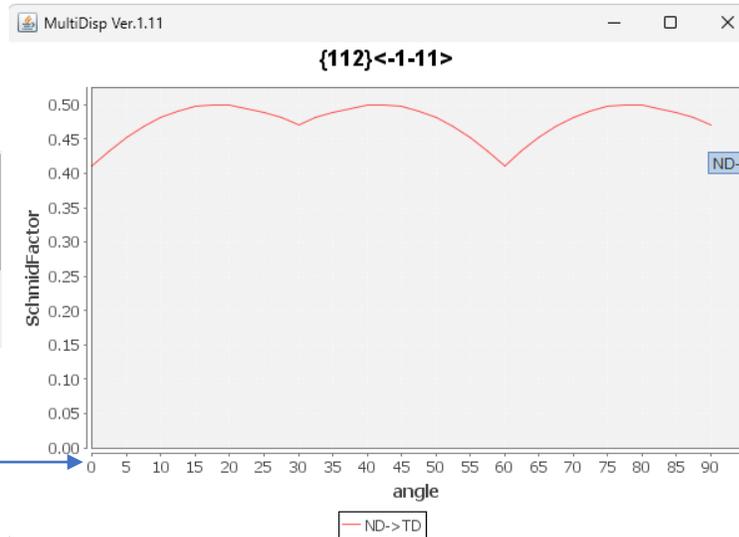
AlongRD(X) 3 90 AlongTD(Y)<=0 2 0 AlongND(Z) 1 0 4 0

{1.0 -1.0 0.0}<-1.0 -1.0 1.0> {1 -1 0}<-1 -1 1>

SchmidFactorProfile
 ND->TD all Step 2.5

TD方向は{TD}<uvw>

RD-axisで回転



ND->TD: (90, 0.471)

BCCSchmidFactorCalc3 3.10T[23/12/31] by CTR

File Help Text SlipProfile RD(TDRotate) abs(SF) Orthorhombic

InputFile(TXT) _____

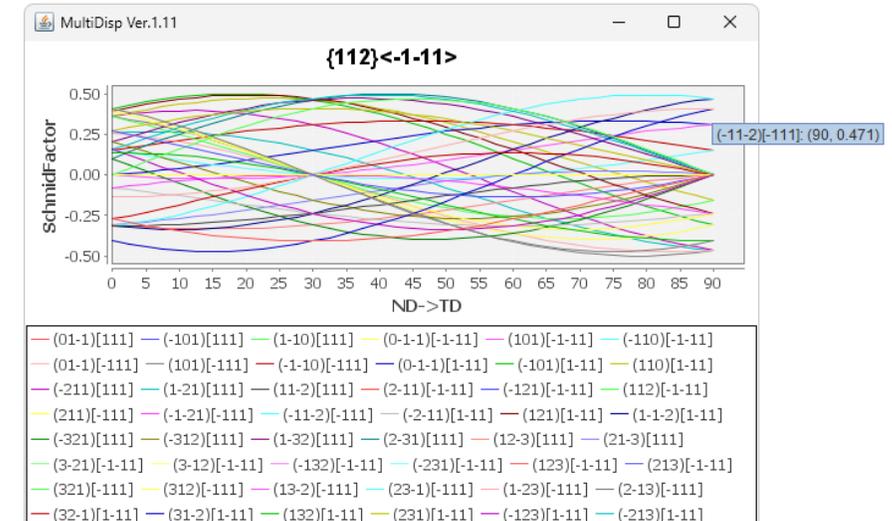
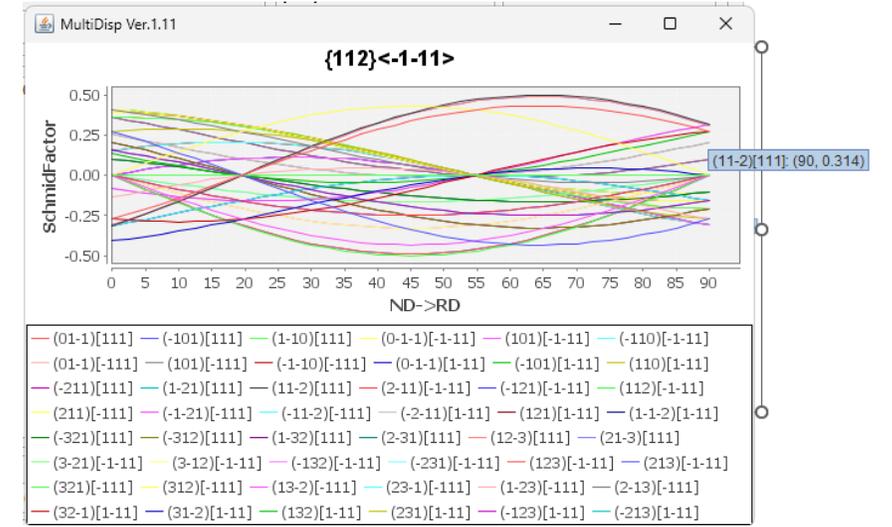
LaboTex VolumeFraction _____

