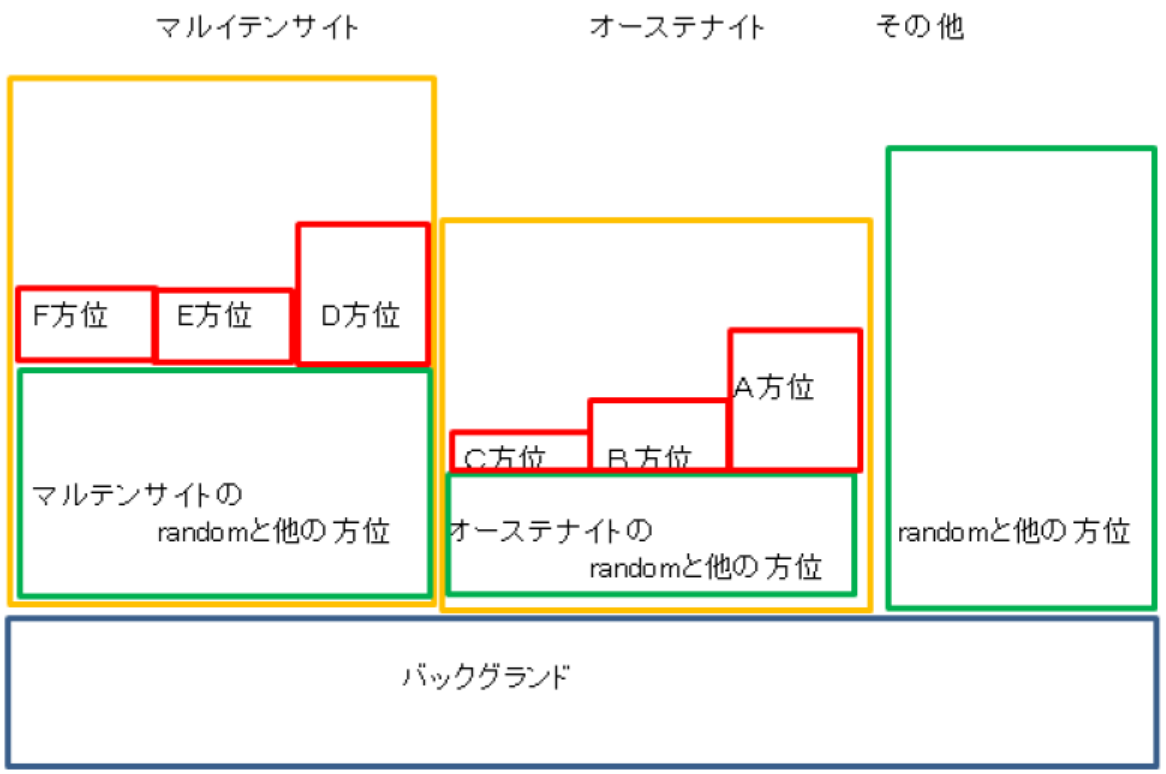
SmartLabデータの解析

測定状況
極点処理
ODF解析
ODF解析結果の評価
（Θ／ΘプロファイルからND方位）
（データ蓄積によるDatabaseの検索）

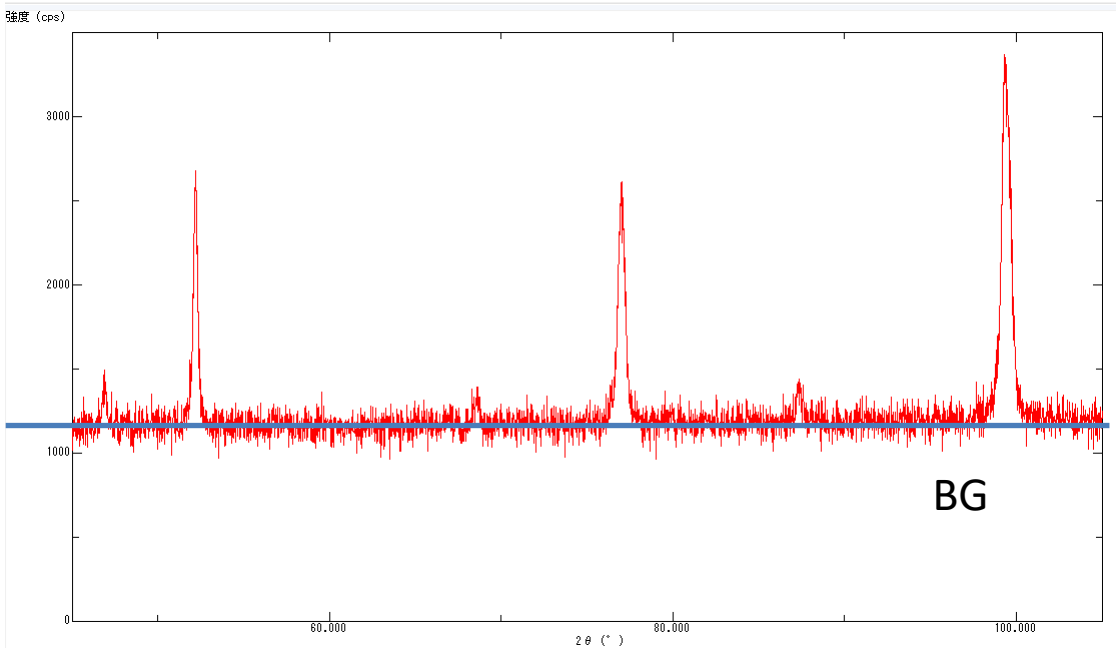
2022年01月06日
HelperTex　Office

測定状況

- コンプトン散乱などのバックグランド
- 光学系に依存するdefocus
- 複数相による畳み込み
- 配向とrandom



バックグランド



Ras

```
*MEAS_3DE_BG_HIGH_ANGLE "55.1700"
*MEAS_3DE_BG_HIGH_EXEC "1"
*MEAS_3DE_BG_HIGH_INT "1230"
*MEAS_3DE_BG_HIGH_TIME "0.50"
*MEAS_3DE_BG_LOW_ANGLE "49.1700"
*MEAS_3DE_BG_LOW_EXEC "1"
*MEAS_3DE_BG_LOW_INT "1271"
*MEAS_3DE_BG_LOW_TIME "0.50"
```

ASC

```
*SPEED          =  0.5
*SLIT_SPEC      =  0, 1.0deg, 1, 0.000000
*SLIT_SPEC      =  1, 10.000mm, 10, 0.000000
*SLIT_SPEC      =  2, 10.000mm, 10, 0.000000
*KV             =  40
*MA             =  40
*LOW            =  91512
*HIGH           =  88560
```

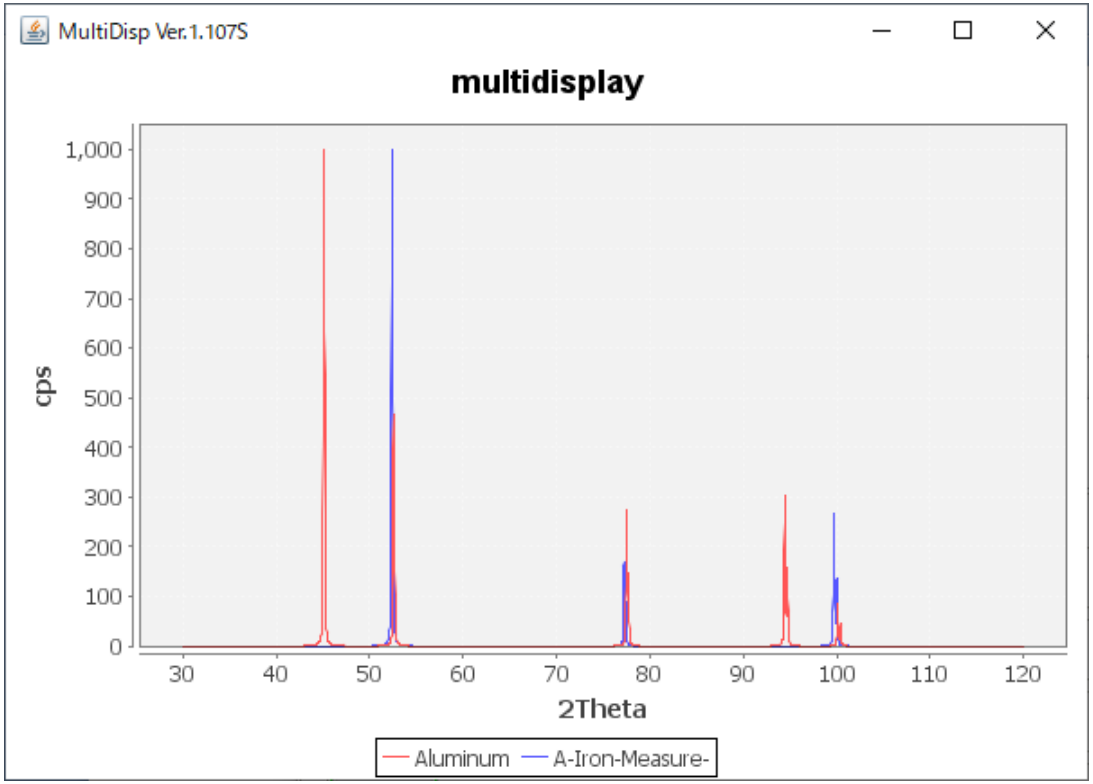
プロファイル測定でバックグランドの概要を把握する
極点測定ではバックグランドも同時に測定する

RasとASCのバックグランドの関係
ASCはCPSに変換されている。更に、lowからhighの間の面積で表示される
よって

ASC＝Ras／FT－time＊（360／step／2）
ASCHIGH＝88560＝1230／0．5＊36

defocus

Defocusは、受光スリット幅、測定2θ角度に依存する
Fe系サンプルはrandom試料が得にくい、アルミニウムを代用する



アルミニウム

1.78897				
6				
1	1	1	100.0	45.082
2	0	0	47.7	52.546
2	2	0	28.7	77.511
3	1	1	31.9	94.454
2	2	2	9.1	100.116

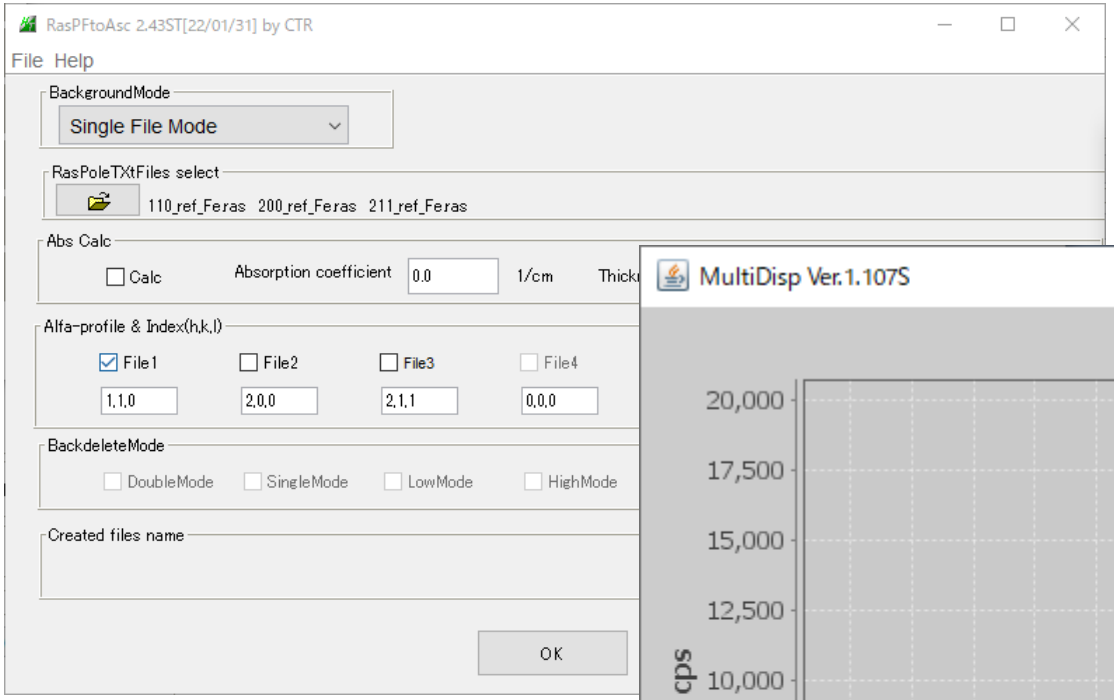
Fe

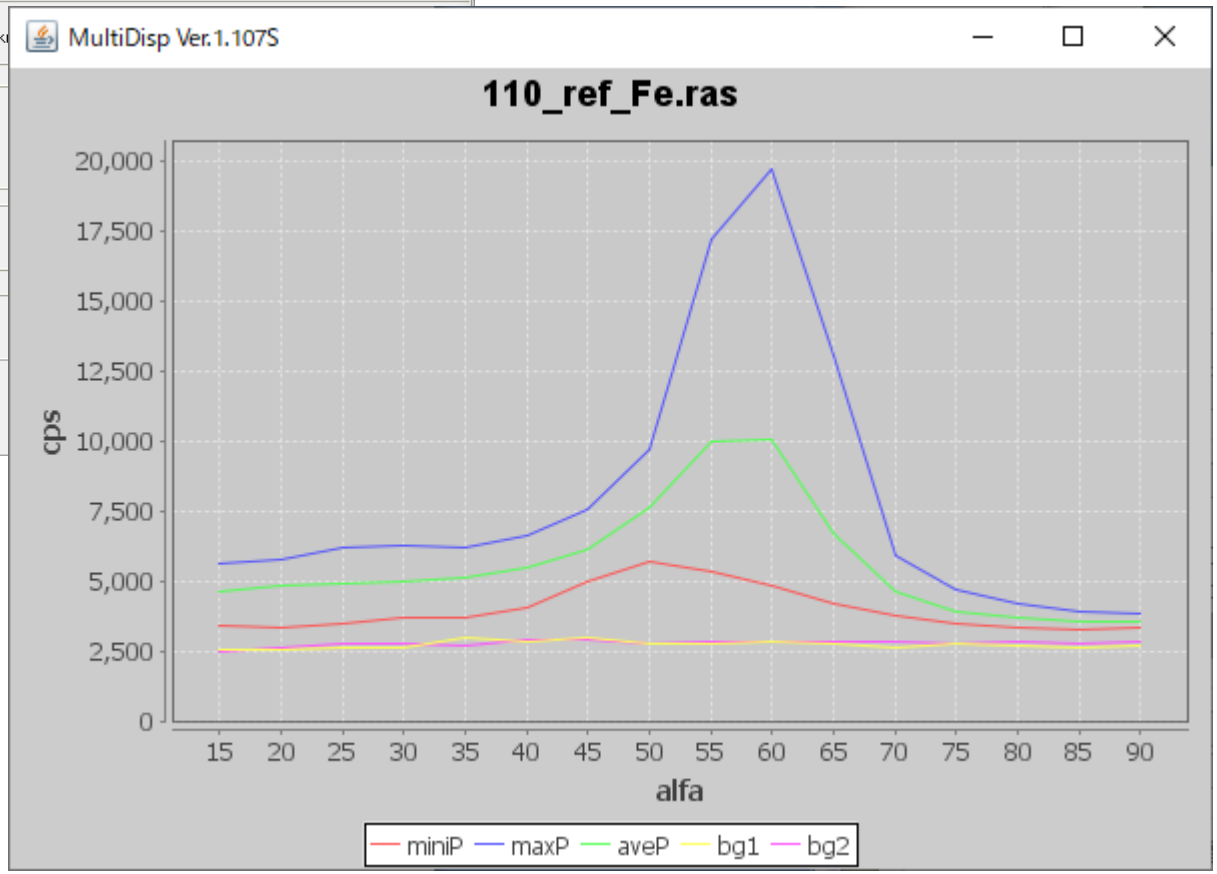
1.78897				
12				
1	1	0	100.0	52.376
2	0	0	17.53	77.235
2	1	1	27.85	99.705
2	2	0	7.8	123.924

