r a n d o m レベル大小極点図の d e f o c u s 補正

randomレベルが少ない

実データrandom補正	計算random補正	再defocus補正	LaboTexRp%	CTRRp%	ODFMax	ODFMin
×	X	X	13.10%	8.40%	22.41	0.004
0	X	X	7.36%	3.50%	21.24	0.004
Х	0	X	6.75%	3.70%	21.19	0.005
Х	×	0	8.89%	4.60%	20.73	0.003
0	×	0	6.27%	2.30%	20.59	0.003
X	0	0	5.72%	2.00%	20.68	0.003

Rp%の差が少ない

randomレベルが比較的大きい

計算random補正	再defocus補正	LaboTexRp%	CTRRp%	ODFMax	ODFMin
X	X	19.67%	19.20%	47.04	0.130
0	X	14.23%	14.80%	41.78	0.073
Х	0	9.23%	7.60%	42.96	0.053
0	0	9.11%	7.60%	42.24	0.051
x 0	0	9.23% 9.11%	7.60% 7.60%	42.96 42.24	0.0 0.0

Rp%の差が大きい

r a n d o m レベルが少ないと、d e f o c u s 補正ありなしでもR p %の差が少なく r a n d o m レベルが大きいと、d e f o c u s 補正ありなしでR p %の差が大きくなる。 再 d e f o c u s の効果が大きい

ODFPoleFigureの再defocus補正はCubicを対象とし Cubic以外はValueODFVFに同一の機能があります。

r a n d o m レベルは、OD F 解析後のV o l u m e F r a c t i o n (VF%)を求める Background (その他の方位+random レベル)の指標になります。

> 2019年12月28日 HelperTex Office

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 - 2.2.1結晶系の選択
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1. 概要

d e f o c u s は、r a n d o m レベルにより多く作用することが知られている。 http://helpertex.sakura.ne.jp/Soft/DOC2/randomLevel-Rp-VolumeFraction.pdf

一方、ODFPoleFigure2 ソフトウエアでは、defocus 補正として
 実測定の random 試料による補正
 内部 defocus 計算による補正(ODFPoleFigure1.5 には付属しない)
 再 defocus 機能(入力極点図とrandomデータのErrorを最小にする機能)
 をサポートしている。

2. アルミニウム実測定データ (C:¥CTR¥DATA¥Aluminium-H-O¥Aluminium-O¥)



を各 defocus 補正を行い、R p % で比較を行ってみます。

2. 1アルミニウムrandomデータ(C:¥DATA¥Al-powder-random¥)



2. 2データ処理

ODFPoleFigure2 ソフトウエア

実データの平滑化

_□ Smoothing fo	or ADC —				
✓ Cycles	5 v	Weight	5	~	Disp
	After o	connection			

実測定のアルミニウムは分散が大きいため、平滑化を行う

2.2.1結晶系の選択

CTRシステムでは、DataBaseを内蔵し、選択、追加、編集が行えます。 結晶系の選択は、ODFPoleFigureのメニューから選択します。

<u>34</u>		ODFPolefigure1.5 1.63 by CTR PDuser CTR HelperTex -
File Linear(3D) T	oolKit Help InitSet Rp% Min	umum All background Transmissionblinds=30.0
Files select ASC(RINT-PC)	PFtoODF3	
Calcration Condition	SoftWare	Nu Countries
Previous	ImageTools	0,0,0 Change □ + α 5 ∨ Arithmetic mean ∨ Disp
Backgroud delete	PopLATools	
AhsGalo	ODFAfterTools	
🗌 Ref 🔄 Tra	PoleOrientationTools	v Change Absorption coefficien 133.0 1/cm Thickness 0.2 cm v Set 2Theta 0.0 deg. ● 1/Kt Profile
Defocus file Se	DataBaseTools	
Smoothing(for A	FiberTools	
Cycles	StandardODFTools	nection Disp CTR Connect Search minimum EqualAngleRp0((Cubic only) Ras Asc @ TXT2 TXT
	DefocusTools	ValueODF-B ValuODF-A Cancel Calc Connect ODF File
	ClusterTools	
	InverseTools	Select crystal : Cubic 19/12/29
	MeasureDatatoAscTools	
THE STATE	OrientationDisplayTools	
	VectorTools	Canon Sub-

🖬 🛛 🖉 🗖 DatabaseIndex 1.05S by CTR SPuser 🚽 🗖 🔜						
File Help						
ICDD data	MakeMyICDD	MaterialData create				
-data disp Data Select	MaterialData	Data Display				
Profile disp Data Select	CreateProfile	Profile Display				
TXT Data TXTData(hkl d 2Theta)	MeasureDatatoMYICDD	Material Data create				
TXT Data Material Data	DataBaseGurad	Error Display				
Database Material Data	TetragonalBtoF	Data Display				
data disp create Data Select Create	MaterialDataManual	Data Display				
Filter Terget	Filter	Data Display				
Pprofile disp Data Select	OrientationProfile	Profile Dsiplay				

