

極点データ処理(VolumeFractionの為)

ソフトウェア 4 種類 ODFPoleFigure1_5(S), ODFPoleFigure2(S)

バックグラウンド処理 (バックグラウンドの最適化)

RD処理

吸収補正

D e f o c u s 補正

内部データベースによる D e f o c u s 補正(ODFPoleFigure2)

平滑化 (定量時使用しない)

規格化

最適化Rp% (ODFPoleFigure2)

複数極点図の平均化 (S)

以降、ODFPoleFigure2Sについて説明を行う

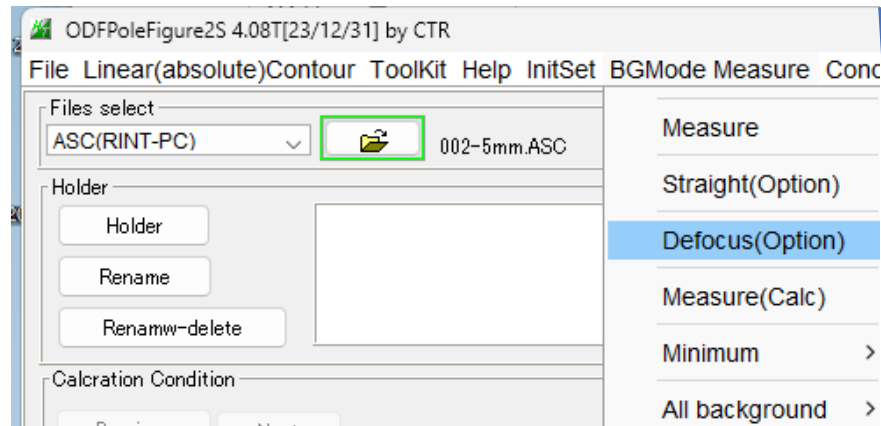
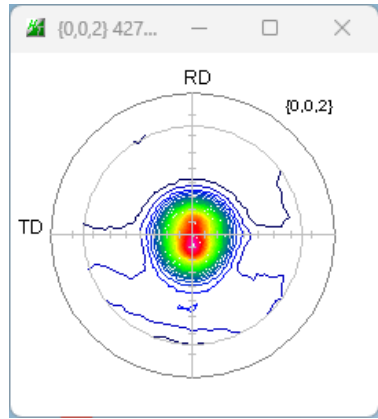
ODFPoleFigure2S

The screenshot shows the ODFPoleFigure2S software interface with the following settings and annotations:

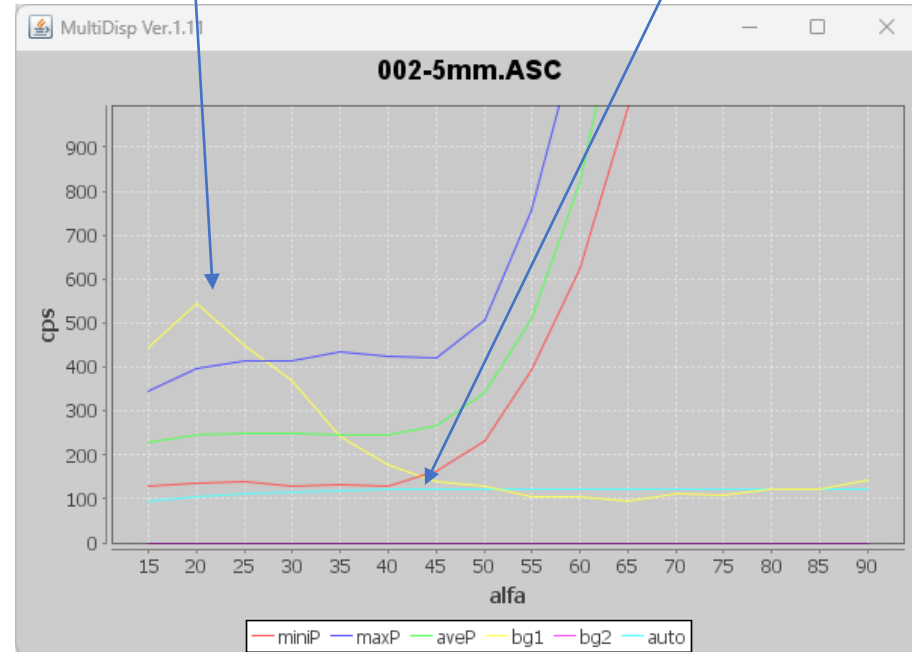
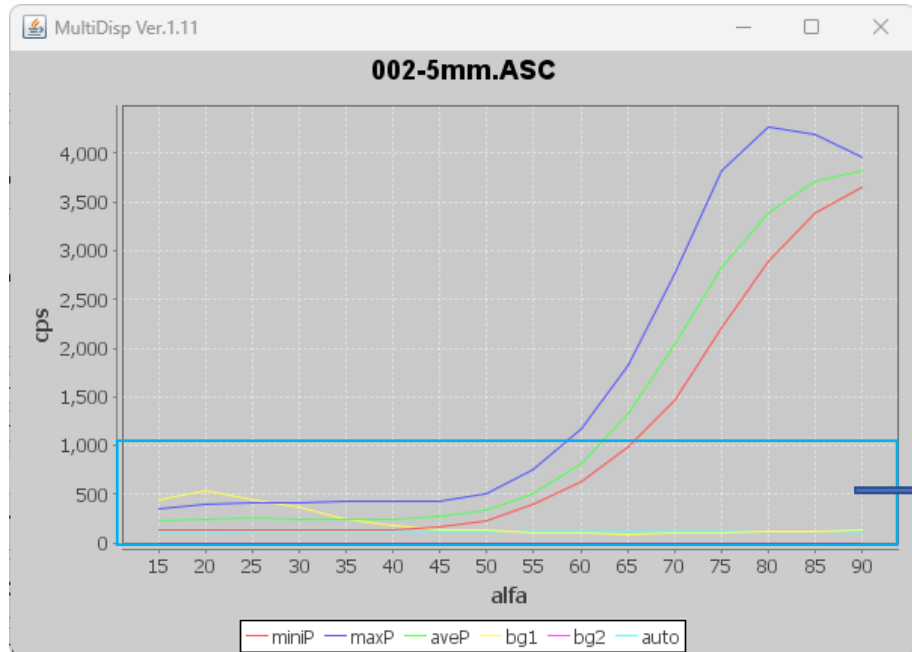
- Files select:** ASC(RINT-PC) (Annotation: バックグラウンドの平滑化)
- Holder:** Holder (Annotation: 平均化を行う局点図の複数枚の選択)
- Calculation Condition:**
 - Background delete mode: Nothing (Annotation: バックグラウンド処理)
 - BG defocus: DSH1.2mm+Schulz+RSH5mm (Annotation: 吸収補正処理)
 - defocus補正処理 (Annotation: defocus補正処理)
 - Smoothing: + α 3 Arithmetic mean (Annotation: 平滑化処理)
 - RD: 0.0 Interpolation Full (Annotation: RD処理)
- AbsCalc:**
 - Ref: Trans: Schulz reflection method
 - Absorption coefficient: 133.0 1/cm
 - Thickness: 0.2 cm
 - 2Theta: 0.0 deg. 1/Kt Profile
- Defocus file:**
 - Select Transmission defocus HKL+T: Defocus(1) functions file (Annotation: Random試料defocus処理)
 - Make defocus function files by TXT2: Files (Annotation: Defocusデータベース処理)
 - Limit Alfa Defocus value: Free(LimitValue=0.0) (Annotation: 最適化Rp%)
 - Defocus(3) function files folder: BB285mm-Slit-1mm-7mm
 - Defocus(2) function files folder: DSH1.2mm+Schulz+RSH5mm
 - Search minimum Equal Angle Rp%(Cubic only)
 - 1/Ra Profile
- Smoothing for ADC:**
 - Cycles: 2 Weight: 10 (Annotation: 平滑化処理)
 - Normalization: CTR Connect Average
 - CenterData: Average
 - OutFiles: ASC MTexAsc Ras TXT TXT2
- Buttons:** ValueODFVF-B, ValueODFVF-A, Average, Exit&ODF, ODF, ALLODFFiles
- Footer:** CTRHome : C: Select crystal : Cubic 23/04/10 (Annotation: Rp%の確認)
- Bottom Right:** 複数極点図の平均化