Al	Al-2theta	Fe	Fe-2theta
{2 0 0}	52.546	{1 1 0}	52.376
{2 2 0}	77.511	{2 0 0}	77.235
{3 1 1}	94.511	{2 1 1}	99.705

アルミニウムで測定したデータをFe指数に変更

RasからASC変換

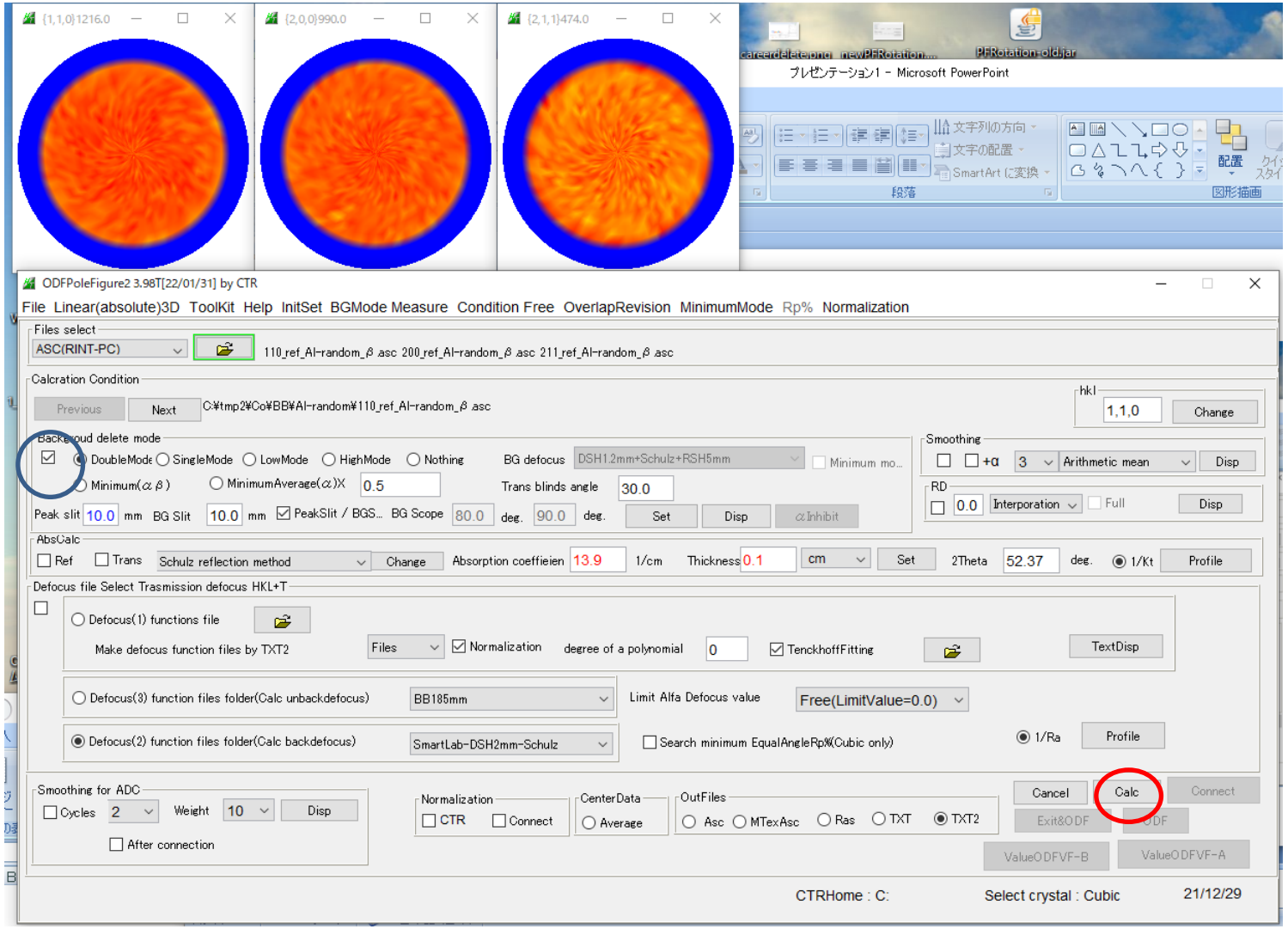




OKでASCに変換される。

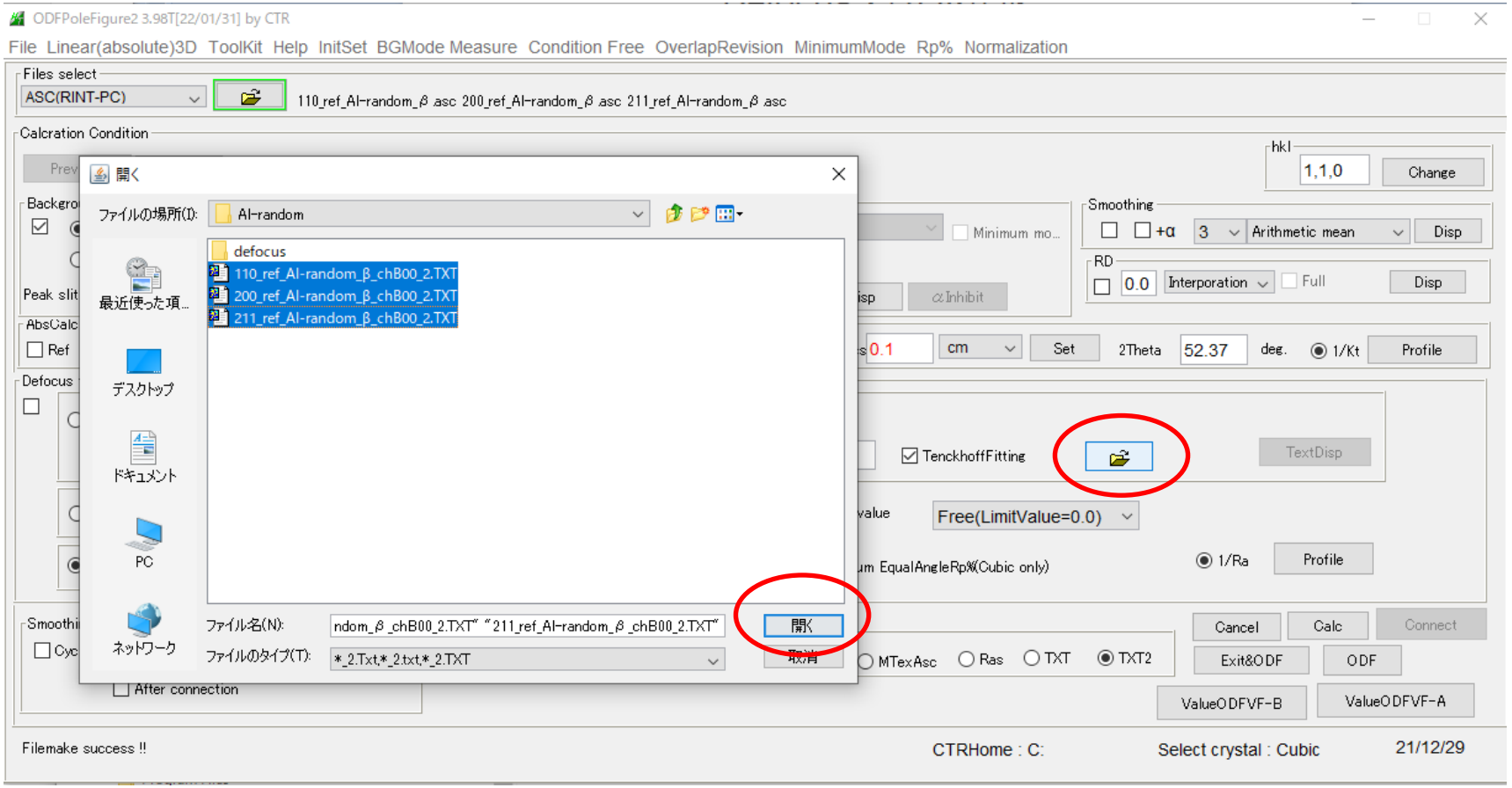
すべてCPSで表示

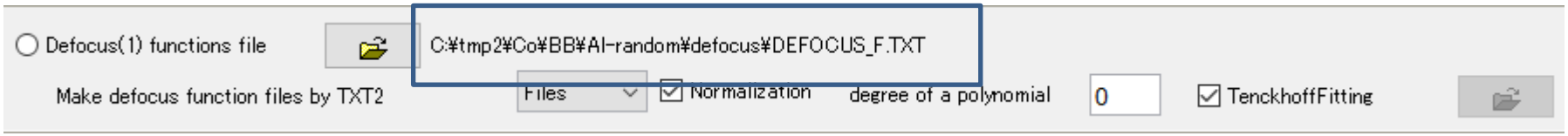
Defocus補正ファイル作成



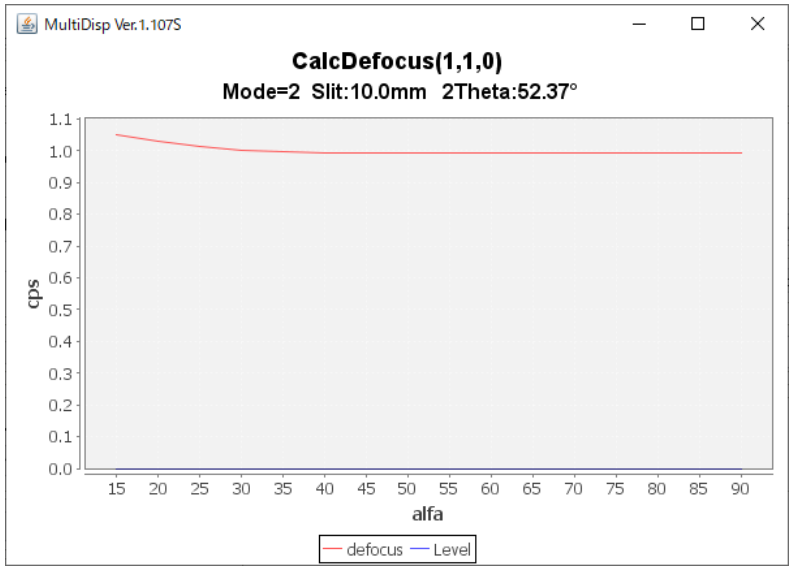
バックグランド削除のみ行う

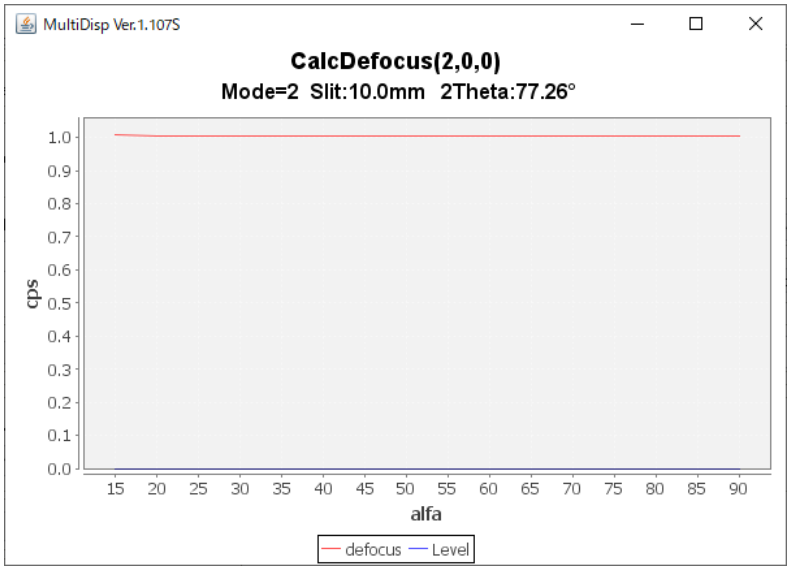
Defocusファイル作成

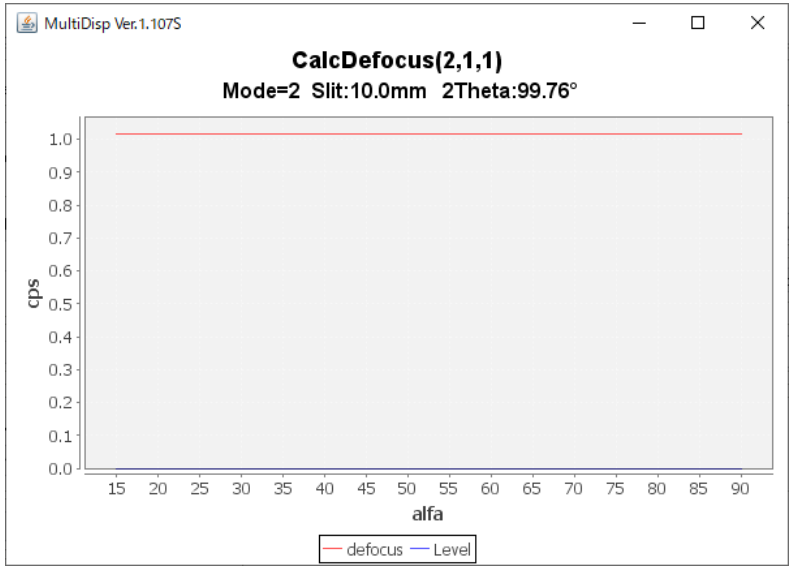




Defocusプロファイル確認

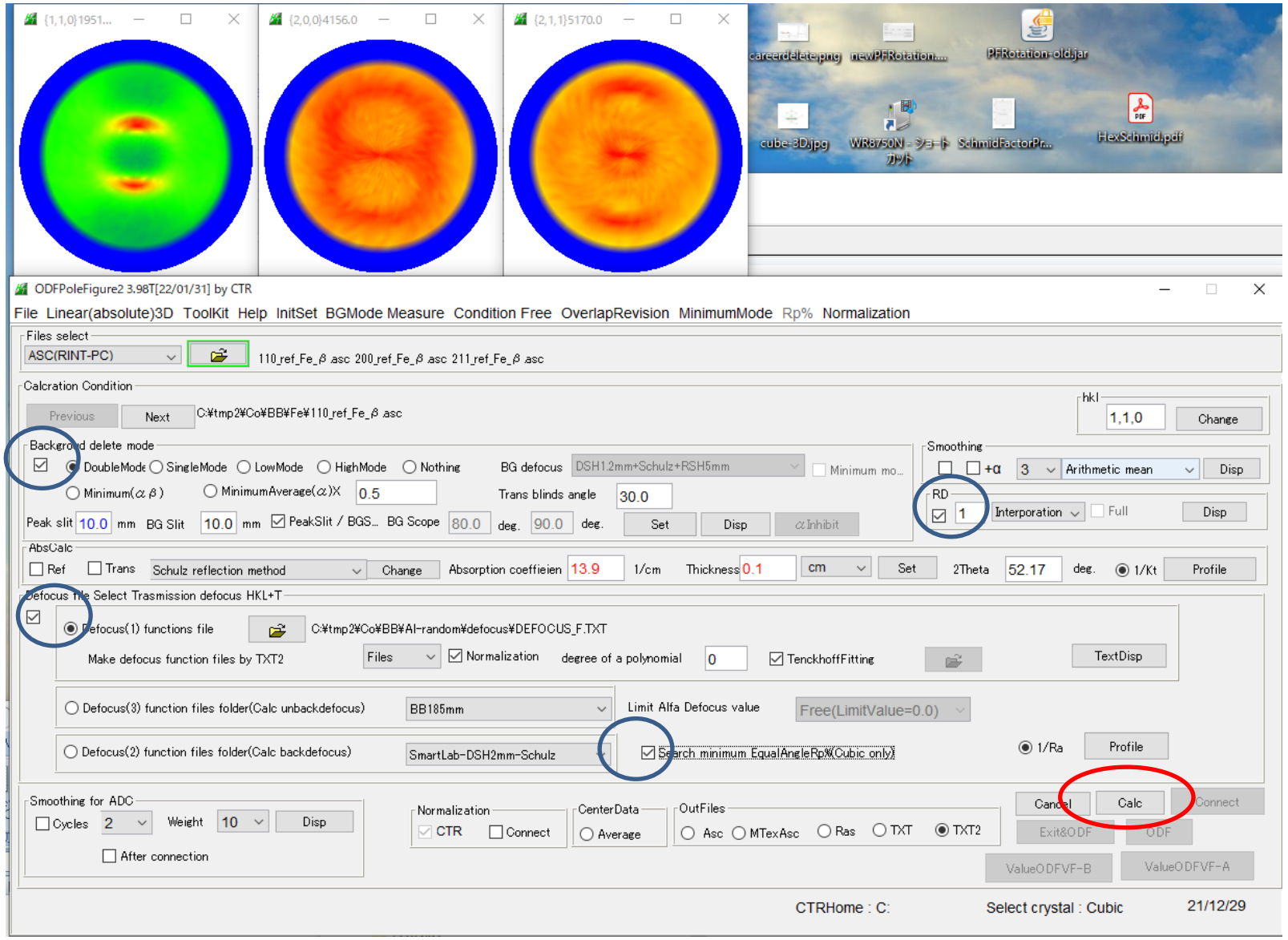




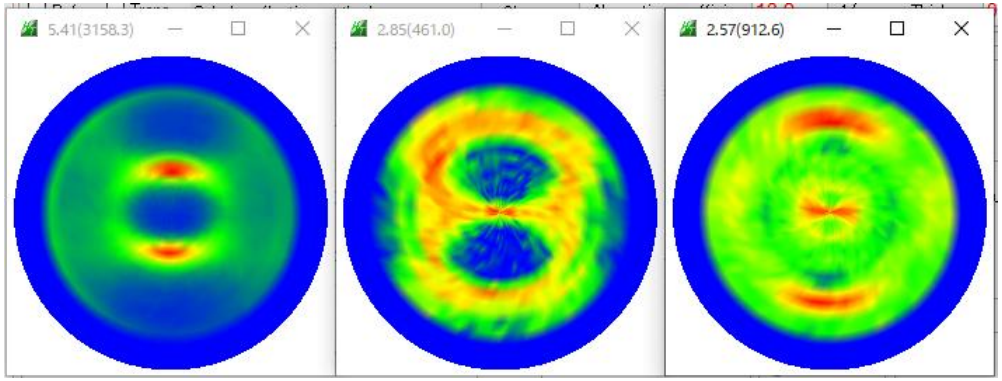


プロファイルに異常があれば修正
バックグランドの点検修正
補正曲線の修正
（TenckhoffCalc、DefocusLineEditer）

Feサンプル極点処理

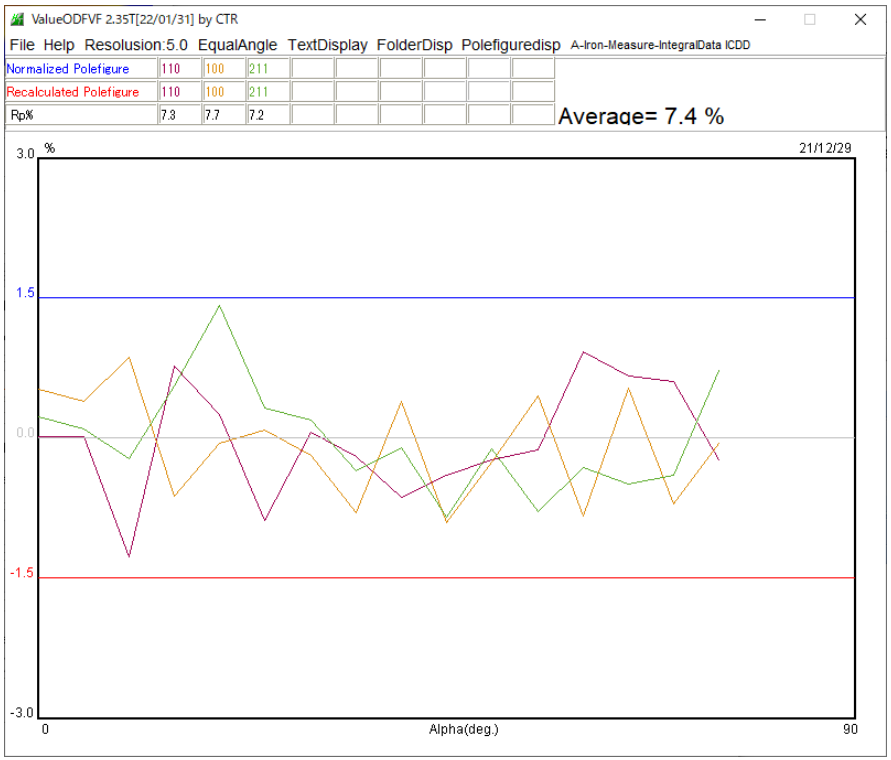

{1,1,0}1951...
{2,0,0}4156.0
{2,1,1}5170.0
careerdelete.png
newPFRotation....
PFRotation-old.jar
cube-3D.jpg
WR8750N - ショートカット
SchmidFactorPr...
HexSchmid.pdf
ODFPoleFigure2 3.98T[22/01/31] by CTR
File Linear(absolute)3D ToolKit Help InitSet BGMode Measure Condition Free OverlapRevision MinimumMode Rp% Normalization
Files select
ASC(RINT-PC)
110_ref_Fe_β.asc 200_ref_Fe_β.asc 211_ref_Fe_β.asc
Calcration Condition
Previous
Next
C:¥tmp2¥Co¥BB¥Fe¥110_ref_Fe_β.asc
hkl
1,1,0
Change
Background delete mode
DoubleMode SingleMode LowMode HighMode Nothing
BG defocus
DSH1.2mm+Schulz+RSH5mm
Minimum mo...
Minimum(α β)
MinimumAverage(α)X