MaterialData 1.37 by CTR PDuser CTR HelperTex -
File Help Disp
Search
Cubic
LaboTex(a<=b<=c α<=90 β <=90 γ <=90)
Wave length
1.54056 ¥
Select
Aluminum.TXT v
Aluminum Formula: Al
Disp Cancel Return Structure Chemical formula Input(e. g. C2 H4) Al Change

結晶系と材料を選択し、Dispで システムの結晶系と材料が決まる。

- 2. 3 r a n d o m 補正曲線作成
- 2. 3. 1入力データ







2.3.2バックグランド削除+規格化



2. 3. 3 d e f o c u s 曲線登録 (次数0を指定すると最適次数で Fitting を行う)

O Defocus(1) functions file	Files V Normalization	degree of a polynomial	0 TenckhoffFitting	`	TextDisp
Defocus(1) functions file	C:¥CTR¥DATA¥Al-powder-random¥defocus	#DEFOCUS_F.TXT			
Make defocus function files by TXT2	Files 🗸 🗌 Normalization	degree of a polynomial	0 TenckhoffFitting		TextDisp

Tenckhoff 次数11で登録されている。(Flat 部が強調されています)

filename,alfanumber,alfastartangle,alfastep,function-n,mm, 19/12/28 3.10 for DefocusCalc,

111-random_S_chB00S_2.TXT,16,0.0,5.0,11,7.0,1.0000002766480862,2.3372113588644705E-4,-1.228704757495626E-4 200-random_S_chB00S_2.TXT,16,0.0,5.0,11,7.0,1.000000971853573,2.3437636451493834E-4,-1.2013125946688044E-220-random_S_chB00S_2.TXT,16,0.0,5.0,11,7.0,0.9999999427361566,-1.6882312291022938E-4,8.654134844747387E-5

実測データの Fitting

補正曲線







3. 計算defocus曲線(測定に使用した受光スリット幅と20角度から計算)







ζ.,

2

LaboTexのような直接法のODFは最小方位がrandomレベルを示す

(Hermonic法では、ゴーストの影響を受け評価できない、マイナスを表示することもあります。)



0 0

5

90 Ø 1

¢_-0-90 Δ=5.00

90 •

5. アルミニウムの解析

5. 1 d e f o c u s 補正なしでアルミニウム解析

Marco ODFPoleFigure2	- D 🗙
File Linear(absolute)3D ToolKit Help InitSet BGMode Measure Condition Free OverlapRevision MinimumMode Rp% Normalization	
	hkl
Previous Next C#CTR#DATA#Aluminum=H=O#Aluminum=O#TTTASC	1,1,1 Change
	Smoothing
Minimum (cr. 8) Minimum Average(cr.)X 0.5	PD
	0.0 Interporation V Full Disp
AbsCalc	
□ Ref □ Trans Schulz reflection method v Change Absorption coefficien 133.0 1/cm Thickness 0.2 cm v Set	2Theta 38.59 deg. () 1/Kt Profile
Defocus file Select Trasmission defocus HKL+T	
Defocus(1) functions file	
Make defocus function files by TXT2 Files V Normalization degree of a polynomial 0	TextDisp
O Defocus(3) function files folder(Calc unbackdefocus) BB185mm V Limit Alfa Defocus value Free(LimitValue=0.	.0) 🗸
	1/Ba Profile
DSH12mm+Schulz+RSH5mm V	
Smoothing for ADC	Cancel Calc Connect
Vormalization V	TXT2 Exit&ODF ODF
	ValueODFVF-A
Filemake success !!	Select crystal : Cubic 19/12/28
	×
4.64 (2966.4) - 6	Cubic 以外を表示して
	いス担今
	マ・つ 3 7 日
	MaterialData で
	Cubic を選択

L a b o T e x による O D F 解析結果

Cycle	Iteration(Max.= 30)	Iteration (total)	Rp[%](Lim.= 1.00)	dRp[%](Lim.= 1.00)	
3	5	35	13.06	1.11	~
3	6	36	13.01	0.42	



				-
Normalized Polefigure	111	200	220	
Recalculated Polefigure	111	200	220	
Rp%	5.4	12.3	7.6	