バックグラウンド処理

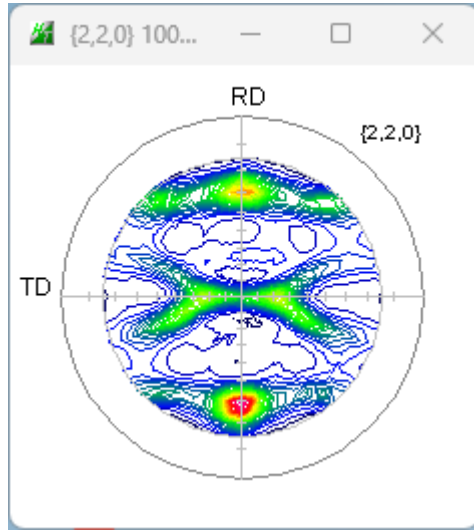
Mgの{002}の測定、バックグラウンド(黄色) が外周部で盛り上がりが見られる



バックグラウンドをDefocus(水色) モードで修正
バックグラウンドもdefocusの影響を受ける

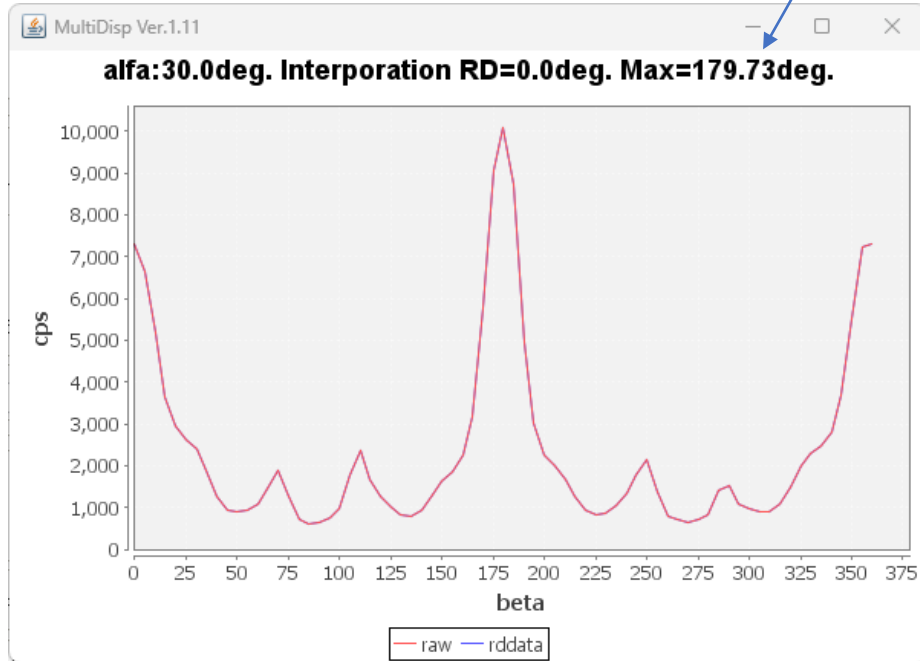
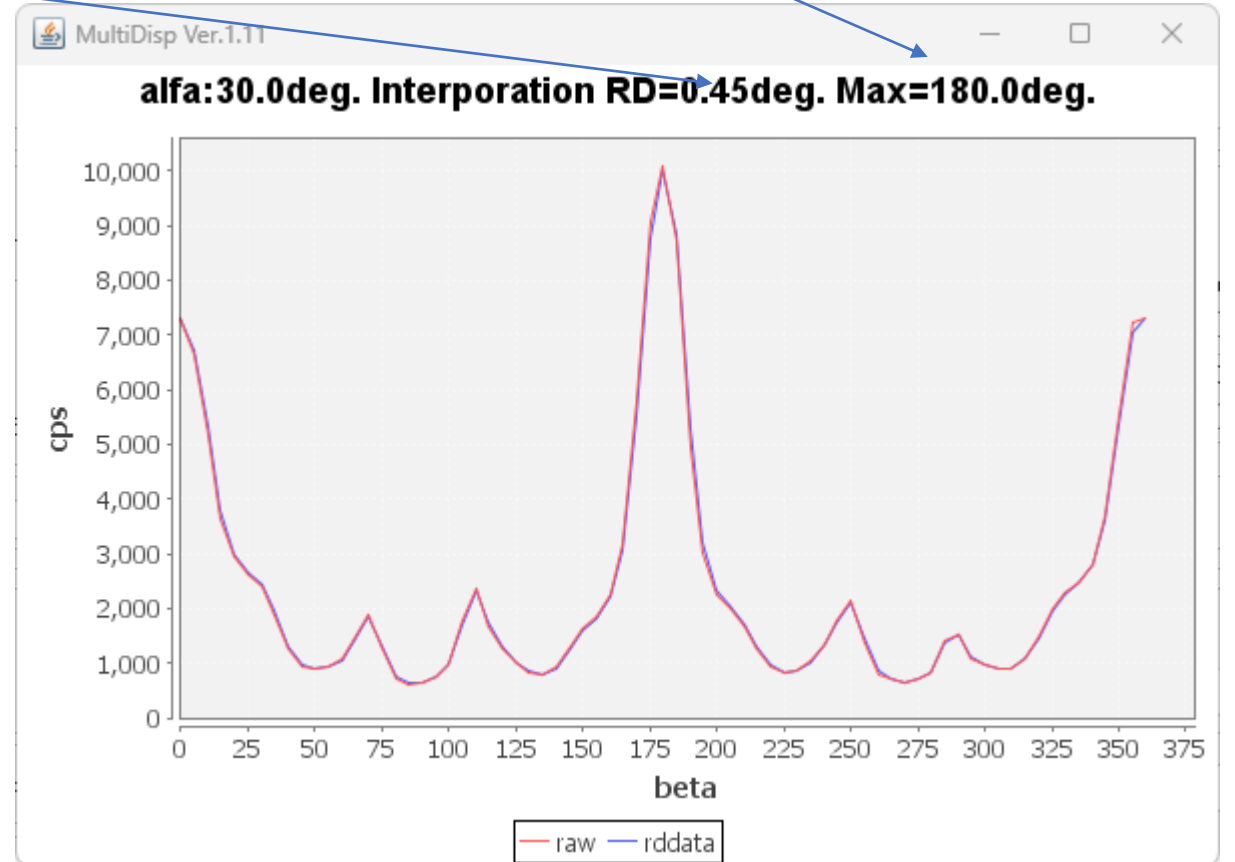
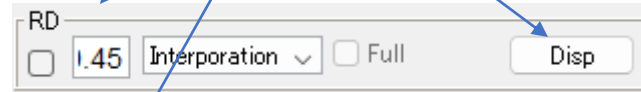