ND(NDRotate) _____

TD(RDRotate) _____

RD(TDRotate)

表示は絶対値ではなくプラスマイナスの最大値で表現



連続回転

{112}<-1-11>をND(90)、TD(-90)、ND(-90)で{-110}<-11-1>が計算され、SF=0.471を得る

BCCSchmidFactorCalc 3.10T[23/12/31] by CTR

File Help Text SlipProfile ND(NDRotate) abs(SF) Orthorhombic

InputFile(TXT)
LaboTex VolumeFraction(SumVFmode) {1 1 2}<-1 -1 1> 100.0

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

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

{1 1 2}<-1 -1 1> 100.0

	-0.408	0.0	0.408	-0.236
	0.471	-0.236	0.0	0.0
	0.0	0.0	0.0	0.0
	-0.236	0.471	-0.236	-0.309
	-0.154	0.463	0.463	-0.309
	-0.154	0.0	0.0	0.0
	0.0	0.0	0.0	0.0
	0.0	0.0	0.0	0.0
	0.0	0.309	0.154	0.463
	0.463	0.309	0.154	0.463
input	VF%	Schmid	VF*Schmid%	
{1.01.02.0}<-1.0-1.01.0>	100.0	0.471	0.471	
VFsum=100.0%		VF*Schmidsum=0.471		
SchmidFactor(SumVF)=0.471				

AlongRD(X) AlongTD(Y)<=0 AlongND(Z)

3 0 2 -90 1 90 4 -90

{-1 0 1 0 0}<1 0 1.0 -1.0> toOrthorhombic {1 0 1}<-1 -1 1>

SchmidFactorProfile
 ND->RD all Step 1

AXISRotation HKLDouble

Clear SlipDisp SchmidCalc Symmetry SchmidCalc SchmidFDisp

CrystalRotation 1.08T[23/12/31] by CTR

File Help ND [hkl]<uvw> {112}<-1-11> RV:integer Orthorhombic

Material
Material Cubic
1.0 1.0 1.0 90.0 90.0 90.0

[hkl]Kuvw>
1 0 1 -1 -2 1 Disp

Rotation vector of crystal axis
 1 0 1 SET CTD

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

Result

```
RD TD ND
-1.0 -1.0 1.0
-2.0 1.0 0.0
1.0 1.0 1.0
RDaxis [-1 -2 1]
TDaxis [-1 1 1]
NDaxis [1 0 1]
1.0 0.0 1.0 (1 0 1)
{101}<-1-21> eulerangle:(35.264,45.0,90.0)
Eulerangle g(phi1 phi2)=
-0.4082 0.5774 0.7071
-0.8165 -0.8165 0.0
0.4082 -0.5774 0.7071
Rotation [1,0,1] angle:-90.0
Calc-d=(0.7071,0.0,0.7071)
a(1.0,0.0,1.0),-90.0
Rotated Eulerangle
0.5 -0.7071 0.5
0.7071 0.0 -0.7071
0.5 0.7071 0.5
Rotated RD TD ND
0.5774 0.5774 0.7071
-0.5774 0.8165 0.0
-0.5774 -0.5774 0.7071
Calc Miller indices
{1.0 0.0 1.0}<1.0 -1.0 -1.0>
{1 0 1}<-1 -1 1>
```