0.5
Trans blinds angle
30.0
Peak slit
10.0
mm
BG Slit
10.0
mm
PeakSlit / BGS...
BG Scope
80.0
deg.
90.0
deg.
Set
Disp
αInhibit
Smoothing
+α
3
Arithmetic mean
Disp
RD
1
Interporation
Full
Disp
AbsCalc
Ref
Trans
Schulz reflection method
Change
Absorption coeffieien
13.9
1/cm
Thickness
0.1
cm
Set
2Theta
52.17
deg.
1/Kt
Profile
Defocus file Select Trasmission defocus HKL+T
Defocus(1) functions file
C:¥tmp2¥Co¥BB¥Al-random¥defocus¥DEFOCUS_F.TXT
Make defocus function files by TXT2
Files
Normalization
degree of a polynomial
0
TenckhoffFitting
TextDisp
Defocus(3) function files folder(Calc unbackdefocus)
BB185mm
Limit Alfa Defocus value
Free(LimitValue=0.0)
Defocus(2) function files folder(Calc backdefocus)
SmartLab-DSH2mm-Schulz
Search minimum EqualAngleRp%(Cubic only)
1/Ra
Profile
Smoothing for ADC
Cycles
2
Weight
10
Disp
After connection
Normalization
CTR
Connect
CenterData
Average
OutFiles
Asc
MTexAsc
Ras
TXT
TXT2
Cancel
Calc
Connect
Exit&ODF
ODF
ValueODFVF-B
ValueODFVF-A
CTRHome : C:
Select crystal : Cubic
21/12/29

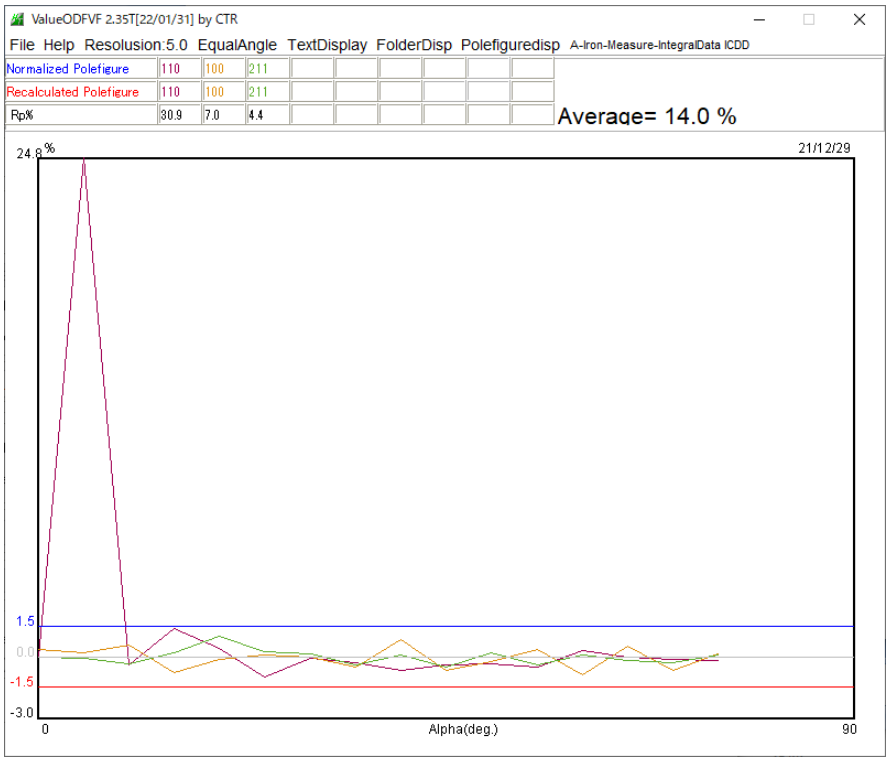
処理結果の検証



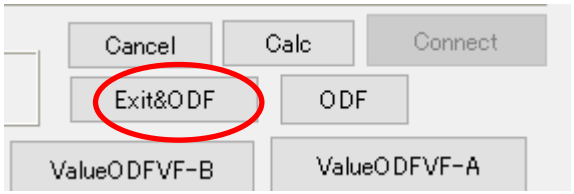
最適化Rp%では、1か所不一致のため採用しない

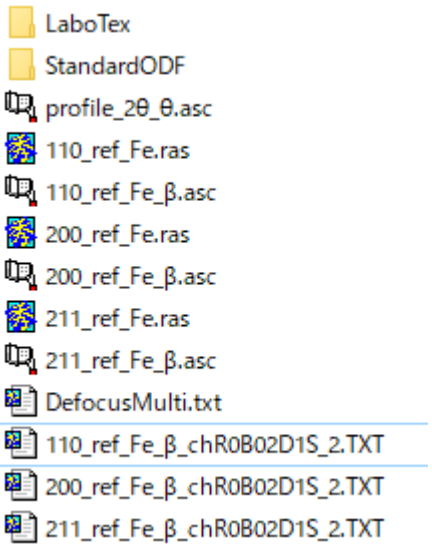
$$RP_{\{hkl\}} = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{\{PF_{exp.}\}_i - \{PF_{calc.}\}_i}{\{PF_{exp.}\}_i}\right| \cdot 100\%$$