D0.TPF Average= 8.4 %

R p %は

入力極点図のErrorを表します

5. 2 d e f o c u s なし+再d e f o c u s 補正でアルミニウム解析

🖬 ODFPoleFigure2 – 🗆 🔼
File Linear(absolute)3D ToolKit Help InitSet BGMode Measure Condition Free OverlapRevision MinimumMode Rp% Normalization
Files select ASC(RINT-PC) V 200 ASC 220 ASC
Calcration Condition
Previous Next C#CTR#DATA#Aluminum=H=O#Aluminum=O#111ASC 1,1,1 Change
Minimum mo
Peak slit 7.0 mm BG Slit 7.0 mm ✔ PeakSlit / BGS BG Scope 80.0 deg. 90.0 deg. Set Disp ∞ Inhibit
AbsCalc AbsCalc Ref Trans Schulz reflection method v Change Absorption coefficien 133.0 1/cm Thickness 0.2 Cm v Set 2Theta 38.59 deg. • 1/kt Profile
Defocus file Select Trasmission defocus HKL+T
Defocus(1) functions file C#CTR#DATA#Al-powder-random#defocus#DEFOCUS_F.TXT
Make defocus function files by TXT2 Files v 🗋 Normalization degree of a polynomial 0 🗹 TenckhoffFitting 📻 TextDisp
O Defocus(3) function files folder(Calc unbackdefocus) BB185mm V Limit Alfa Defocus value Free(LimitValue=0.0) V
Defocus(2) function files folder(Calc backdefocus) DSH12mm+Schulz+RSH5mm DSH12mm+Schulz+RSH5mm
Smoothing for ADC Cancel Calc Connect
✓ Cycles 5 ✓ weight 5 ✓ bisp ✓ CYcles 5 ✓ weight 5 ✓ bisp ✓ CTR Connect ○ Average ○ Asc ○ MTexAsc ○ Ras ○ TXT ● TXT2 Exit&ODF ODF
After connection ValueO DFVF-B ValueO DFVF-A
Filemake success !! Select crystal : Cubic 19/12/28
4.47(2966.4) - □ × 4.74(1153.2) - □ × 2.64(1060.4) - □ ×

L a b o T e x によるODF 解析結果

Cycle	Iteration(Max.= 30)	Iteration (total)	Rp[%](Lim.= 1.00)	dRp[%](Lim.= 1.00)	
3	7	44	8.97	1.27	~
3	8	45	8.89	0.92	
		Creation of	f pole figures files NPF an	d RPF	



Normalized Polefigure	111	200	220
Recalculated Polefigure	111	200	220
Rp%	2.5	5.1	6.3

DOR.TPF

Average= 4.6 %

5. 3 実測 d e f o c u s 曲線によるデータ処理

M ODFPoleFigure2 - 🗆 🗙
File Linear(absolute)3D ToolKit Help InitSet BGMode Measure Condition Free OverlapRevision MinimumMode Rp% Normalization
Files select ASC(RINT-PC) v 200 ASC 220 ASC
Calcration Condition
Previous Next C#CTR#DATA#Aluminum-H-O¥Aluminum-O¥111.ASC 1,1,1 Change
Minimum (α, β) Minimum Average(α)X 0.5 Trans blinds angle 20.0
Peak slit 7.0 mm BG Slit 7.0 mm ✔ PeakSlit / BGS_ BG Scope 80.0 deg. 90.0 deg. Set Disp ∞Inhibit
AbsCalc
Devicus file Select Trasmission defocus HKL+T
C#CTR#DATA#AI-powder-random#defocus#DEFOCUS_F.TXT
Make defocus function files by TXT2 Files V Normalization degree of a polynomial 0 V TenckhoffFitting TextDisp
○ Defocus(3) function files folder(Calc unbackdefocus) BB185mm v Limit Alfa Defocus value Free(LimitValue=0.0) v
O Defocus(2) function files folder(Calc backdefocus) DSH12mm+Schulz+RSH5mm ✓ □ Search minimum EqualAngleRpX(Cubic only) ④ 1/Ra Profile
Smoothing for ADC Cancel Calc Connect
Image: Weight 5 Weight 5 Disp Ownedization Ownedization Image: Weight 5 V Disp Image: Weight 0 Image: Weight 5 V Disp Ownedization Ownedization Image: Weight 5 V Disp Image: Weight 0 Image: Weight 5 V Disp Ownedization Ownedization Image: Weight 5 V Disp Ownedization Ownedization
After connection ValueODFVF-B ValueODFVF-A
Select crystal : Cubic 19/12/28
₩ 4.45(3227.7) - □ × ₩ 5.0(1265.1) - □ × ₩ 2.64(1098.1) - □ ×



L a b o T e x によるODF解析結果





Normalized Polefigure	111	200	220	_
Recalculated Polefigure	111	200	220	
Rp%	1.1	6.0	3.7	