{1 1 0}<1 -1 1> set[hkl]Kuvw>

Result: {101}<1-1-1> toOrthorhombic {110}<-1-11>

繰り返し

[hkl]Kuvw>
1 1 2 -1 -1 1 Disp

Rotation vector of crystal axis
 1 1 2 SET CTD

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

Result: {112}<-110> toOrthorhombic {112}<-1-10>

[hkl]Kuvw>
1 1 2 1 -1 0 Disp

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

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

Result: {-110}<112> toOrthorhombic {101}<-1-21>

[hkl]Kuvw>
1 0 1 -1 -2 1 Disp

Rotation vector of crystal axis
 1 0 1 SET CTD

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

Result: {101}<1-1-1> toOrthorhombic {110}<-1-11>

CrystalRotationは回転毎に整数化、Orthorhombicチェックが行われているが、BccSchmidFactorCalcは実数のままで計算し、最後に整数化Orthorhombicチェック

Orthorhombic ↔ Triclinic Orthorhombic(90,90,90) Triclinic(360,90,90)

BCCSchmidFactorCalc3 3.10T[23/12/31] by CTR

File Help Text SlipProfile ND(NDRotate) abs(\$F) **Orthorhombic**

InputFile(TXT): LaboTex VolumeFraction(SumVFmode) {3 1 2}<4 -6 -3> 100

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

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

{3 1 2}<4 -6 -3> 100 InputData {3 1 2}<4 -6 -3> 100 **変換あり**

Calc Schmid's Factor abs(\$F)mode
{2.01.03.0}<-3.0-6.04.0> rotation (2[0.0],1[-90.0],0[90.0]3[-90.0])

slip0	slip1	slip2	slip3	slip4
slip5	slip6	slip7	slip8	slip9
slip10	slip11	slip12	slip13	slip14
slip15	slip16	slip17	slip18	slip19
slip20	slip21	slip22	slip23	slip24
slip25	slip26	slip27	slip28	slip29
slip30	slip31	slip32	slip33	slip34
slip35	slip36			

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

{-22 17 9}<11 10 8> toOrthorhombic {17 22 9}<-10 -11 8>

SchmidFactorProfile: ND->RD all Step 1

AXISRotation HKLDouble

[22 9 17] --> 54.43 22.25

{2.01.03.0}<-3.0-6.04.0> 100.0 0.477
 VFsum=100.0% VF*Schmidsum=0.477
 SchmidFactor(SumVF)=0.477

BCCSchmidFactorCalc3 3.10T[23/12/31] by CTR

File Help Text SlipProfile ND(NDRotate) abs(\$F) **Triclinic**

InputFile(TXT): LaboTex VolumeFraction(SumVFmode) {3 1 2}<4 -6 -3> 100

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

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

{3 1 2}<4 -6 -3> 100 InputData {3 1 2}<4 -6 -3> 100 **変換なし**

Calc Schmid's Factor abs(\$F)mode
{3.01.02.0}<4.0-6.0-3.0> rotation (2[0.0],1[-90.0],0[90.0]3[-90.0])

slip0	slip1	slip2	slip3	slip4
slip5	slip6	slip7	slip8	slip9
slip10	slip11	slip12	slip13	slip14
slip15	slip16	slip17	slip18	slip19
slip20	slip21	slip22	slip23	slip24
slip25	slip26	slip27	slip28	slip29
slip30	slip31	slip32	slip33	slip34
slip35	slip36			

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

{1.8918 1.0 4.9552}<3.1891 -1.0781 -1.0> {17 7 44}<3 -1 -1>

SchmidFactorProfile: ND->RD all Step 1

AXISRotation HKLDouble

[17 7 44] --> 22.68 22.38

{3.01.02.0}<4.0-6.0-3.0> 100.0 0.494
 VFsum=100.0% VF*Schmidsum=0.494
 SchmidFactor(SumVF)=0.494