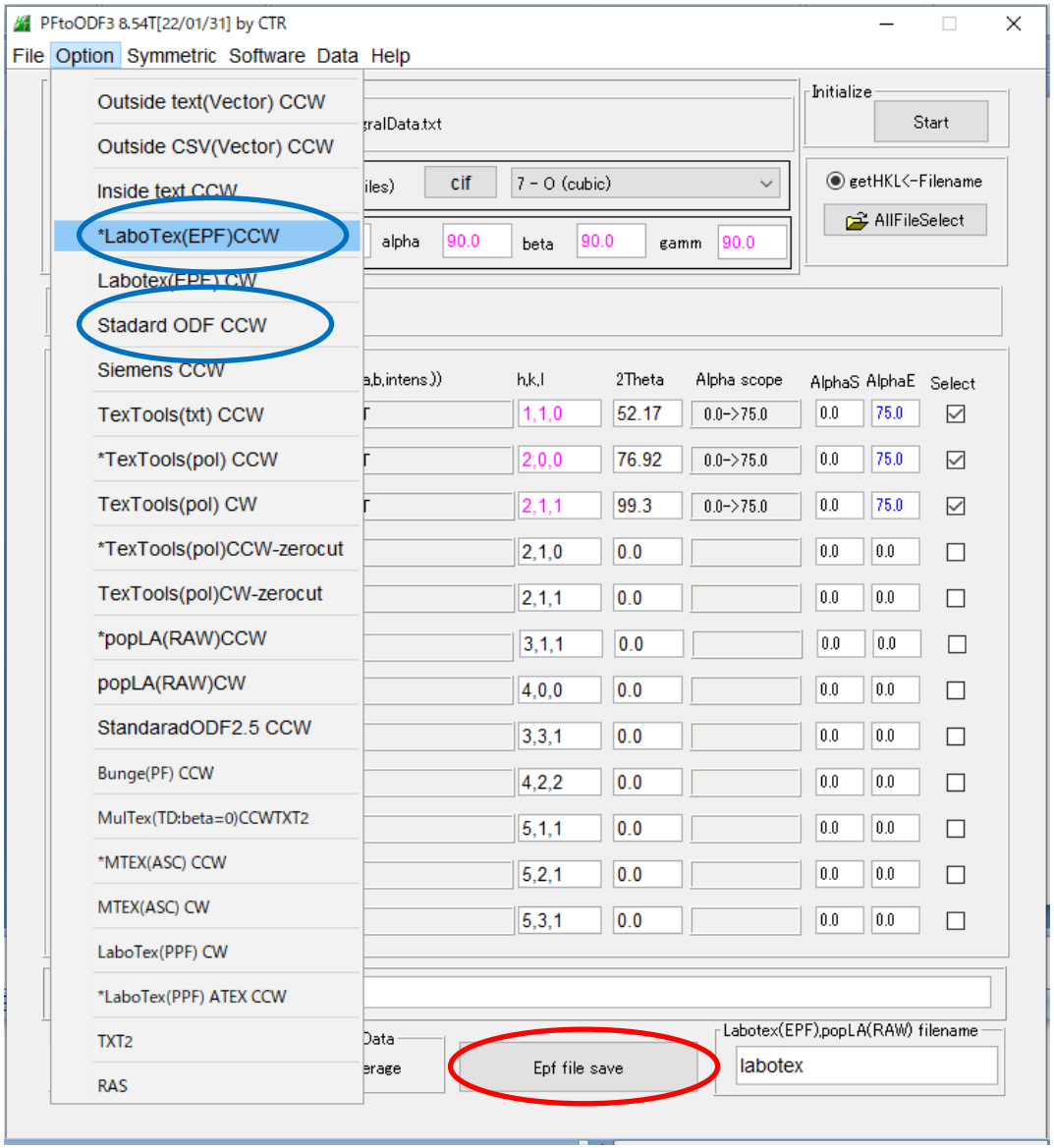




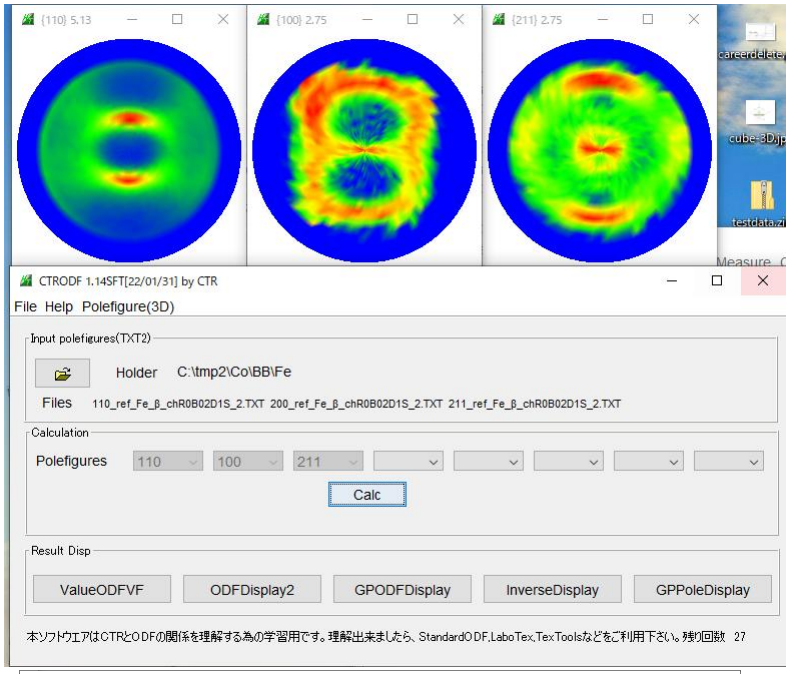
ODF入力データ作成

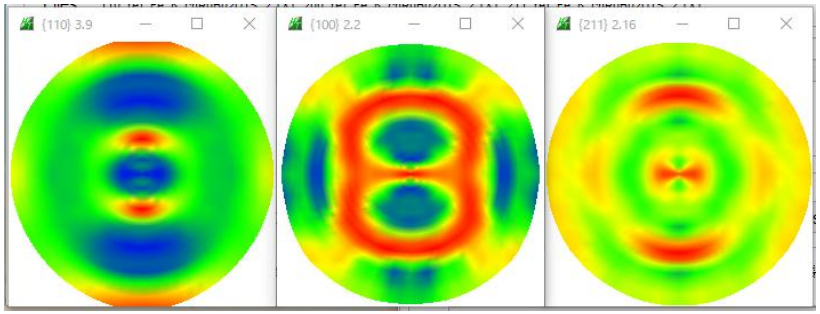

Cancel
Calc
Connect
Exit&ODF
ODF
ValueODFVF-B
ValueODFVF-A

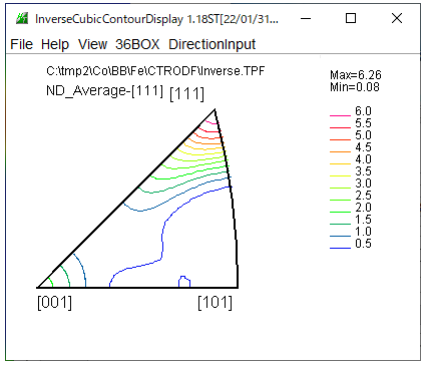

LaboTex
StandardODF
profile_2θ_θ.asc
110_ref_Fe.ras
110_ref_Fe_β.asc
200_ref_Fe.ras
200_ref_Fe_β.asc
211_ref_Fe.ras
211_ref_Fe_β.asc
DefocusMulti.txt
110_ref_Fe_β_chR0B02D1S_2.TXT
200_ref_Fe_β_chR0B02D1S_2.TXT
211_ref_Fe_β_chR0B02D1S_2.TXT

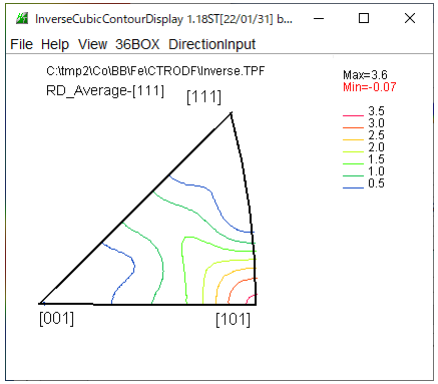

PFtoODF3 8.54T[22/01/31] by CTR
File
Option
Symmetric
Software
Data
Help
Outside text(Vector) CCW
Outside CSV(Vector) CCW
Inside text CCW
*LaboTex(EPF)CCW
Labotex(EPF) CW
Stadard ODF CCW
Siemens CCW
TexTools(txt) CCW
*TexTools(pol) CCW
TexTools(pol) CW
*TexTools(pol)CCW-zerocut
TexTools(pol)CW-zerocut
*popLA(RAW)CCW
popLA(RAW)CW
StandaradODF2.5 CCW
Bunge(PF) CCW
MulTex(TD:beta=0)CCWTXT2
*MTEX(ASC) CCW
MTEX(ASC) CW
LaboTex(PPF) CW
*LaboTex(PPF) ATEX CCW
TXT2
RAS
Initialize
Start
cif
7 - O (cubic)
getHKL<-Filename
AllFileSelect
alpha
90.0
beta
90.0
gamm
90.0
h,k,l
2Theta
Alpha scope
AlphaS
AlphaE
Select
1,1,0
52.17
0.0->75.0
75.0
2,0,0
76.92
2,1,1
99.3
Epf file save
Labotex(EPF),popLA(RAW) filename
labotex

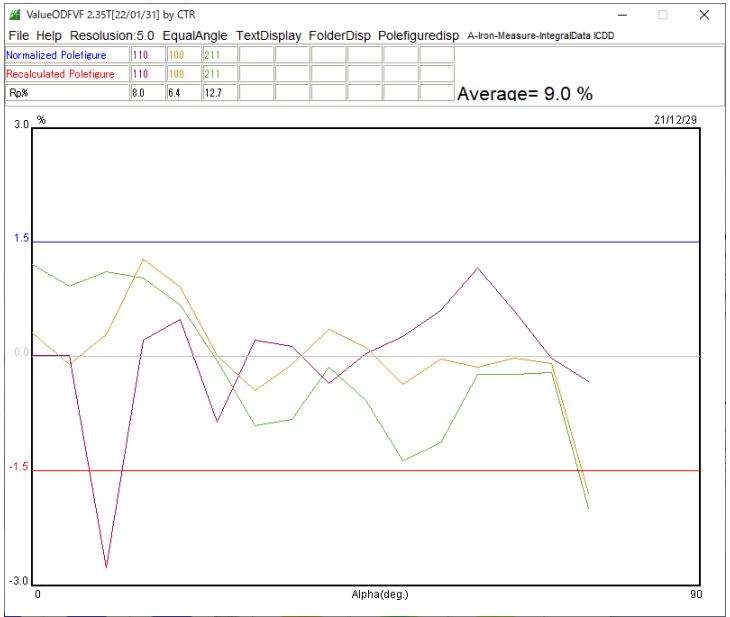
ODF解析の概念

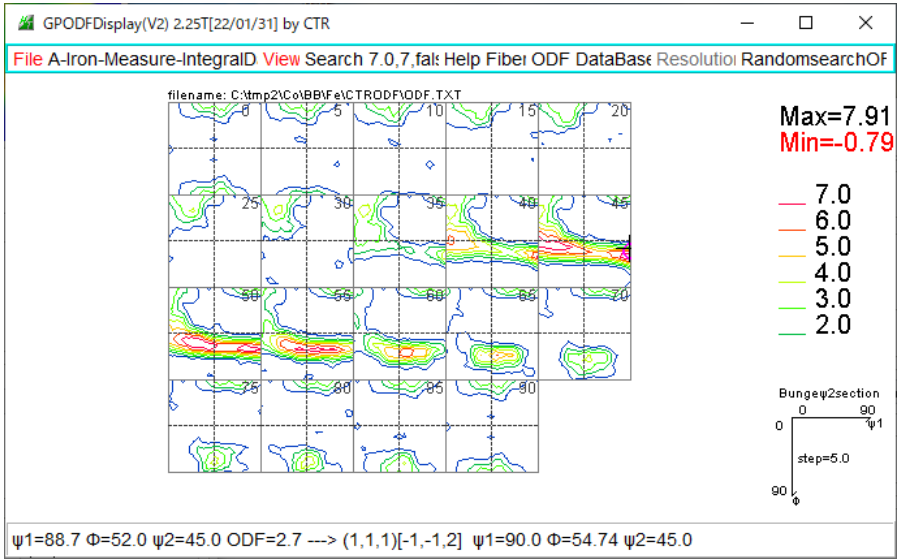

{110} 5.13
{100} 2.75
{211} 2.75
CTRODF 1.14SFT[22/01/31] by CTR
File Help Polefigure(3D)
Input polefigures(TXT2)
Holder C:\tmp2\Co\BB\Fe
Files 110_ref_Fe_β_chR0B02D1S_2.TXT 200_ref_Fe_β_chR0B02D1S_2.TXT 211_ref_Fe_β_chR0B02D1S_2.TXT
Calculation
Polefigures 110 100 211
Calc
Result Disp
ValueODFVF
ODFDisplay2
GPODFDisplay
InverseDisplay
GPPoleDisplay
本ソフトウエアはCTRとODFの関係を理解する為の学習用です。理解出来ましたら、StandardODF,LaboTex,TexToolsなどをご利用下さい。残り回数 27


{110} 3.9
{100} 2.2
{211} 2.16

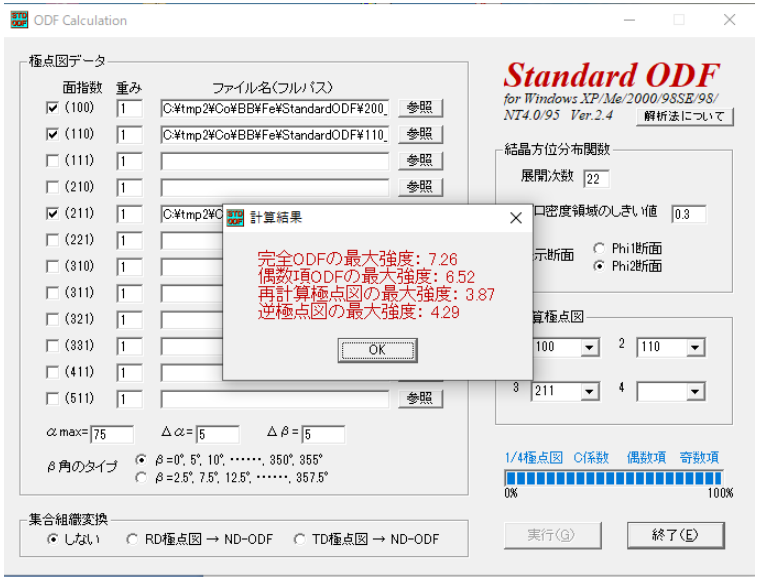

InverseCubicContourDisplay 1.18ST[22/01/31...
File Help View 36BOX DirectionInput
C:\tmp2\Co\BB\Fe\CTRODF\Inverse.TPF
ND_Average-[111] [111]
Max=6.26
Min=0.08
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
[001]
[101]