RD処理



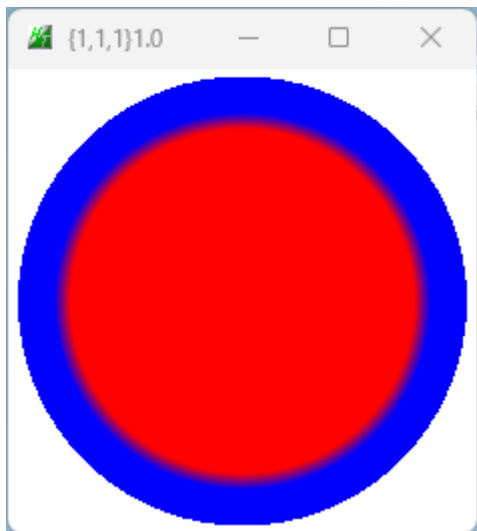
最大極密度位置の確認(179.73deg)

RD入力によりMax位置(180deg)の確認でRD補正値が得られる

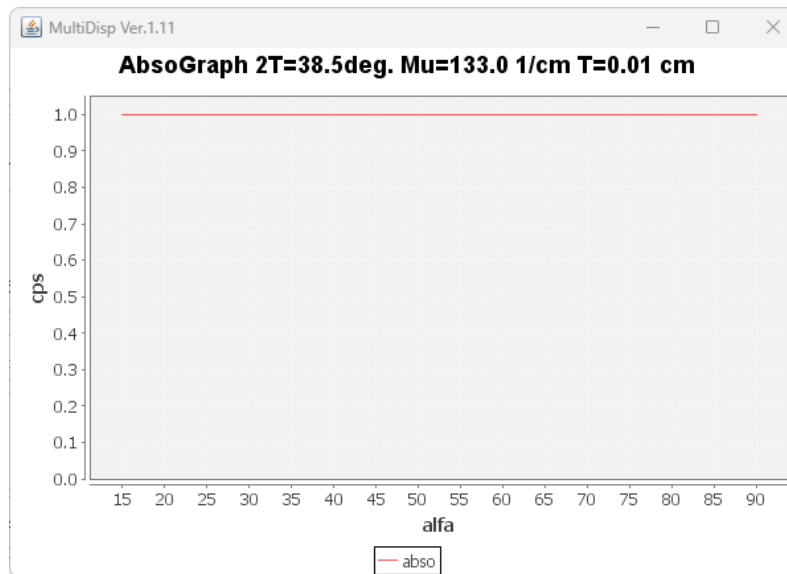


吸収補正

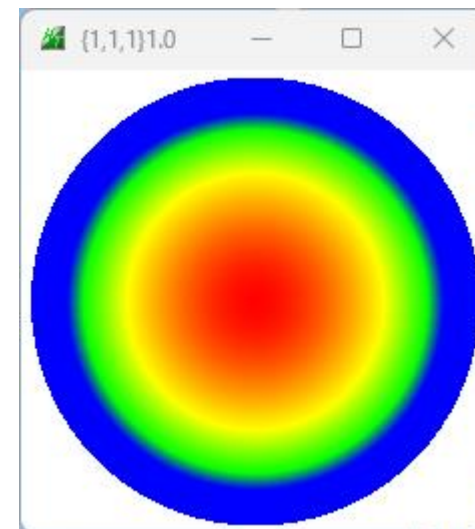
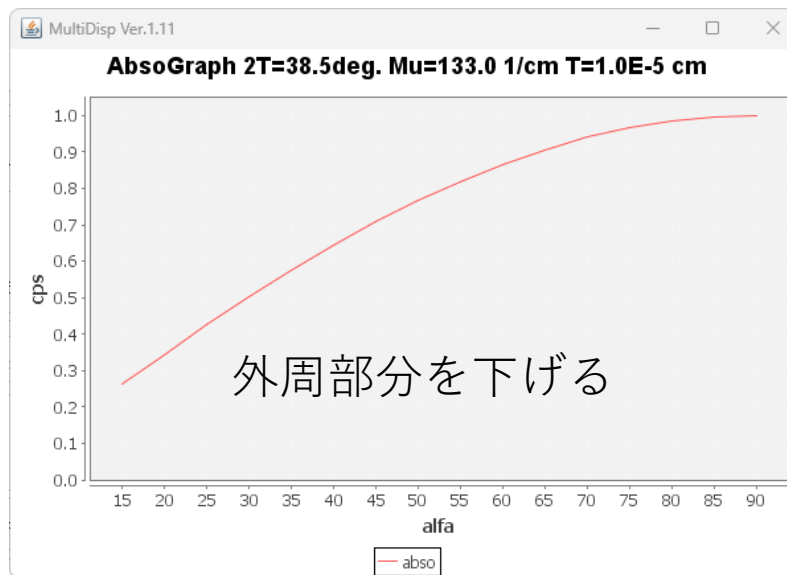
Absorption coefficient 1/cm Thickness mm 2Theta deg. 1/Kt



