

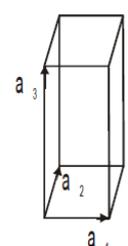
1面配向のPolyethyleneの非対称解析

2023年01月09日

HelperTex Office

概要

Polyethyleneの解析では格子定数の指定の仕方でもODF図が異なる。
 本資料ではLaboTexでシュミレーションデータを作成し各種比較を行う。
 LaboTexは、面配向（ {xxx} - Fiber ）を作成する。
 作成した極点図をExportしRotationから軸配向データを作成し比較する。
 LaboTexでrthorhombicを扱う場合、以下の注意が必要

Orthorhombic	D_2	D_{2h}, D_2	$a < b < c$	$90^\circ \ 90^\circ \ 90^\circ$	
	C_2	C_{2v}			

指数変換

ICDD

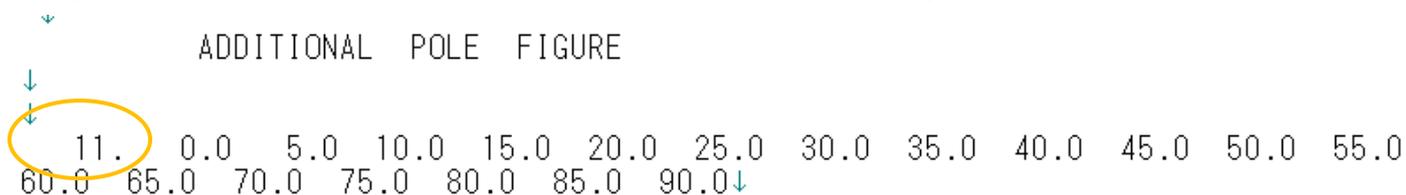
LaboTex

Orthorhombic					Orthorhombic				
7.4	(1.0)				2.54	(1.0)			
4.93	(0.6662)				4.93	(1.9409)			
2.54	(0.3432)				7.4	(2.9134)			
90.0					90.0				
90.0					90.0				
90.0					90.0				
1.54056					1.54056				
9					9				
1	1	0	100.0	4.1029	0	1	1	100.0	4.1029
2	0	0	35.0	3.7	0	0	2	35.0	3.7
2	1	0	5.0	2.9593	0	1	2	5.0	2.9593
0	2	0	20.0	2.465	0	2	0	20.0	2.465
0	1	1	25.0	2.2579	1	1	0	25.0	2.2579
3	1	0	20.0	2.206	0	1	3	20.0	2.206
1	1	1	20.0	2.1596	1	1	1	20.0	2.1596
2	2	0	15.0	2.0514	0	2	2	15.0	2.0514
3	1	1	25.0	1.6655	1	1	3	25.0	1.6655