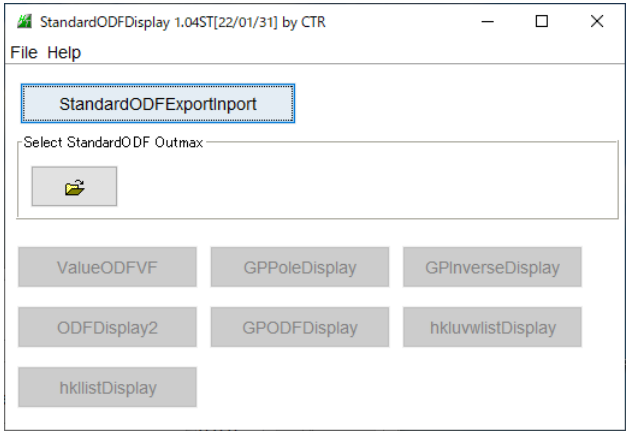

InverseCubicContourDisplay 1.18ST[22/01/31] b...
File Help View 36BOX DirectionInput
C:\tmp2\Co\BB\Fe\CTRODF\Inverse.TPF
RD_Average-[111] [111]
Max=3.6
Min=-0.07
3.5
3.0
2.5
2.0
1.5
1.0
0.5
[001]
[101]


ValueODFVF 2.35T[22/01/31] by CTR
File Help Resolusion:5.0 EqualAngle TextDisplay FolderDisp Polefiguredisp A-Iron-Measure-IntegralData ICDD
Normalized Polefigure 110 100 211
Recalculated Polefigure 110 100 211
Rp% 8.0 6.4 12.7
Average= 9.0 %
21/12/29
3.0
1.5
0.0
-1.5
-3.0
%
0
Alpha(deg.)
90

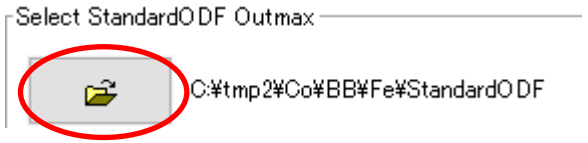

GPODFDisplay(V2) 2.25T[22/01/31] by CTR
File A-Iron-Measure-IntegralD View Search 7.0,7,fals Help Fiber ODF DataBase Resolutio RandomsearchOF
filename: C:\tmp2\Co\BB\Fe\CTRODF\ODF.TXT
Max=7.91
Min=-0.79
7.0
6.0
5.0
4.0
3.0
2.0
Bungeψ2section
step=5.0
ψ1=88.7 Φ=52.0 ψ2=45.0 ODF=2.7 ---> (1,1,1)[-1,-2,2] ψ1=90.0 Φ=54.74 ψ2=45.0

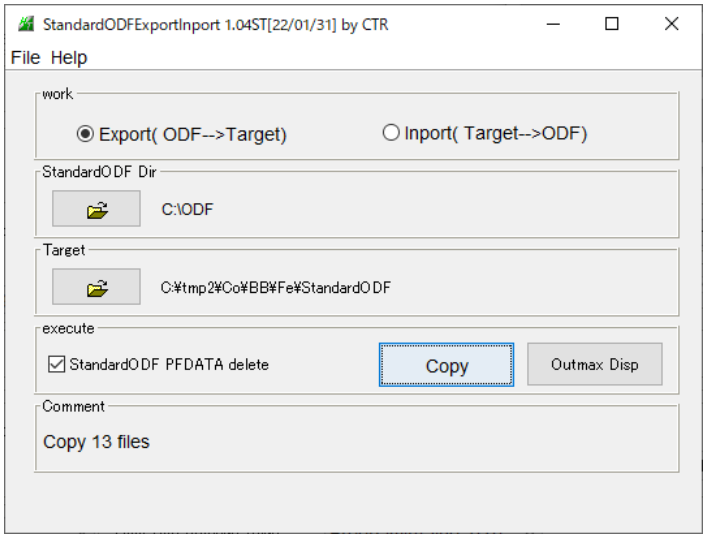
StandardODF解析

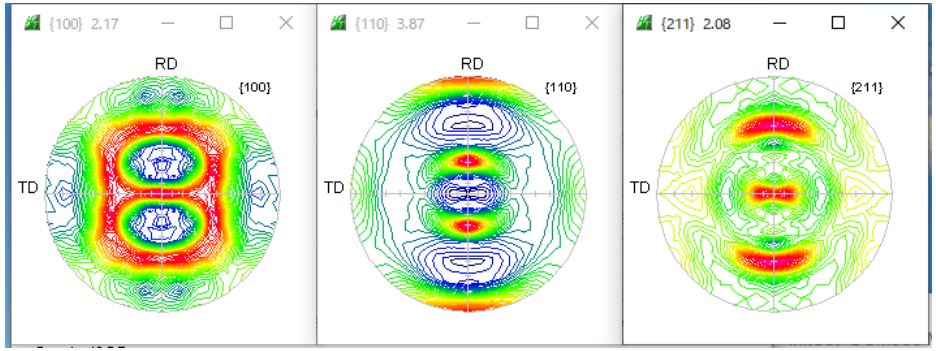




Outmaxを選択

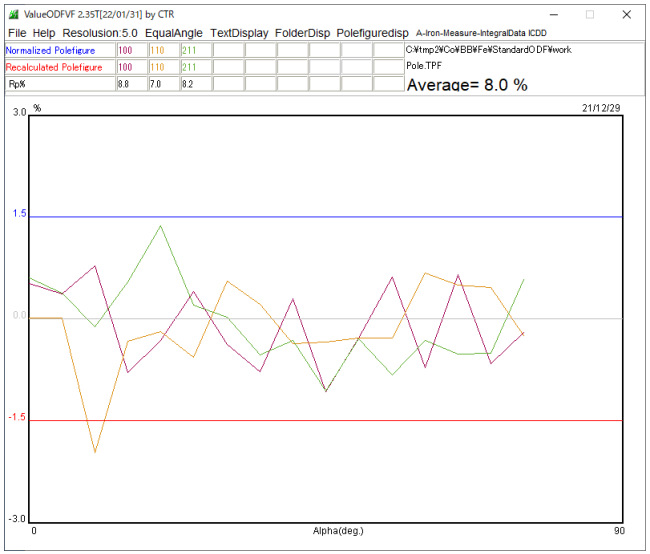


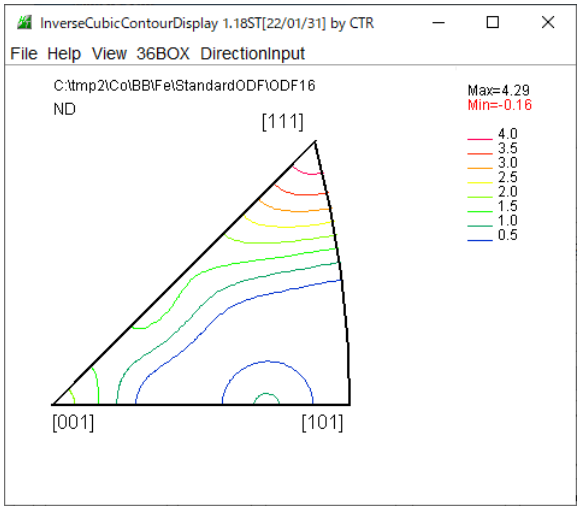


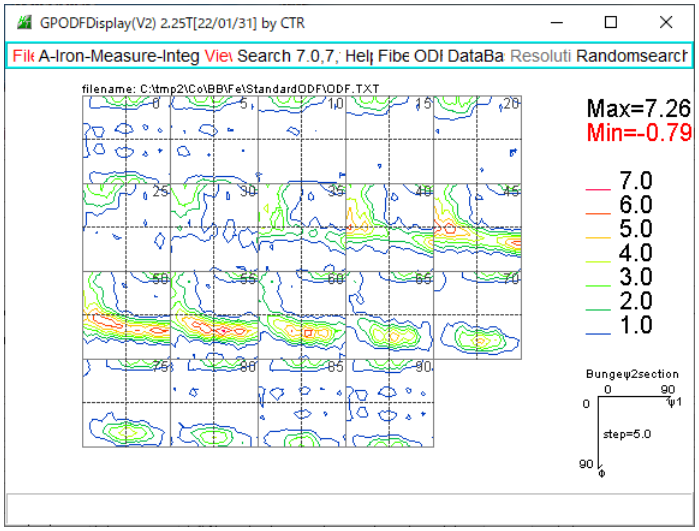


ワークエリアC:￥ODFから解析データの退避

StandardODFの解析

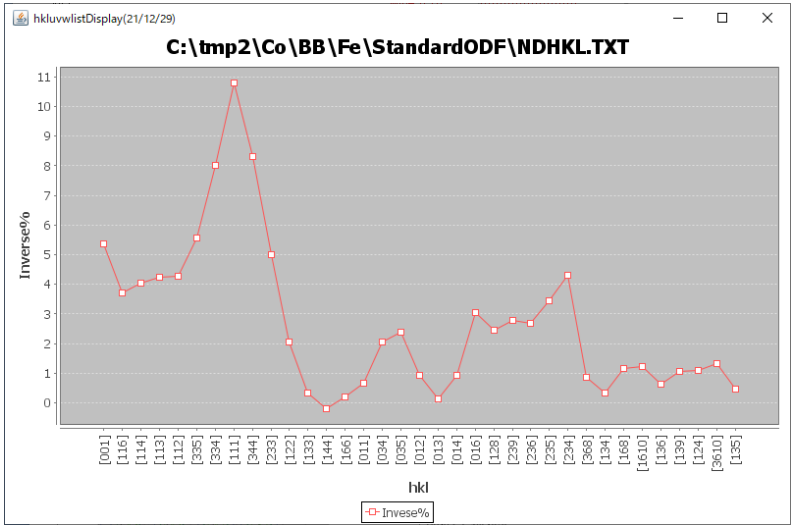






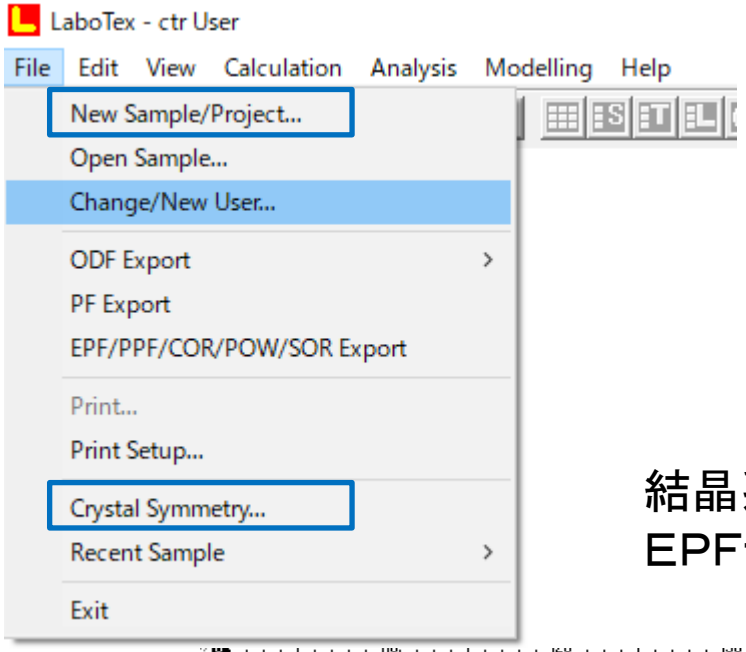

```
Average{hkl}<uvw>,standardodf
{001}<100>,0.64
{101}<-1-21>,0.05
{112}<-1-11>,0.09
{011}<100>,1.54
{001}<1-10>,2.87
{110}<1-11>,0.0
{111}<-1-12>,4.45
{011}<2-55>,0.0
{525}<1-51>,1.34
{013}<100>,0.0
{122}<2-21>,0.91
{113}<1-10>,5.11
{112}<1-10>,5.84
{233}<0-11>,1.36
{111}<0-11>,3.72
{213}<-1-42>,0.0
{132}<6-43>,0.0
{114}<-1-72>,0.53
{4411}<-11-118>,0.26
{001}<2-10>,2.53
{012}<100>,0.94
{113}<-3-32>,0.48
{362}<8-53>,0.02
{011}<5-22>,0.35
```