Thickness mm



Thickness um

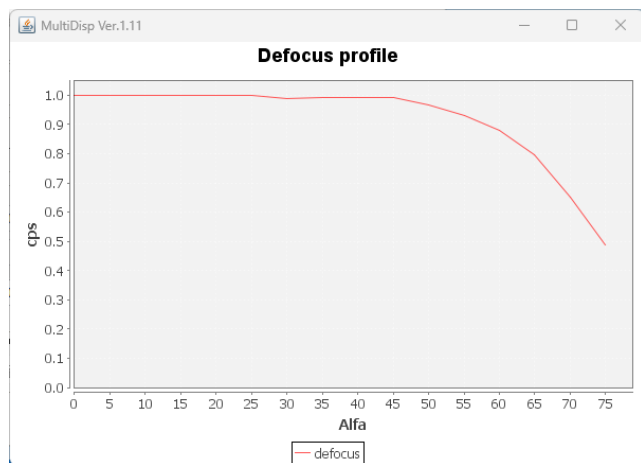
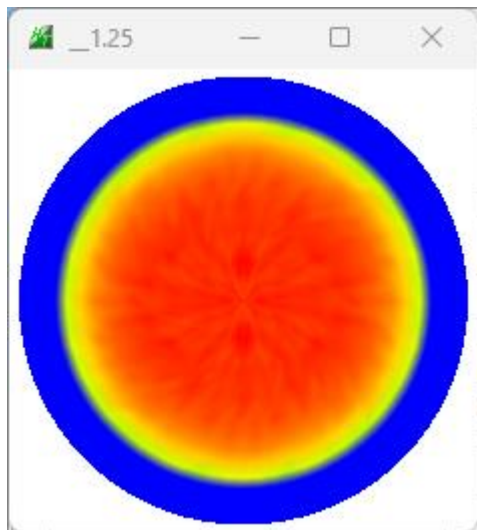


試料が薄い場合、
極点図の外周に向けて散乱体積が増える
補正が行われる、補正量の確認

Random試料によるdefocus補正

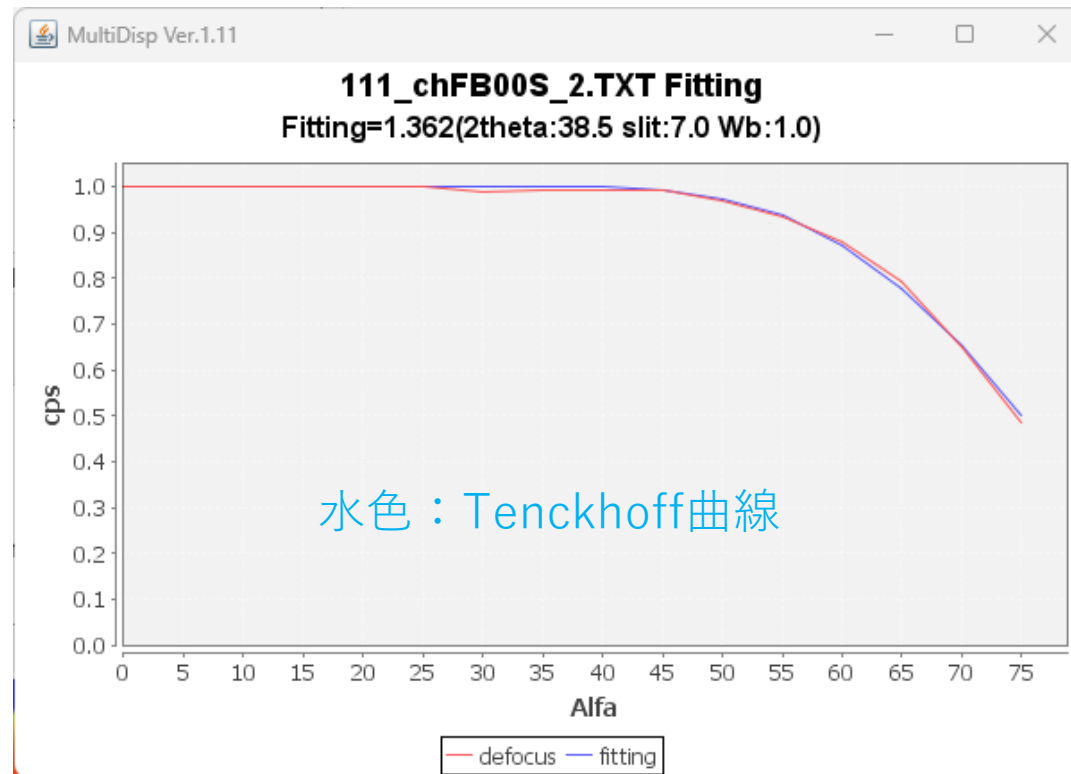
Random試料によるdefocus曲線はTenckhoff曲線に近似されます。