実際は {001} は測定できない

{100} は測定出来ない

ExportしたTPFファイルの指数部分はdoubleで登録されている。

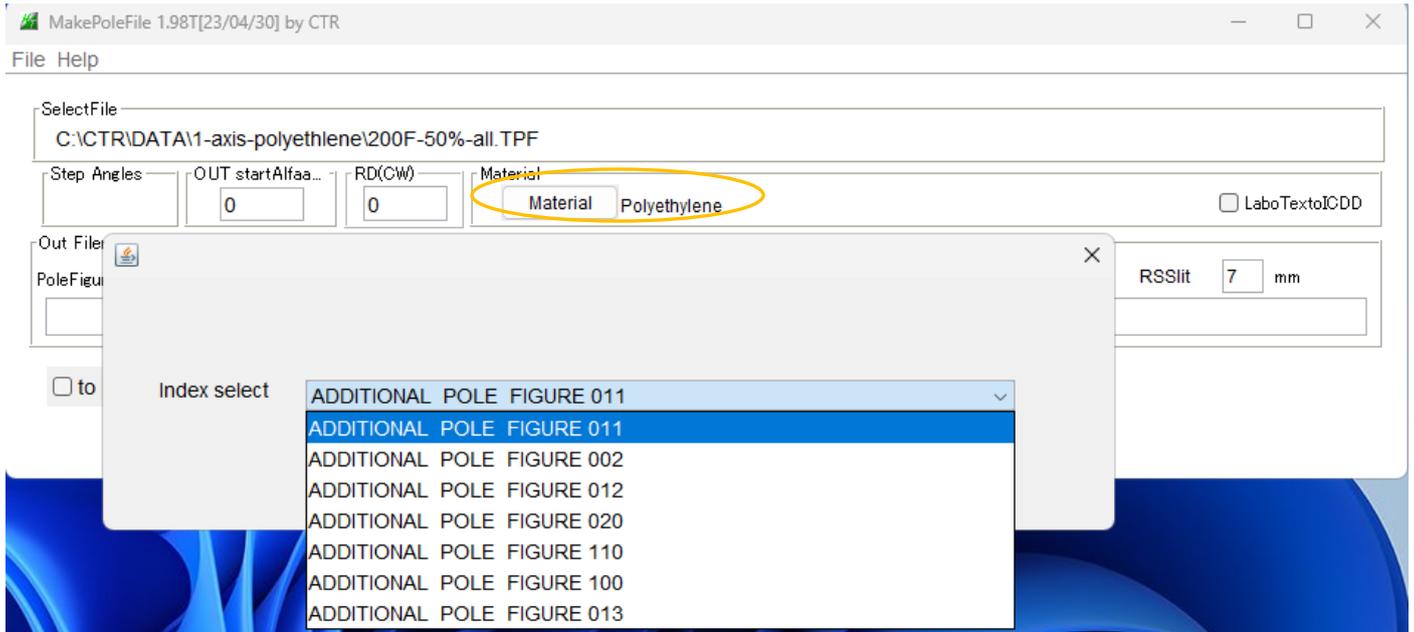


LaboTex 指数 String

TPFファイル

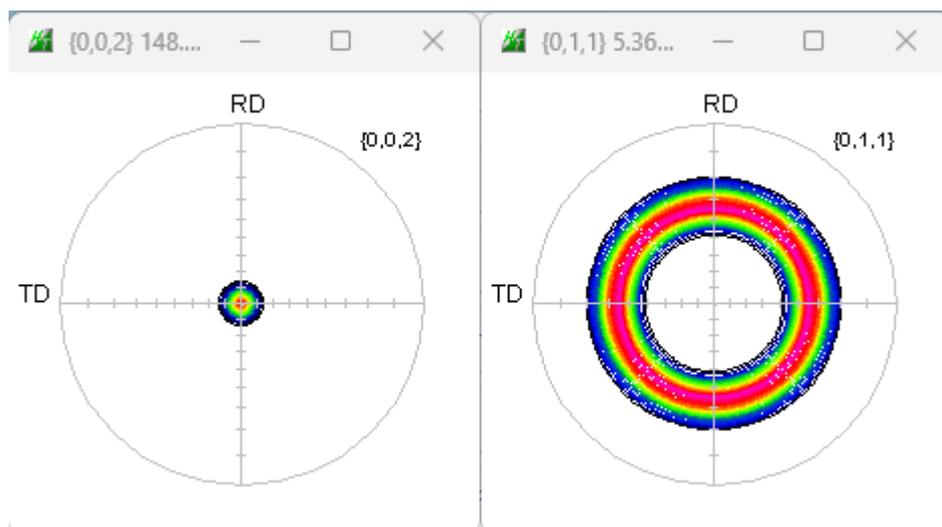
0 1 1	1 1 .
0 0 2	2 .
0 1 2	1 2 .
0 2 0	2 0 .
1 1 0	1 1 0 .
1 0 0	1 0 0 .
0 1 3	1 3 .