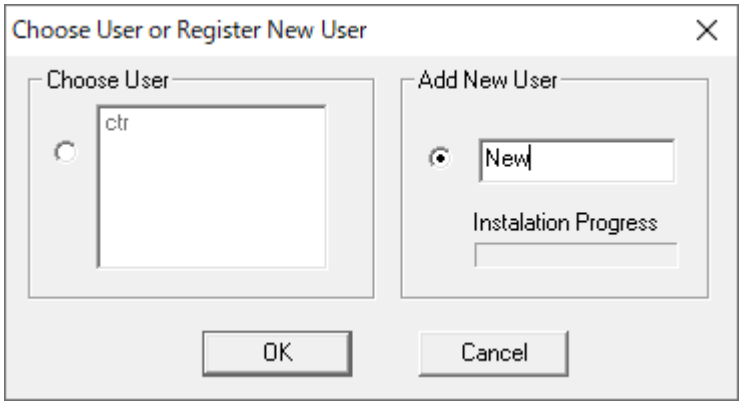
Inverse36Box



LaboTexによる解析

LaboTexでは、解析データを以下の階層で管理しています
User－結晶系－Project－sample名



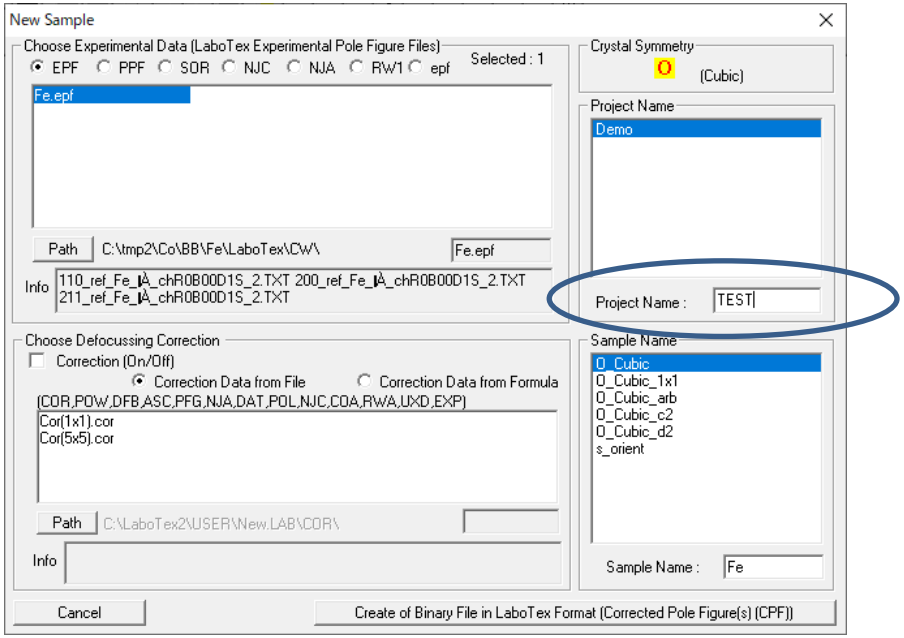


結晶系じは変更しなければCubicで扱われる
EPFデータを読み込むと、EPFの結晶系に登録

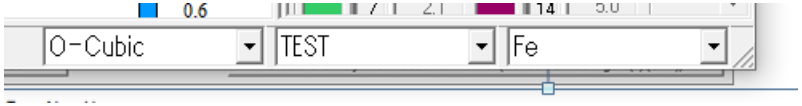
```
110_ref_Fe_β_chROBOOD1S_2.TXT 200_ref_Fe_β_chROBOOD1S_2.TXT 211_ref_Fe_β_chRO
BOOD1S_2.TXT ↓
↓
Structure Code a     b     c     alfa    beta    gamma↓
    7    1.0    1.0    1.0    90.0    90.0    90.0↓
3↓
2Theta    alf-s    alf-e    d-alf    bet-s    bet-e    d-bet   index  H K L  P/B↓
52.17    0.0    75.0    5.0    0.0    355.0    5.0    0    1 1 0    1↓
76.92    0.0    75.0    5.0    0.0    355.0    5.0    0    2 0 0    1↓
99.3    0.0    75.0    5.0    0.0    355.0    5.0    0    2 1 1    1↓
```

EPFファイルの読み込みは、New Sampleで読み込む

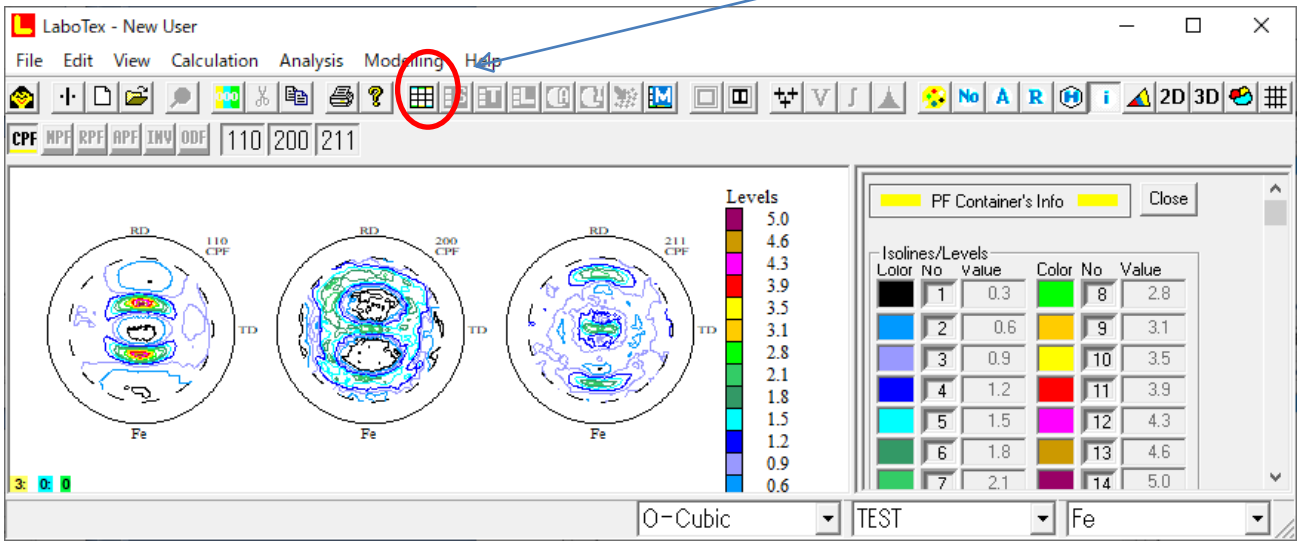
LaboTexの解析



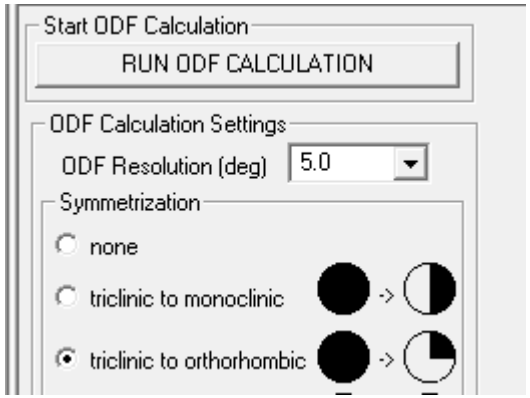
結晶系　　Project　　sample名

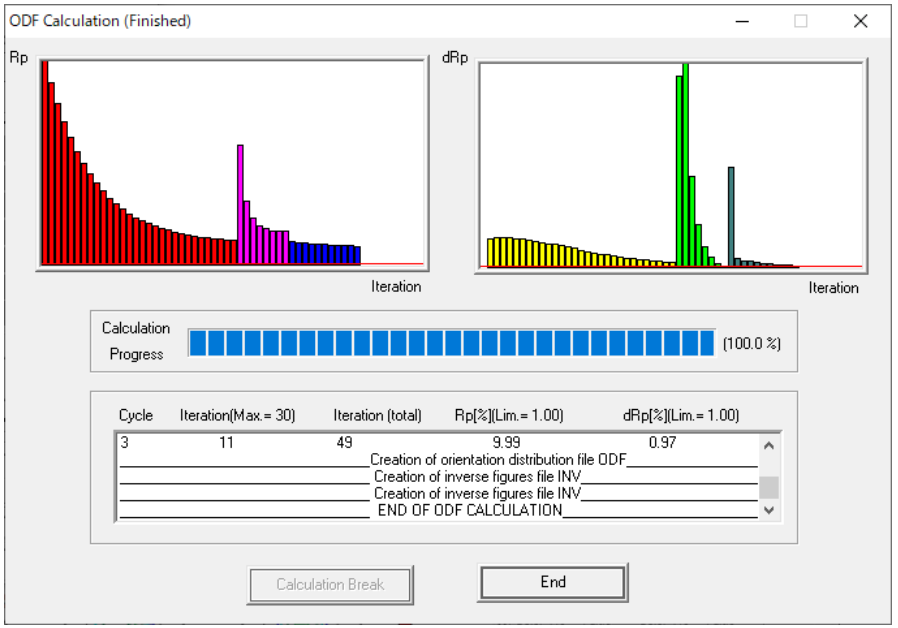


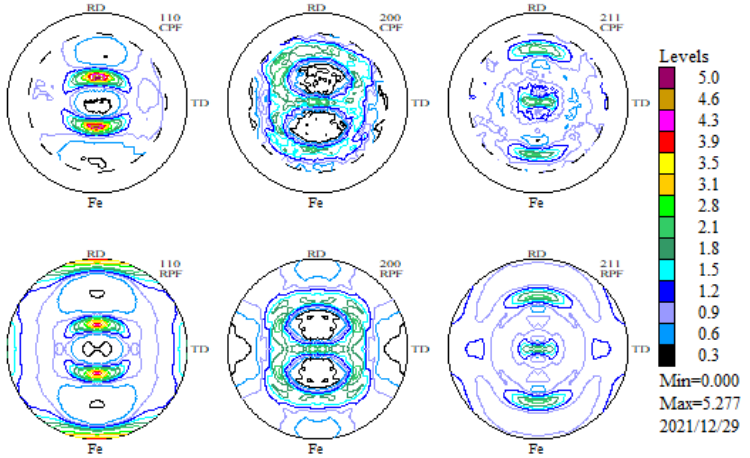
ODF解析は碁盤の目をクリック

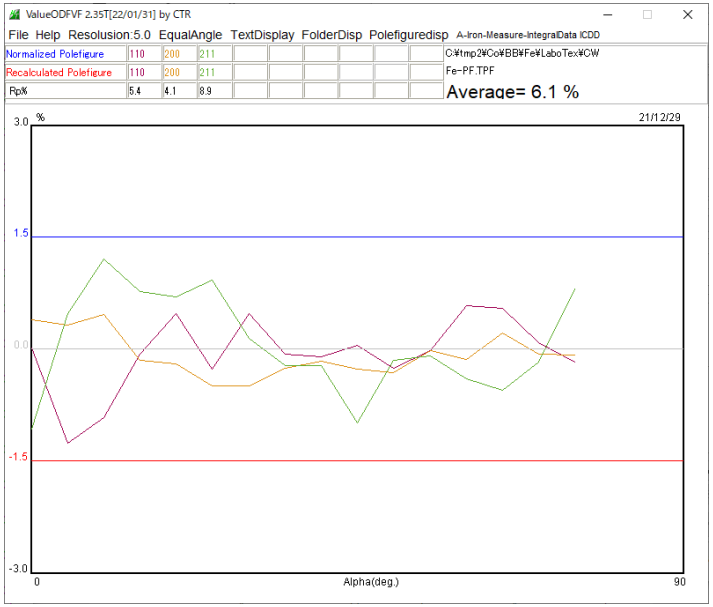


LaboTexの解析

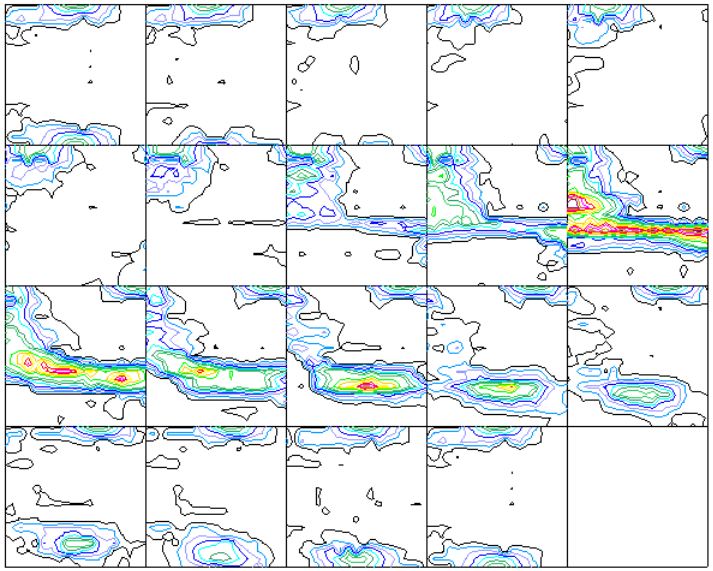

Start ODF Calculation
RUN ODF CALCULATION
ODF Calculation Settings
ODF Resolution (deg)
5.0
Symmetrization
none
triclinic to monoclinic
triclinic to orthorhombic

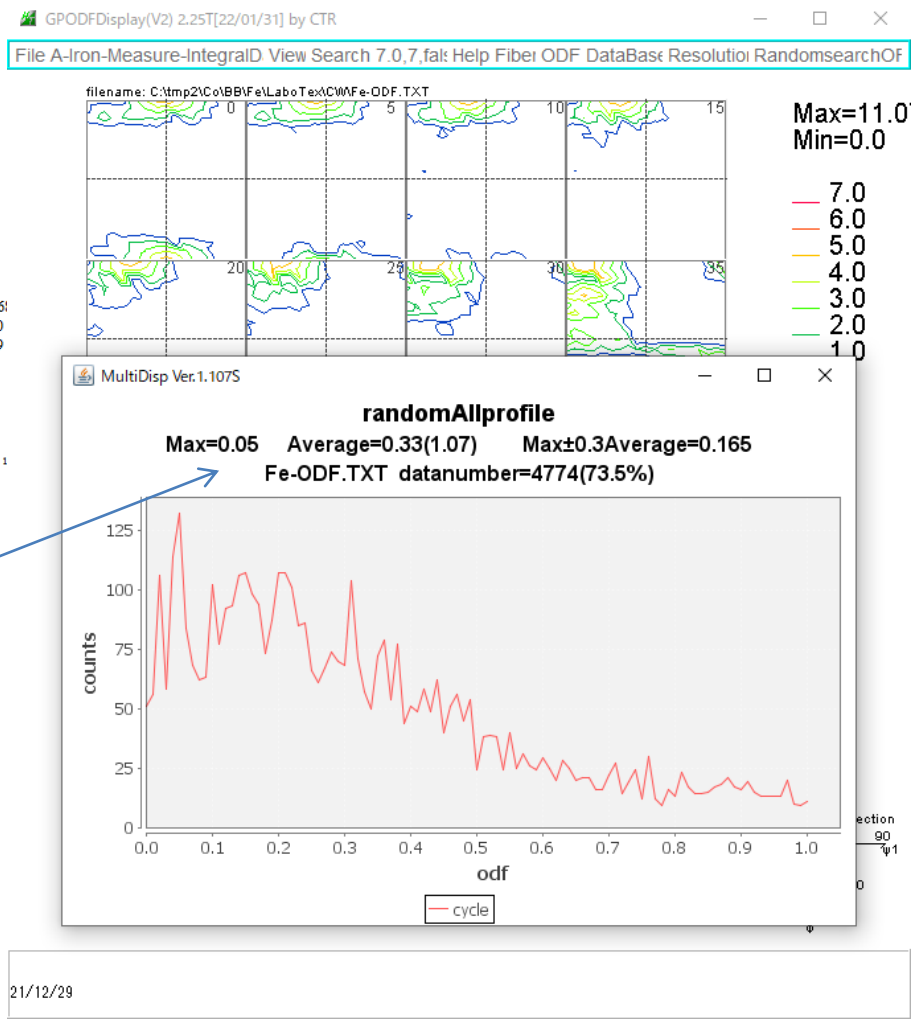

ODF Calculation (Finished)
Rp
dRp
Iteration
Iteration
Calculation Progress
(100.0 %)
Cycle
Iteration(Max.= 30)
Iteration (total)
Rp[%](Lim.= 1.00)
dRp[%](Lim.= 1.00)
3
11
49
9.99
0.97
Creation of orientation distribution file ODF
Creation of inverse figures file INV
Creation of inverse figures file INV
END OF ODF CALCULATION
Calculation Break
End

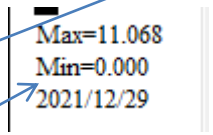

RD
110 CPF
200 CPF
211 CPF
TD
Fe
110 RPF
200 RPF
211 RPF
Levels
5.0
4.6
4.3
3.9
3.5
3.1
2.8
2.1
1.8
1.5
1.2
0.9
0.6
0.3
Min=0.000
Max=5.277
2021/12/29


ValueODFVF 2.35T[22/01/31] by CTR
File Help Resolusion:5.0 EqualAngle TextDisplay FolderDisp Polefiguredisp
Normalized Polefigure
Recalculated Polefigure
Rp%
Average= 6.1 %
21/12/29
3.0
1.5
-1.5
-3.0
0
90
Alpha(deg.)