バックグランド処理極点図





凸凹が目立つ

Tenckhoff曲線は受光スリット幅、 2θ 角度に影響される



Defocus file Select Trasmission defocus HKL+T

Defocus(1) functions file 

Make defocus function files by TXT2 Files Normalization degree of a polynomial TenckhoffFitting  TextDisp

バックグランド処理後極点図をTenckhoff曲線にFittingで登録

内部データベースによるDefocus補正(ODFPoleFigure2)

The screenshot displays the MultiDisp Ver.1.11 software interface. On the left, three circular pole figures are shown, illustrating the defocus correction process. The main window features a control panel with various settings for background deletion, peak slit, and defocus calculation. A graph on the right, titled "CalcDefocus(1,1,1)", plots counts per second (cps) against the angle α (alfa). The curve shows a sharp initial drop followed by a plateau around 1.0 cps. A red text overlay on the graph reads "2 θ 、受光スリット、dataBaseより計算".

Defocus curve confirmation

Correction effect

Density of peripheral part u_p



The bottom right shows two circular plots. The left plot, labeled "補正効果" (Correction effect), shows a uniform red center with a blue outer ring. The right plot, labeled "外周部分の密度 u_p " (Density of peripheral part u_p), shows a gradient from red in the center to blue at the periphery, indicating the distribution of the peripheral density.

最適化Rp%

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

Rp%はODF解析後、入力データ評価の指標であり、defocusの状態により影響を受けます。
CTRソフトウェアの最適化Rp%は、defocusの見直しによって、Rp%の改善を行っています。

Defocus file Select Transmission defocus HKL+T

Defocus(1) functions file  Make defocus function files by TXT2 Files Normalization degree of a polynomial 0 TenckhoffFitting  TextDisp

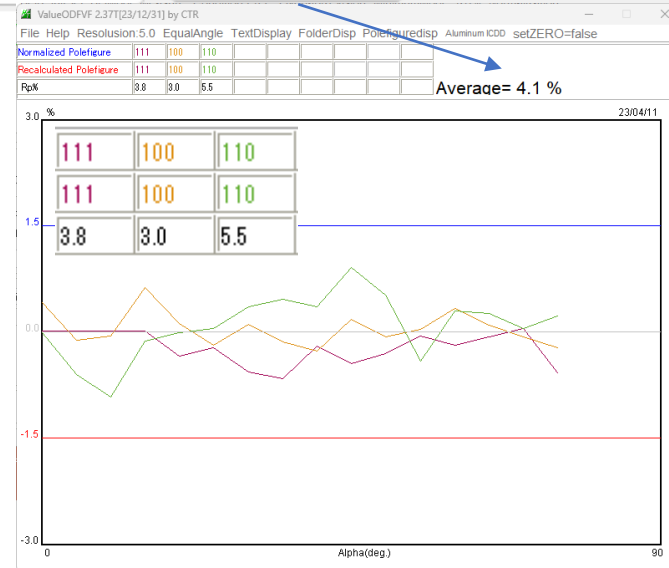
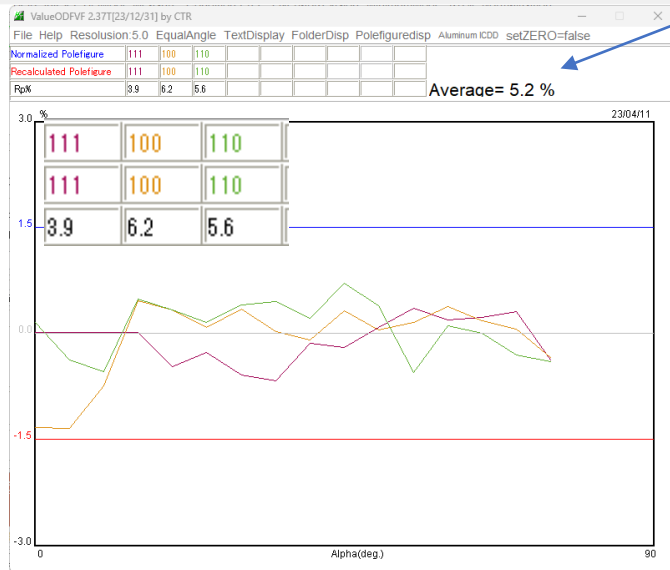
Defocus(3) function files folder(Calc unbackdefocus) BB285mm-Slit-1mm-7mm Limit Alfa Defocus value Free(LimitValue=0.0)