D1.TPF

Average= 3.5 %

5. 4 実測defocus曲線+再defocusによるデータ処理

File Linear(absolute)3D ToolKit Help InitSet BGMode Measure Condition Free OverlapRevision MinimumMode Rp% Normalization
Files select ASC(RINT-PC) V III.ASC 200.ASC 220.ASC
Calcration Condition
Previous Next C#newCTR#DATA#Aluminum-H-O#Aluminum-O#111.ASC 1,1,1 Change
O Minimum (α β) O Minimum Average(α)X 0.5 Trans blinds angle 30.0
Peak slit 7.0 mm BG Slit 7.0 mm ✔ PeakSlit / BGS_ BG Scope 80.0 deg. 90.0 deg. Set Disp ∞ Inhibit
Hoscvaic Ref Trans Schulz reflection method v Change Absorption coefficien 133.0 1/cm Thickness 0.2 cm v Set 2Theta 38.59 deg. () 1/kt Profile
Defogus file Select Trasmission defocus HKL+T
C*newCTR¥CTR¥DATA¥AI-powder-random¥defocus¥DEFOCUS_F.TXT Make defocus function files by TXT2 Files Normalization degree of a polynomial O TenckhoffFitting TextDisp
○ Defocus(3) function files folder(Calc unbackdefocus) BB185mm Limit Alfa Defocus value Free(LimitValue=0.0) ✓ ○ Defocus(3) function files folder(Calc unbackdefocus) BB185mm ✓ Imit Alfa Defocus value Free(LimitValue=0.0) ✓
DEHL2mm+Schulz+RSHbmm V Beardn minimum Equal/Miglerpx/Cubic only
Smoothing for ADC Cancel Calc Connect
Smoothing for ADC Normalization CenterData OutFiles Cancel Calc Connect Cycles 5 v Weight 5 Disp CTR Connect Average Asc MTexAsc Ras TXT TXT2 Exit&ODF ODF
Smoothing for ADC Image: Connection Normalization Image: CTR Connect After connection ValueODFVF-B ValueODFVF-A
Smoothing for ADC Normalization CenterData OutFiles Cancel Calc Connect Opened After connection After connection Asc MTexAsc Ras TXT TXT2 Exit&ODF ODF ValueODFVF-B ValueODFVF-A ValueODFVF-A ValueODFVF-A Select crystal : Cubic 19/12/28
Smoothing for ADC Image: Cycles Image: Cycles
Smoothing for ADC Normalization CenterData OutFiles Cancel Calc Connect Cycles 5 v Weight 5 Disp CTR Connect Average Asc MTexAsc Ras TXT TXT2 Exit&ODF ODF After connection ValueODFVF-B ValueODFVF-B ValueODFVF-A Select crystal : Cubic 19/12/28 4.4(3227.7) - × 4.68(1265.1) - × 2.54(1098.1) - ×
Smoothing for ADC Normalization Center Data OutFiles Cancel Calc Connect Opcles 5 Velue 0 Asc MTexAsc Ras TXT TXT2 Exit&ODF ODF After connection Value Value 0 FVF-B Value Value Value 19/12/28 4.4(3227.7) - × 4.68(1265.1) - × 2.54(1098.1) - ×
Smoothing for ADC Cycles 5 v Weight 5 v Disp After connection ValueODFVF-B ValueODFVF-A Select crystal : Cubic 19/12/28 4.68(1265.1) - × 2.54(1098.1) - ×



L a b o T e x によるODF 解析結果

Cycle	Iteration(Max.= 30)	Iteration (total)	Rp[%](Lim.= 1.00)	dRp[%](Lim.= 1.00)	
3	13	51	6.33	1.12	~
3	14	52	6.27	0.90	
		Creation of	[;] pole figures files NPF an	d RPF	



Normalized Polefigure	111	200	220	
Recalculated Polefigure	111	200	220	
Rp%	1.3	3.3	2.5	