LaboTexの解析(random評価）

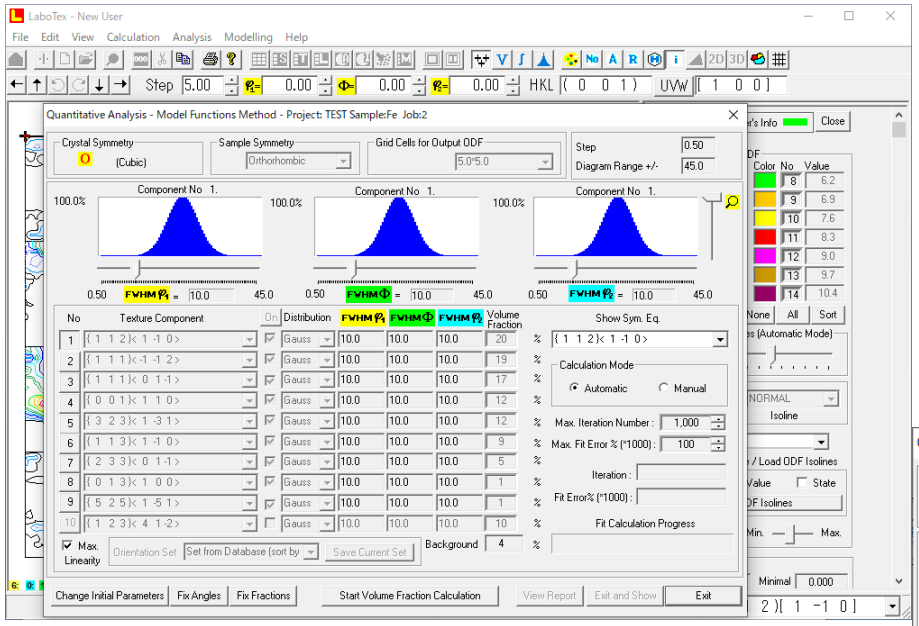




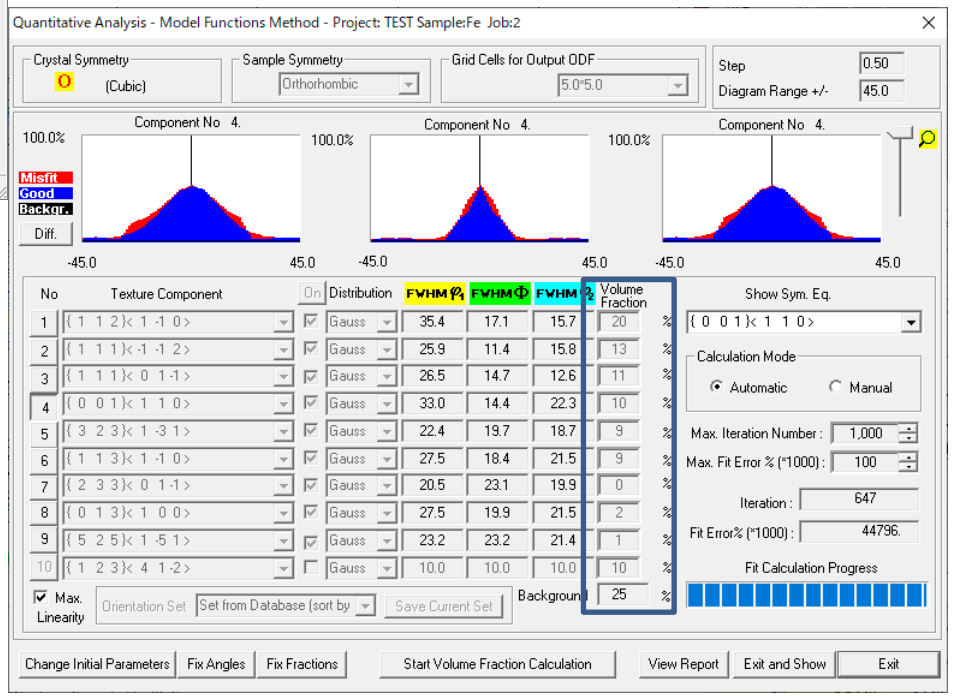


Random成分は存在しない。

LaboTexの解析(VolumeFractionを求める）



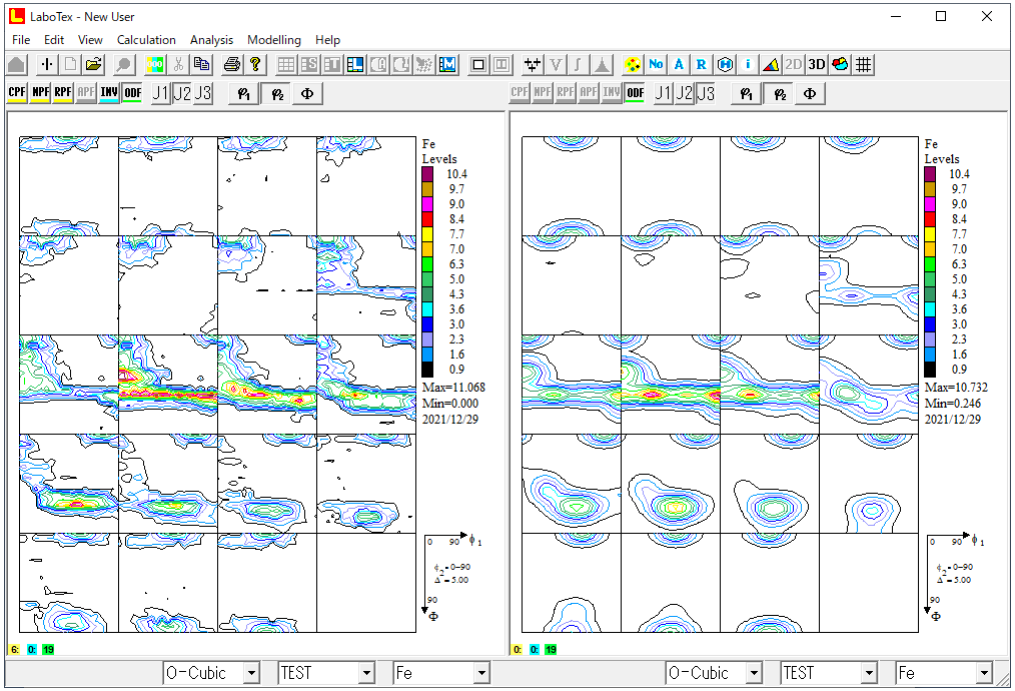
内部に登録された方位に対してVF%を求める
足りない場合はDataBaseに追加する

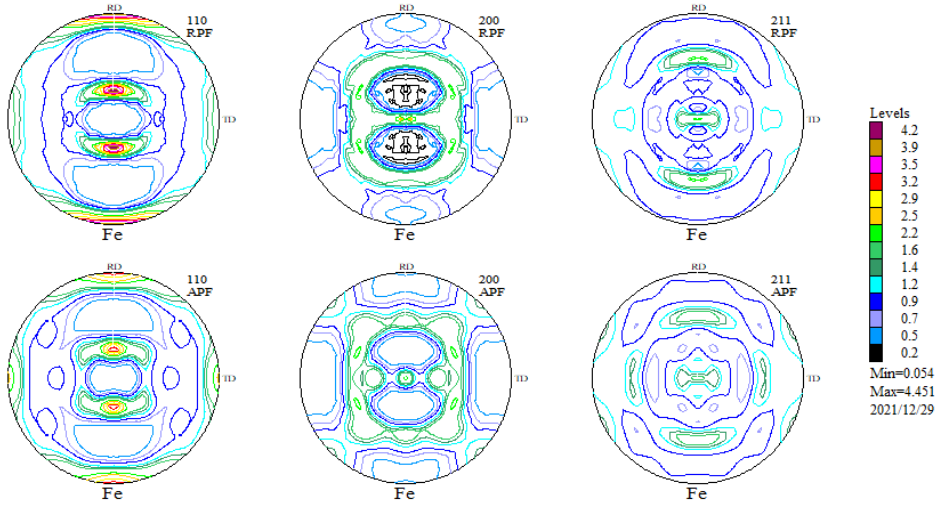


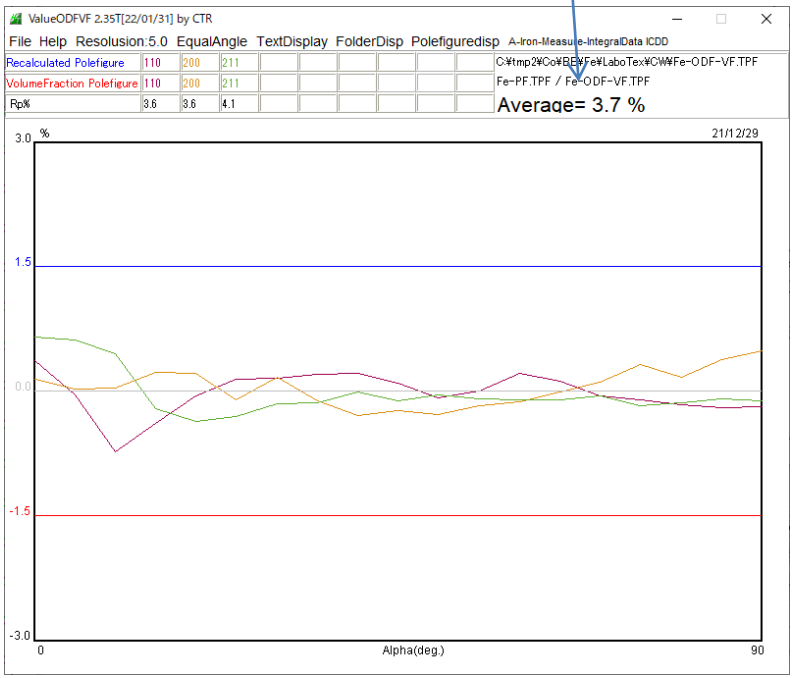
Errorの変化が小さくなったら計算を中止する

LaboTexの解析（VolumeFractionのRp%）

VolumeFractionの一致度を評価







LaboTex(VolumeFraction)

C:) › LaboTex2 › USER › New.LAB › O-Cubic.LAB › TEST.LAB › Fe.LAB › Job03

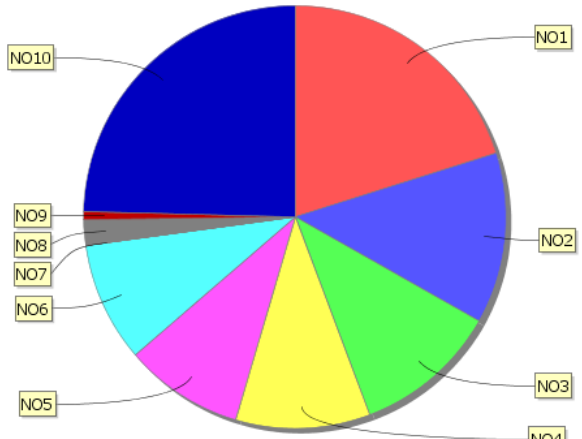
名前	更新日時	種類	サイズ
Fe.APF	2021/12/29 14:26	APF ファイル	6 KB
Fe.ODF	2021/12/29 14:22	ODF ファイル	27 KB
Fe.POD	2021/12/29 14:24	POD ファイル	2 KB

ODFVFGraph 1.12T[22/01/31] by CTR

File Help

Job JOB3 Sample : Fe Project : TEST

2:	13.05	25.9	11.4	15.8	{ 1 1 1 }< -1	-1	2 >
3:	11.07	26.5	14.7	12.6	{ 1 1 1 }< 0	1	-1 >
4:	10.31	33.0	14.4	22.3	{ 0 0 1 }< 1	1	0 >
5:	9.11	22.4	19.7	18.7	{ 3 2 3 }< 1	-3	1 >
6:	9.12	27.5	18.4	21.5	{ 1 1 3 }< 1	-1	0 >
7:	0.01	20.5	23.1	19.9	{ 2 3 3 }< 0	1	-1 >
8:	1.96	27.5	19.9	21.5	{ 0 1 3 }< 1	0	0 >
9:	0.67	23.2	23.2	21.4	{ 5 2 5 }< 1	-5	1 >
10:	24.56	Background Volume Fraction					



BCCSchmidFactorCalc3 3.03T[22/01/31] by CTR

File Help Text SlipProfile

InputFile(TXT)

LaboTex VolumeFraction(SumVFmode) {1 1 0}<1 -1 2> 100.0

C:\LaboTex2\USER\New.LAB\O-Cubic.LAB\TEST.LAB\Fe.LAB\Job03\Fe.POD Disp DISP

Slip Systems

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

Data input

[h k l] or [h k l] ND Input

[h k l]<u v w> Input

phi1 PHI phi2 Input

{1 1 2}<1 -1 0> 20.13
{1 1 1}<-1 -1 2> 13.05
{1 1 1}<0 1 -1> 11.07
{0 0 1}<1 1 0> 10.31
{3 2 3}<1 -3 1> 9.11
{1 1 3}<1 -1 0> 9.12
{2 3 3}<0 1 -1> 0.01
{0 1 3}<1 0 0> 1.96
{5 2 5}<1 -5 1> 0.67