Defocus(2) function files folder(Calc backdefocus) DSH1.2mm+Schulz+RSH5mm Search minimum EqualAngleRp%(Cubic only) 1/Ra Profile

Smoothing for ADC Cycles 2 Weight 10 Disp After connection

Normalization CTR Connect Center Data Average OutFiles ASC MTextAsc Ras TXT TXT2

ValueODFVF-B ValueODFVF-A Average Exit&ODF ODF ALLODFFiles



Defocusの影響は極点図の外周に現れる
補正量見直しでRp%の最適化を行っている
Rp% = 5.2% → 4.1%に改善

複数極点図の平均化 (S)

圧延版の平均極点図や、粒径の大きい試料の平均極点図を求める 試料数 6, 極点図 4 の平均極点図を求める (試料数、極点数は無制限)

```
C:\¥A1100P¥NO001¥111-7mm.ASC  
C:\¥A1100P¥NO001¥200-7mm.ASC  
C:\¥A1100P¥NO001¥220-7mm.ASC  
C:\¥A1100P¥NO001¥311-7mm.ASC  
C:\¥A1100P¥NO002¥111-7mm.ASC  
C:\¥A1100P¥NO002¥200-7mm.ASC  
C:\¥A1100P¥NO002¥220-7mm.ASC  
C:\¥A1100P¥NO002¥311-7mm.ASC  
C:\¥A1100P¥NO003¥111-7mm.ASC  
C:\¥A1100P¥NO003¥200-7mm.ASC  
C:\¥A1100P¥NO003¥220-7mm.ASC  
C:\¥A1100P¥NO003¥311-7mm.ASC  
C:\¥A1100P¥NO004¥111-7mm.ASC  
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C:\¥A1100P¥NO006¥200-7mm.ASC  
C:\¥A1100P¥NO006¥220-7mm.ASC  
C:\¥A1100P¥NO006¥311-7mm.ASC
```

ファイル名が異なる場合
予め統一する

sample毎に、
BG(defocusモード)、内部defocus計算
最適化Rp%を行う。

指数毎に平均化を行い
NO001ホルダに平均極点図を作成

The screenshot displays the ODFPol software interface. At the top, four circular pole figures are shown in a row, each representing a different sample. Below them is a large settings window titled 'ODFPol:Figure2S 4.08T[23/12/31] by CTR'. The 'Files select' section shows a list of files: '111-7mm.ASC 200-7mm.ASC 220-7mm.ASC 311-7mm.ASC'. The 'Holder' section lists sample identifiers: 'C:\¥A1100P¥NO002', 'C:\¥A1100P¥NO003', 'C:\¥A1100P¥NO004', 'C:\¥A1100P¥NO005', and 'C:\¥A1100P¥NO006'. The 'Calculation Condition' section includes 'Background delete mode' (DoubleMo selected), 'Peak slit' (7.0 mm), 'BG Slit' (7.0 mm), and 'AbsCalc' (Schulz reflection method). The 'Defocus file' section is set to 'Defocus(2) function files folder(Calc backdefocus)'. The 'Smoothing for ADC' section has 'Cycles' set to 2 and 'Weight' set to 10. The 'OutFiles' section has 'TXT2' selected. The 'Average' button is highlighted with a yellow circle. The status bar at the bottom shows 'CTRHome : C:', 'Select crystal : Cubic', and the date '23/04/11'.

まとめ

- 正確なVolumeFractionを求めるには正確なrandom定量が必要
- バックグラウンド削除が最も重要、正確なバックグラウンド曲線
- 平滑化は行わない（randomレベルに影響する）
- 極点図が粗い場合、試料を増やし、平均極点図を求める
- R a n d o mサンプルが得られない場合、計算defocus補正
- 常に補正量は確認した上で補正を行い、結果への影響を把握

不明な点は問い合わせください。 HelperTex Office