D1R.TPF

Average= 2.3 %

5. 5 内部 d e f o c u s 計算によるデータ処理

🖬 ODFPoleFigure2 3.94 by CTR PDuser CTR HelperTex – 🗖
File Linear(absolute)3D ToolKit Help InitSet BGMode Measure Condition Free OverlapRevision MinimumMode Rp% Normalization
Files select ASC(RINT-PC) V III ASC 200 ASC 220 ASC
Caloration Condition
Previous Next C#newCTR#CTR#DATA#Aluminum-H-O#Aluminum-O#111.ASC 1,1,1 Change
Backgroud delete mode
🗹 💿 DoubleMode 🔾 SingleMode 🔾 LowMode 🔾 HighMode 🖉 Nothing 🛛 BG defocus DSH1.2mm+Schulz+RSH5mm 📉 🗌 Minimum mo
\bigcirc Minimum($\alpha\beta$) \bigcirc MinimumAverage(α)X 0.5 Trans blinds angle 30.0 RD RD RD \bigcirc 0.0 Interpretation \downarrow Full Dipp
Peak slit 7.0 mm BG Slit 7.0 mm ✔ PeakSlit / BGS_ BG Scope 80.0 deg. 90.0 deg. Set Disp ∞Inhibit
Peter illeris Schulz reflection method V Change Absorption coefficien 133.0 17cm Inickness 0.2 Ciri V Set 21neta 38.39 Uee. • 17kt Profile
Defocus(1) functions file C*newCTR#DATA¥AI-powder~random#defocus#DEFOCUS_F.TXT
Make defocus function files by TXT2 Files 🗸 🗌 Normalization degree of a polynomial 0 🗹 TenckhoffFitting
O Defocus(3) function files folder(Calc unbackdefocus) BB185mm v Limit Alfa Defocus value Free(LimitValue=0.0) v
Descure(2) function files folder(Cale backdetorus) Descure up L L Dours Search minimum Equal Ref(Cubic cale) O 1/Ra Profile
Smoothing for ADC Cancel Calc Connect
Cycles 5 ▼ Weight 5 ▼ Disp Normalization CenterData Outlines Vormalization CenterData Outlines Vormalization CenterData Outlines Vormalization CenterData Outlines Vormalization CenterData
After connection
Value0DFVF-B Value0DFVF-A
Select crystal : Cubic 19/12/
▲ 4.49(3348.4) - □ × ▲ 4.9(1264.1) - □ × ▲ 2.56(1107.2) - □ ×

L a b o T e x によるODF 解析結果

Cycle	Iteration(Max.= 30)	Iteration (total)	Hp[%][Lim.=1.00]	dHp[%](Lim.=1.00)	
3	13	51	6.82	1.02	~
3	14	52	6.76	0.96	
		Creation of	t note figures files NPF an	4 RPF	_



Normalized Polefigure	111	200	220	
Recalculated Polefigure	111	200	220	
Rp%	3.5	5.1	2.7	

D2.TPF

Average= 3.7 %

5. 6内部defocus計算+再defocusによるデータ処理

M ODFPoleFigure2 3.94 by CTR PDuser CTR HelperTex	- • <mark>*</mark> *
File Linear(absolute)3D ToolKit Help InitSet BGMode Measure Condition Free OverlapRevision MinimumMode Rp% Normalization	
Files select ASC(RINT-PC) V 20 ASC 220 ASC	
Calcration Condition	-bkl
Previous Next C#newCTR#CTR#DATA#Aluminum-H-O#Aluminum-O#111ASC	1,1,1 Change
Backgroud delete mode	noothing
■ © DoubleMode () SingleMode () LowMode () HighMode () Nothing BG defocus DSH12mm+Schulz+RSH5mm () Minimum mo	C +α 3 v Arithmetic mean v Disp
$\bigcirc Minimum(\alpha,\beta) \qquad \bigcirc Minimum Average(\alpha) \times 0.5 \qquad \qquad Trans blinds angle \qquad 30.0$	D Internoration Full Disn
Peak slit 7.0 mm BG Slit 7.0 mm ✔ PeakSlit / BGS BG Scope 80.0 deg. 90.0 deg. Set Disp α/Inhibit	
AbsCalc AbsCalc Change Absorption coefficien 133.0 1/cm Thickness 0.2 Cm v Set	2Theta 38,59 deg. I/Kt Profile
Tefosus file Select Trasmission defocus HKL+T	
Mala defense functions file by TVT3	- 2 TextDisp
O Defocus(3) function files folder(Calc unbackdefocus) BB185mm v Limit Alfa Defocus value Free(LimitValue=0.0)	· · ·
	1/Pa Profile
O Defotus(2) function files folder(Calc backdefocus) DSH12mm+Schulz+RSH5mm Searth minimum EqualAngleRpt(Cubic only)	
Smoothing for ADC	Cancel Calc Connect
V Cycles 5 v Weight 5 v Disp V CTR Connect OAverage OAsc OMTexAsc ORas OTXT (TXT2 Exit&ODF ODF
absolute)3D Toolkit Help InitSet BGMode Measure Condition Free OverlapRevision MinimumMode Rp% Normalization P	
	ValueODFVF-B ValueODFVF H
	Select crystal : Cubic 19/12/28
P	
$44(33484) - \Box \times 467(12641) - \Box \times 4253(11072) - \Box \times$	



L a b o T e x によるODF解析結果

Cycle	Iteration(Max.= 30)	Iteration (total)	Rp[%](Lim.= 1.00)	dRp[%](Lim.= 1.00)	
3	15	53	5.77	1.17	~
3	16	54	5.72	0.98	
		Constitution of	Calle Carrier Clark MDD and		



Normalized Polefigure	111	200	220
Recalculated Polefigure	111	200	220
Rp%	1.1	2.9	2.0

D2R.TPF

Average= 2.0 %

6. randomレベルの高い銅材料のdefocus補正

Random データがないため、内部計算 r a n d o m と 再 d e f o c u s 補正を行ってみます。

入力データ (Cu材料)