NewCubicCODisp 1.185T[23/12/31] by CTR

File Help Symmetry Special Index

Miller Indices: (hkl)[uvw] 3 1 2 4 -6 -3 Calc

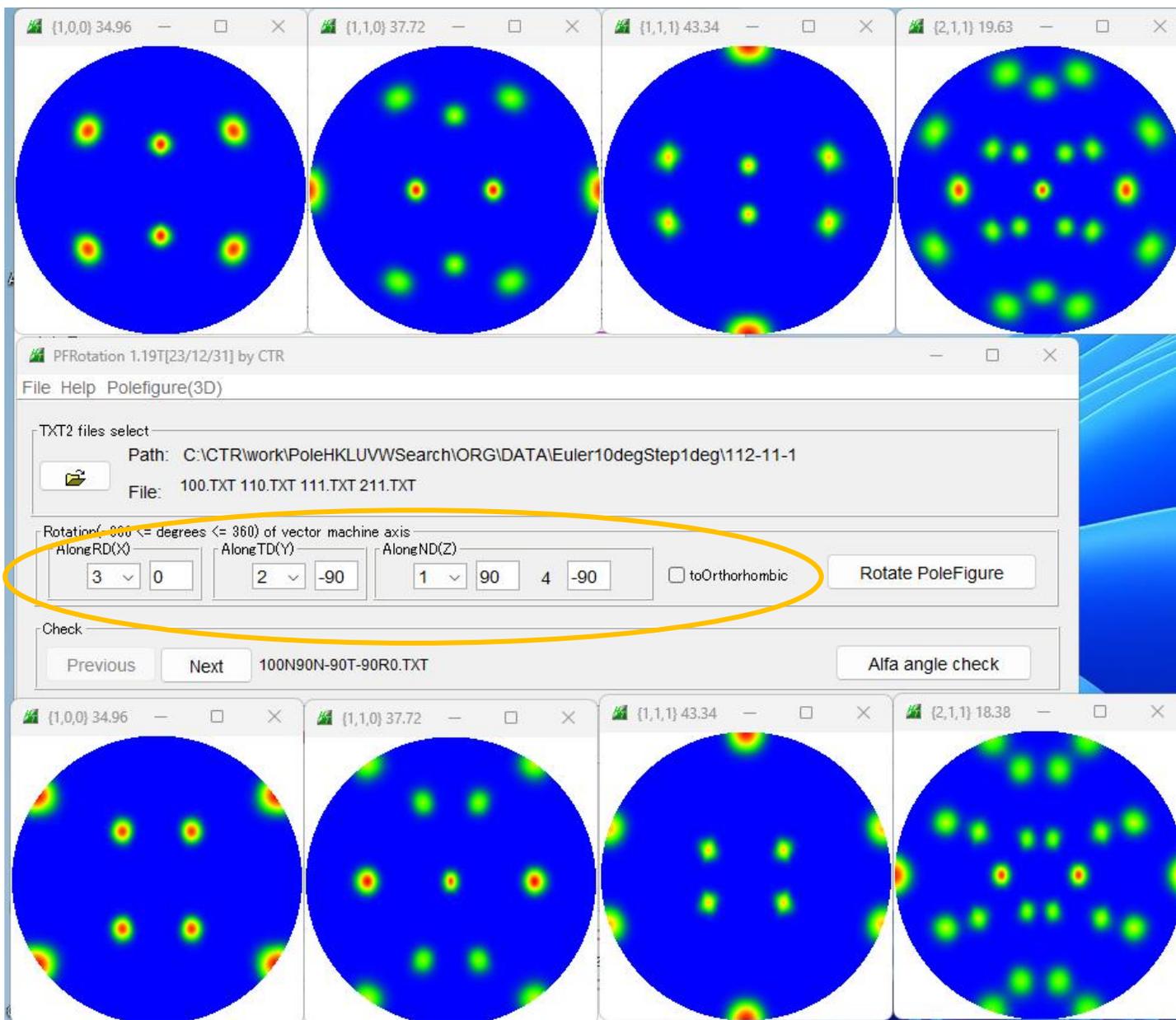
Euler Angle: (p1 P p2) <=90 332.9681 57.6885 71.5651 Calc

Present Condition: Euler Angle

Double Miller Indices

DISP: Position 10 Disp size 400 DISP
 BG color Black Line size 2.0 Minus

連続回転をPFRotationで確認



$\{112\}\langle 111\rangle$

ND 90度回転
TD -90度回転
ND -90度回転
を連続した結果

$\{110\}\langle 111\rangle$