0.045 -0.045 0.151 -0.106
-0.423 0.0 0.423

input	VF%	Schmid	VF*Schmid%
{1.01.02.0}<1.0-1.00.0>	20.13	0.408	0.082
{1.01.01.0}<-1.0-1.02.0>	13.05	0.272	0.036
{1.01.01.0}<0.01.0-1.0>	11.07	0.272	0.03
{0.00.01.0}<1.01.00.0>	10.31	0.408	0.042
{3.02.03.0}<1.0-3.01.0>	9.11	0.371	0.034
{1.01.03.0}<1.0-1.00.0>	9.12	0.445	0.041
{2.03.03.0}<0.01.0-1.0>	0.01	0.371	0.0
{0.01.03.0}<1.00.00.0>	1.96	0.49	0.01
{5.02.05.0}<1.0-5.01.0>	0.67	0.423	0.003

VFsum=75.43% VF*Schmidsum=0.277

SchmidFactor(SumVF)=0.367

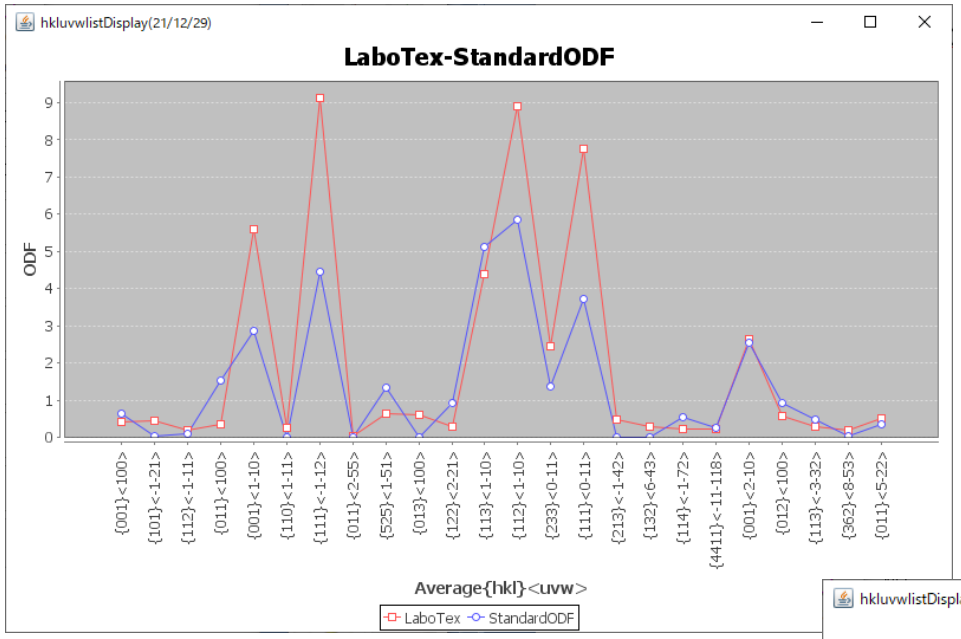
AlongRD(X) 3 0 AlongTD(Y)<=0 2 0 AlongND(Z) 1 0 4 0

SlipDisp Schmidcalc Symmetry SchmidCalc SchmidFDisp

SchmidFactorProfile ND->RD all Step 1

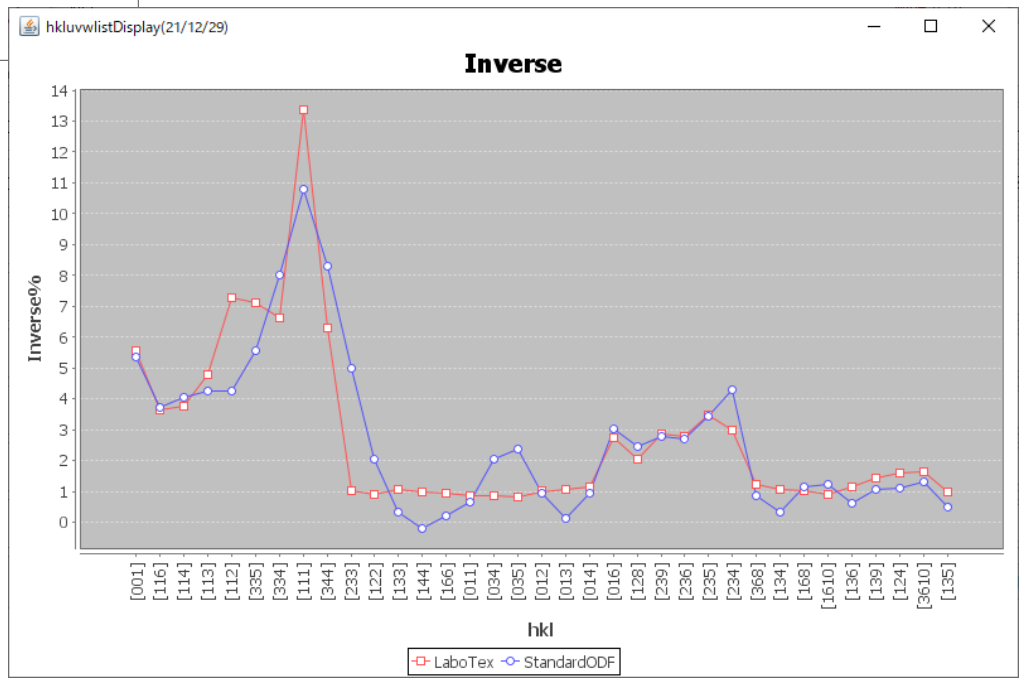
AXISROtation HKLDouble

LaboTex vs StandardODF



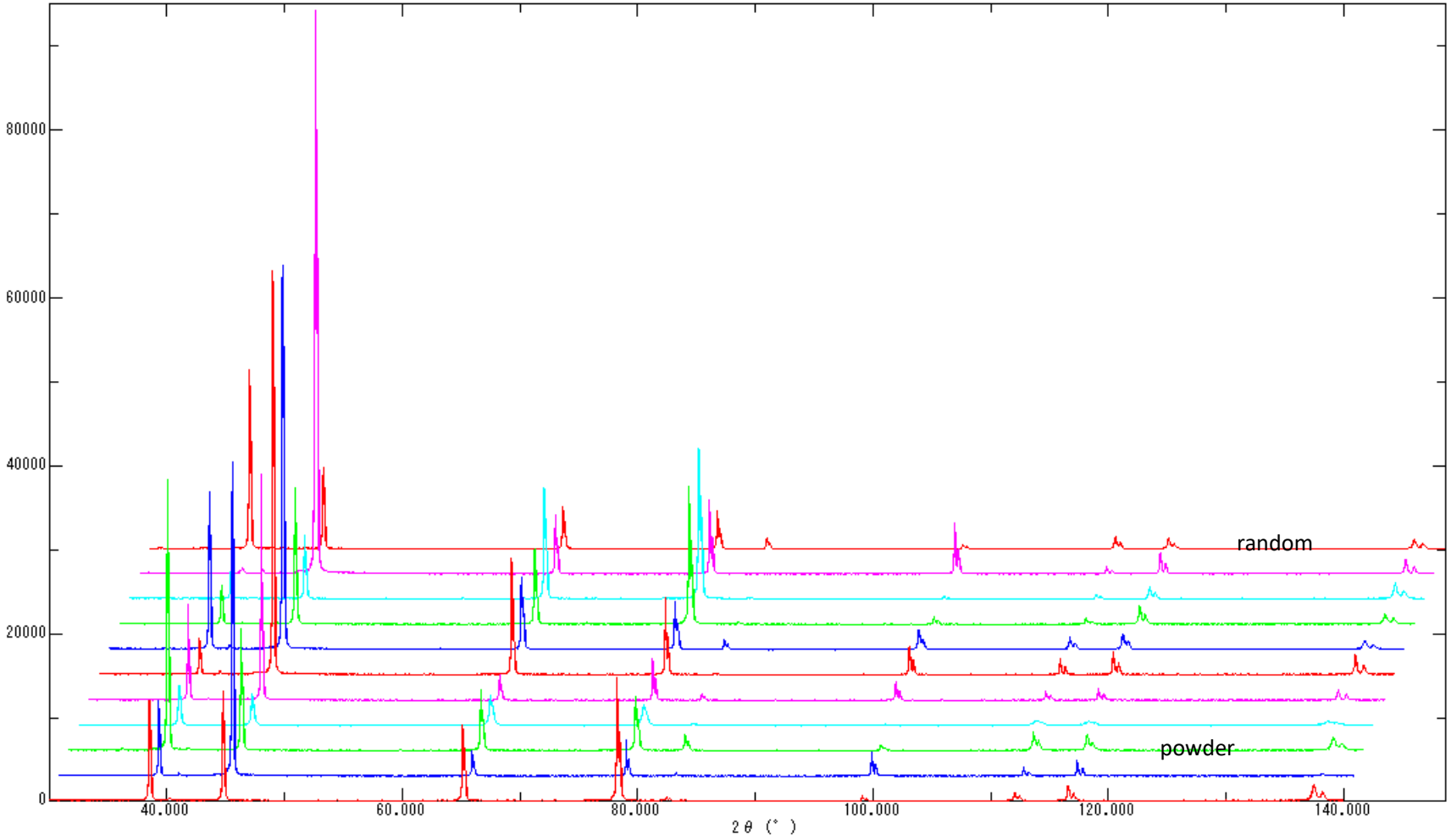
GPODFDisplayで解析した方位分布図
最大8データ比較が可能

GPInverseで解析した36Box
方位分布図、最大8データ比較

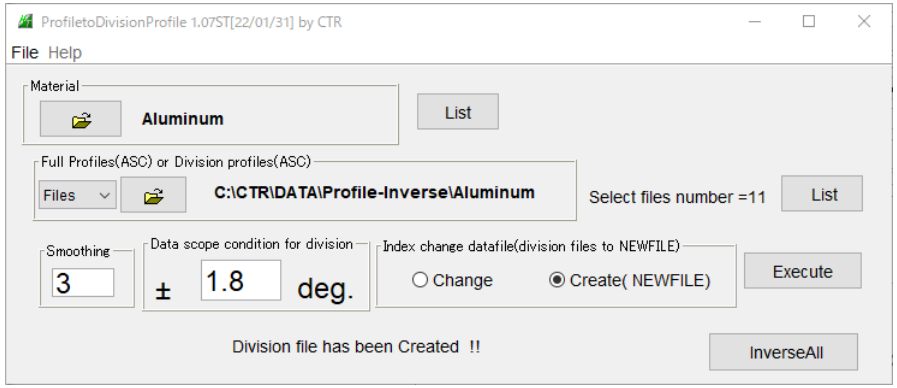


θ／θプロファイルからND方位

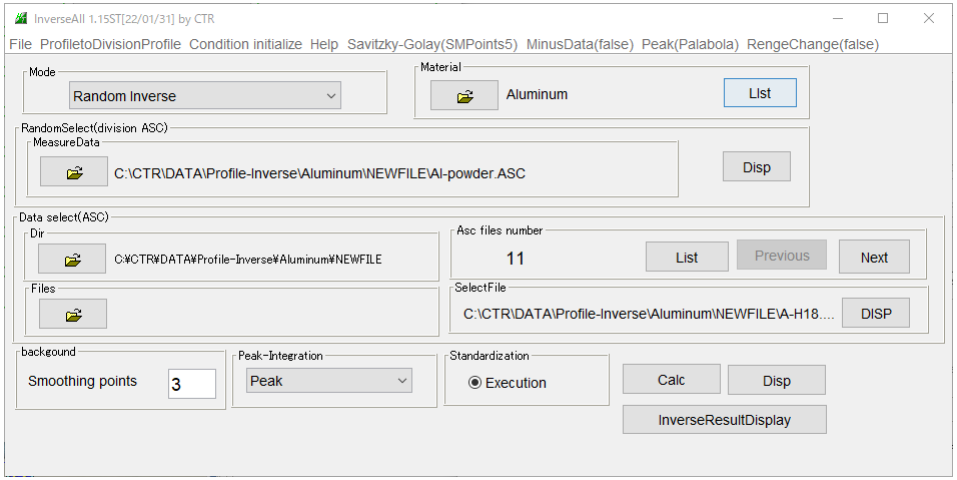
Randomサンプルとの強度比からND方向の逆極点を計算
サンプルチェンジャーなどで測定したデータの一括処理



プロファイルを分割

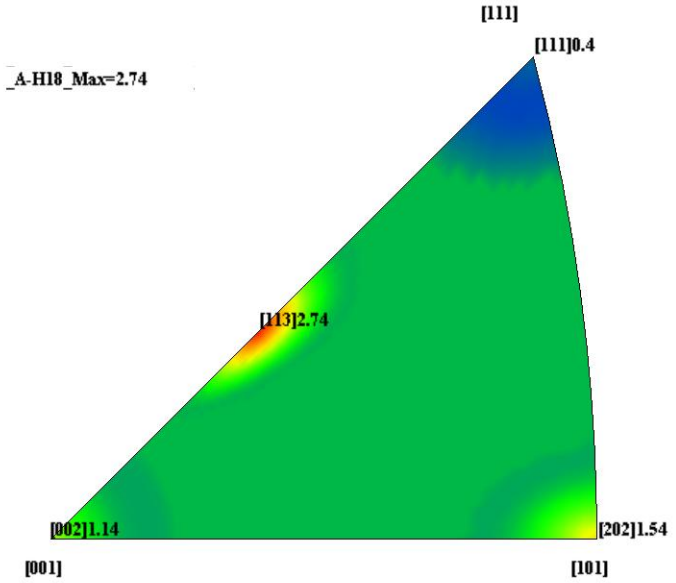


相対強度比率を計算



Randommode Standardization Savitzky-Golay(SMpoinrts5) BGsmpoints=3 PEAK peakPalabola5 Minusdata-OFF

	[111]	[200]	[220]	[311]	[222]	[400]
A-H18	0.475	1.147	1.542	2.743	0.329	1.129
A-T4	0.313	2.898	0.426	0.713	0.195	4.888
Al-powder	1.013	1.007	0.967	0.968	0.96	0.981
B-H18	0.638	1.12	2.036	1.491	0.426	0.849
B-O	0.449	2.413	0.548	0.923	0.549	4.239
C-Bach	0.102	2.701	1.489	1.062	0.056	4.235
C-CAL	0.446	2.457	0.881	0.647	0.443	2.81
D-H14	0.193	1.528	1.604	3.196	0.117	1.859
D-H18	0.178	0.769	2.601	3.9	0.097	0.64
D-O	0.012	3.349	0.633	0.869	0.034	6.276
random-plate	1.0	1.0	1.0	1.0	1.0	1.0



データ蓄積によるdatabaseの検索

同一測定条件で測定しDatabaseを構築
カテゴリー別に登録すると高速検索が可能
新しいデータでDataBaseを検索
極点図のプロファイル化も可能

データ比較