内部計算defocus曲線





平滑化は行いません。

Smoothing fo	or ADC				
Cycles	5 ¥	Weight	5	~	Disp
	After o	connection			

6. 1 d e f o c u s 補正なしによるデータ処理

M ODFPoleFigure2 3.94 by CTR PDuser CTR HelperTex	- 🗆 🗙
File Linear(absolute)3D ToolKit Help InitSet BGMode Measure Condition Free OverlapRevision MinimumMode Rp% Normalization	1
ASC(RIN1-PC) V III-7mm-2BASC 200-7mm-2BASC 220-7mm-2BASC 311-7mm-2BASC	
Calcration Condition	_hkl
Previous Next C#newCTR#DATA#Cu=0#111-7mm-2B.ASC	1,1,1 Change
Backgroud delete mode ☑ ● DoubleMode ○ SingleMode ○ LowMode ○ HighMode ○ Nothing BG defocus DSH12mm+Schulz+RSH5mm ✓ □ Minimum mo	Smoothing
\bigcirc Minimum(α β) \bigcirc MinimumAverage(α)X 0.5 Trans blinds angle 30.0	RD
Peak slit 7.0 mm BG Slit 7.0 mm ✔ PeakSlit / BGS_ BG Scope 80.0 deg. 90.0 deg. Set Disp α2Inhibit	0.0 Interporation v Full Disp
AbsCalc	et 2Theta 43.38 deg. 1/Kt Profile
Contraction defocus HKL+T	
O Defocus(1) functions file C¥newCTR¥CTR¥CTR¥Al-powder-random¥defocus¥DEFOCUS_F.TXT Make defocus function files by TXT2 Files Normalization degree of a polynomial O TenckhoffFitting	TextDisp
O Defocus(3) function files folder(Calc unbackdefocus) BB185mm v Limit Alfa Defocus value Free(LimitValue=	=0.0) 🗸
Defocus(2) function files folder(Calc backdefocus) DSH12mm+Schulz+RSH5mm Search minimum EqualAngleRpX(Cubic only)	0 1/Ra Profile
r Smoothing for ADC	Cancel Calc Connect
Cycles 5 V Weight 5 V Disp	Г ● TXT2 Fxit&ODF ODF
	ValueODFVF-B ValueODFVF-A
Filemake success !!	Select crystal : Cubic 19/12/28
	-
4.53(6587.3) - · · · · · · · · · · · · · · · · · ·	2.97(6147.5) - L

L a b o T e x によるODF 解析結果

Cycle	Iteration(Max.= 30)	Iteration (total)	Rp[%](Lim.= 1.00)	dRp[%](Lim.= 1.00)	
3 3	2 3	14 15	19.06 18.89	2.12 0.91	^
		Carakian at	LEIL CLARK CLARKING LA		



Normalized Polefigure	111	200	220	311	
Recalculated Polefigure	111	200	220	311	
Rp%	20.8	18.7	18.6	18.9	

Cu0.TPF Average= 19.2 %

6. 2 d e f o c u s 補正なし+再 d e f o c u s によるデータ処理

M ODFPoleFigure2 3.94 by CTR PDuser CTR HelperTex – 🗆 🗙
File Linear(absolute)3D ToolKit Help InitSet BGMode Measure Condition Free OverlapRevision MinimumMode Rp% Normalization
Files select ASC(RINT-PC) V 111-7mm-2BASC 200-7mm-2BASC 220-7mm-2BASC 311-7mm-2BASC
Calcration Condition Previous Next C*newCTR#CTR#DATA#Cu=0#111=7mm=2B.ASC hkl
Backgroud delete mode Image: State of the state o
Nosoac Ref Trans Schulz reflection method v Change Absorption coefficien 133.0 1/cm Thickness 0.2 cm v Set 2Theta 43.38 deg. • 1/kt Profile
Oefocus(1) functions file C¥new@CTR¥CTR¥DATA¥AI-powder-random¥defocus¥DEFOCUS_F.TXT Make defocus function files by TXT2 Files Normalization degree of a polynomial ① TenckhoffFitting TextDisp Defocus(3) function files folder(Calc unbackdefocus) BB185mm Limit Alfa Defocus value Free(LimitValue=0.0) ① Defocus(2) function files folder(Calc backdefocus) DSH12mm+Schulz+RSH5mm ① Search minimum EqualAngleRp&Cubic only ① 1/Ra Profile
Smoothing for ADC OutFiles Cancel Calc Connect Cycles 5 Weight 5 OutFiles Cancel Calc Connect After connection After connection OutFiles ValueODFVF-B ValueODFVF-A Select crystal : Cubic 19/12/28
4.71(6587.3) - □ × 4.71(6587.3) - □ × 4.252(6147.5) - □ ×

L a b o T e x によるODF 解析結果

Cycle	Iteration(Max.= 30)	Iteration (total)	Rp[%](Lim.= 1.00)	dRp[%](Lim.= 1.00)	
3	8	32	9.32	1.28	~
3	9	33	9.23	0.97	
		Creation of	f pole figures files NPF an	d RPF	

– 🗆 🗙



Normalized Polefigure	111	200	220	311	
Recalculated Polefigure	111	200	220	311	
Rp%	9.6	10.3	3.3	7.3	

Cu0R.TPF

Average= 7.6 %

6. 3 内部 d e f o c u s 計算によるデータ処理

🛛 ODFPoleFigure 23.94 by CTR PDuser CTR HelperTex – 🗆 🗙
File Linear(absolute)3D ToolKit Help InitSet BGMode Measure Condition Free OverlapRevision MinimumMode Rp% Normalization
Files select ASC(RINT-PC) v 28ASC 200-7mm-2BASC 220-7mm-2BASC 311-7mm-2BASC
Calcration Condition
Previous Next C#newCTR#CTR#DATA#Cu=0#111-7mm=2B.ASC
Backgroud delete mode Smoothing Smoothing Smo
\bigcirc Minimum($\alpha \beta$) \bigcirc MinimumAverage(α)X 0.5 Trans blinds angle 30.0
Peak slit 7.0 mm BG Slit 7.0 mm ✔ PeakSlit / BGS BG Scope 80.0 deg. 90.0 deg. Set Disp ∞ Inhibit
Host action host a
Defecus file Select Trasmission defocus HKL+T
Defocus(1) functions file
Make defocus function files by TXT2 Files Image: Normalization degree of a polynomial Image: Object to the second degree of a polynomi
O Defocus(3) function files folder(Calc unbackdefocus) BB185mm v Limit Alfa Defocus value Free(LimitValue=0.0) v
O Derbcus(2) function files folder(Calc backdefocus) DSH12mm+Schulz+RSH5mm DSH12mm+Schulz+RSH5mm Search minimum EqualAngleRp%(Cubic only) O 1/Ra
-Smoothing for ADC
Oxelans to Theory Weight 5 Disp Operation Operation Center Data Out Files Out Files Operation Operation Operation Operation Operation </td
After connection ValueODFVF-B ValueODFVF-A
Select crystal : Cubic 19/12/28
4.3(7286.0) = -4.42 $4.3(7286.0) = -4.42 $ $4.3(7286.0) = -4.42 $ $4.3(7286.0) = -4.42 $ $4.3(7286.0) = -4.42$

LaboTexによるODF解析結果

.00)	dRp[%](Lim.= 1.	Rp[%](Lim.= 1.00)	Iteration (total)	Iteration(Max.= 30)	Cycle
^	1.09	14.34	22	5	3
	0.81	14.23	23	6	3
	d RPF	of pole figures files NPF and	Creation o		<u> </u>
	- 005	e 1.:	C		



Normalized Polefigure	111	200	220	311	
Recalculated Polefigure	111	200	220	311	
Rp%	12.5	16.8	16.9	13.2	

Cu1.TPF Average= 14.8 %

6. 4内部defcous計算+再defocusによるデータ処理

File Linear(absolute)3D ToolKit Help InitSet BGMode Measure Condition Free OverlapRevision MinimumMode Rp% Normalization
Files select ASC(RINT-PC) V II1-7mm-2BASC 200-7mm-2BASC 210-7mm-2BASC 311-7mm-2BASC
Calcration Condition
Previous Next C#newCTR#CTR#DATA¥Cu=0#111-7mm-2B.ASC 1,1,1 Change
Backgroud delete mode
🗹 🖲 DoubleMode 🔾 SingleMode 🔾 LowMode 🔾 HighMode 🔿 Nothing 🛛 BG defocus DSH12mm+Schulz+RSH5mm 🗸 🔤 Minimum mo_
O MinimumAverage(α)X 0.5 Trans blinds angle 30.0 Peak slit 7.0 mm PeakSlit / BGS BG Scope 80.0 deg. 90.0 deg. Set Disp α Inhibit
AbsCalc
Ref Trans Schulz reflection method v Change Absorption coefficien 133.0 1/cm Thickness 0.2 Cm v Set 2Theta 43.38 deg. (e) 1/Kt Profile
Perforces file Select Trasmission defocus HKL+T
Defocus(1) functions file
Make defocus function files by TXT2 Files V Normalization degree of a polynomial 0 V TenckhoffFitting
Derbocus(2) function files folder(Calc backdefocus) DSH12mm+Schulz+RSH5mm DSH12mm+Schulz+RSH5mm Search minimum EqualAngleRp((Cubic only)) ① 1/Ra Profile
Smoothing for ADC Connect CenterData rOutFiles Cancel Calc Connect
□ Cycles 5 v Weight 5 v Disp V CTR □ Connect ○ Average ○ Asc ○ MTexAsc ○ Ras ○ TXT
ValueODEV/F-B ValueODEV/F-A
ValueODFVF-B ValueODFVF-A
ValueODFVF-B ValueODFVF-A Select crystal : Cubic 19/12/28
ValueODFVF-B ValueODFVF-A Select crystal : Cubic 19/12/28
Value ODFVF-B Value ODFVF-A Select crystal : Cubic 19/12/28 4.66(7286.0) - × 3.22(5148.4) - × 2.44(6379.4) - ×
Value OFVF-B Value OFVF-A Select crystal : Cubic 19/12/28 4.66(7286.0) 7.18(5100.1) - × 3.22(5148.4) - × 2.44(6379.4) - ×
Value OFVF-B Value OFVF-A Select crystal : Cubic 19/12/28 4.66(7286.0) - × 3.22(5148.4) - × 2.44(6379.4) - ×
Image: connection ValueODFVF-B ValueODFVF-A Select crystal : Cubic 19/12/28 #4 4.66(7286.0) - × 3.22(5148.4) - × 2.44(6379.4) - ×
Image: connection ValueODFVF-B ValueODFVF-A Select crystal : Cubic 19/12/28 # 4.66(7286.0) - × 3.22(5148.4) - × 2.44(6379.4) - × # 4.66(7286.0) - × # 3.22(5148.4) - × 4.66(7286.0) - ×
Image: connection ValueODFVF-B ValueODFVF-A Select crystal : Cubic 19/12/28 # 4.66(7286.0) - * 7.18(5100.1) - * 3.22(5148.4) - * 2.44(6379.4) - * 2.44(6379.4) - *
$\frac{1}{\sqrt{alueODFVF-B}} \frac{1}{\sqrt{alueODFVF-A}}$ Select crystal : Cubic 19/12/28 $4.66(7286.0) - 1 \times 7.18(5100.1) - 1 \times 3.22(5148.4) - 1 \times 42.44(6379.4) - 1 \times 42.44(637$
$\frac{1}{44.66(7286.0) - 1} \times 7.18(5100.1) - 1} \times 3.22(5148.4) - 1 \times 2.44(6379.4) - 1 \times 2.4$

L a b o T e x によるODF 解析結果

Cycle	Iteration(Max.= 30)	Iteration (total)	Rp[%](Lim.= 1.00)	dRp[%](Lim.= 1.00)	
3	10	34	9.19	1.03	^
3	11	35	9.11	0.91	



Normalized Polefigure	111	200	220	311	
Recalculated Polefigure	111	200	220	311	
Rp%	8.3	11.6	5.4	5.3	

Cu1R.TPF

Average= 7.6 %

7. ValueODFVFによる再defocus補正

本来Cubic以外を対象にするが、Cubicでも計算可能、以下に流れを説明します。



7. 1ODFPoleFigureによるdefocus補正(再defocusなし)







90 ¢ 1

90 φ

7. 3 Export された極点図をValue ODF VF で処理

34		Valu	eODFVF 2.	.33 by CTR	PDuser (CTR HelperTex -	
File	Help Resolusion:5.0	EqualAngle	TextDisplay	FolderDisp	Polefigure	edisp Aluminum ICDD	
	LaboTex-TPF	200 220 200 220				C¥newCTR¥CTR¥DATA¥Aluminum-H-O¥i AH0.TPF	Aluminum-H¥
	RIGAKU-ODF	4.9 5.5				Average= 4.2 %	
	TexTools-POL						19/12/29
	TexTools-RINTTXT						
	Standard ODF						
	popLA(Raw&Other)						
	NEWODF						
	MTEX						
	TXT2						
	PrintDisplay	\wedge	$ \wedge $				
	Calcdefocus		~~~				
	Exit						
	-						
15							
-1.5							
-3.0							
	0			Alph	a(deg.)		90
· · · · ·							

 ODF入力極点図
 ODF入力極点図と再計算極点図のRp%から計算した再 defocus 曲線



入力極点図を再 defocus 曲線で補正

ODFFiles で ODF 再入力データを作成

7. 4 L a b o T e x で再ODF解析





7. 5再defocus補正結果をValueODFVFで評価



今回Cubicで解析を行ったが、他の結晶系にも利用可能

又、実randomデータを利用したが、ODFPoleFigure2の計算 defocus も利用可能7.6ValueODFVFによる再defocusマトメ

実データrandom補正	再defocus補正	LaboTexRp%	CTRRp%	ODFMax	ODFMin
0	X	7.70%	4.20%	22.06	0.001
	0	6.10%	2.10%	21.96	0.000

再defocus補正を利用することで、Rp%を下げたデータが得られます。