ExportされたTPFファイルからTXT2ファイル作成
ICDDでの変換なしデータを用いる

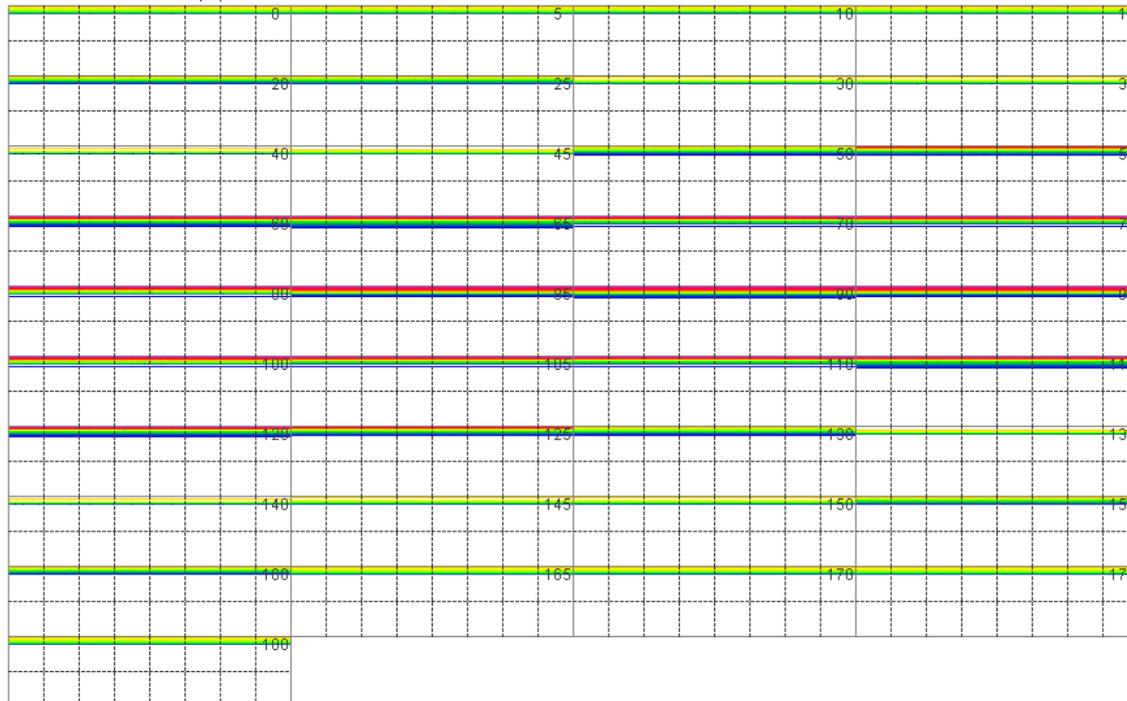


Orthorhombic				
2.54		(1.0)		
4.93		(1.9409)		
7.4		(2.9134)		
90.0				
90.0				
90.0				
1.54056				
9				
0	1	1	100.0	4.1029
0	0	2	35.0	3.7
0	1	2	5.0	2.9593
0	2	0	20.0	2.465
1	1	0	25.0	2.2579
0	1	3	20.0	2.206
1	1	1	20.0	2.1596
0	2	2	15.0	2.0514
1	1	3	25.0	1.6655

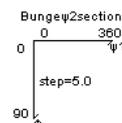
使用する極点図



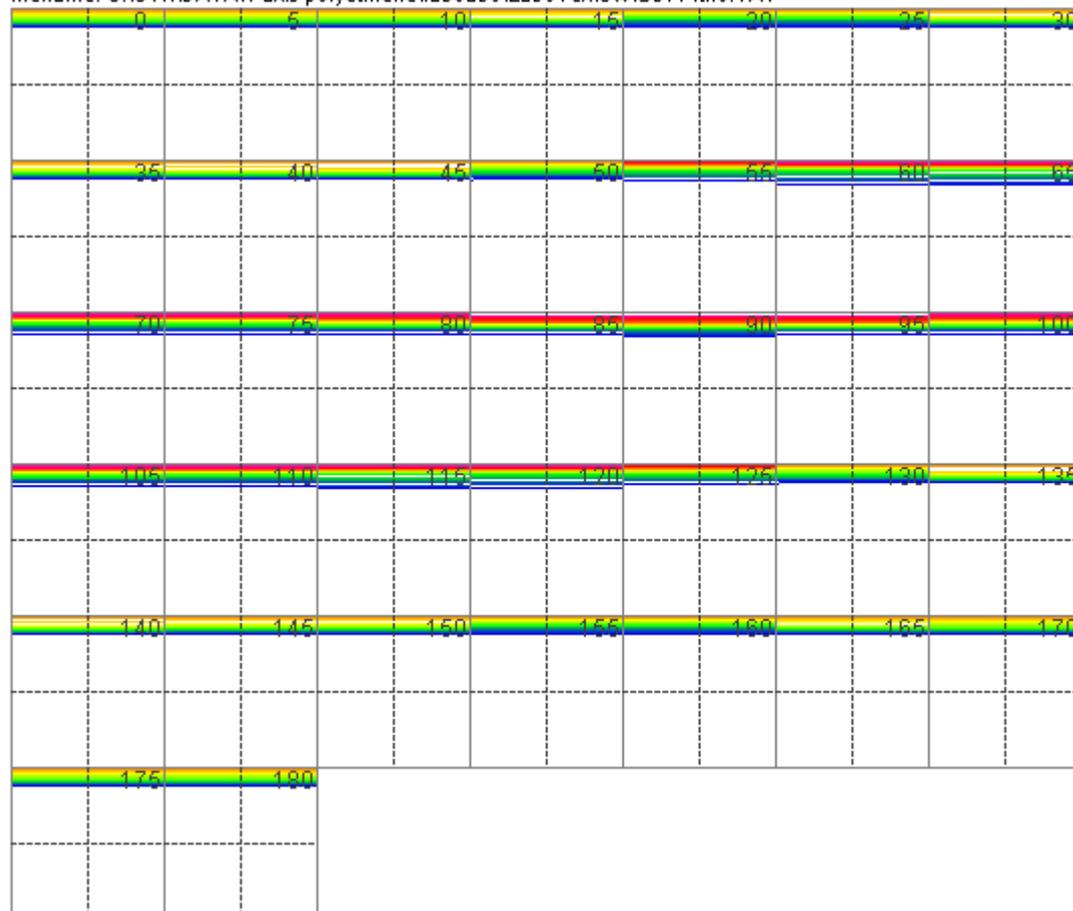
filename: C:\CTR\DATA\1-axis-polyethylene\laboabc\LaboTex\CW\Laboabc-ODF.TXT



Max=180.
Min=0.0



filename: C:\CTR\DATA\1-axis-polyethylene\laboabc\LaboTex\CW\ODFPrho.TXT

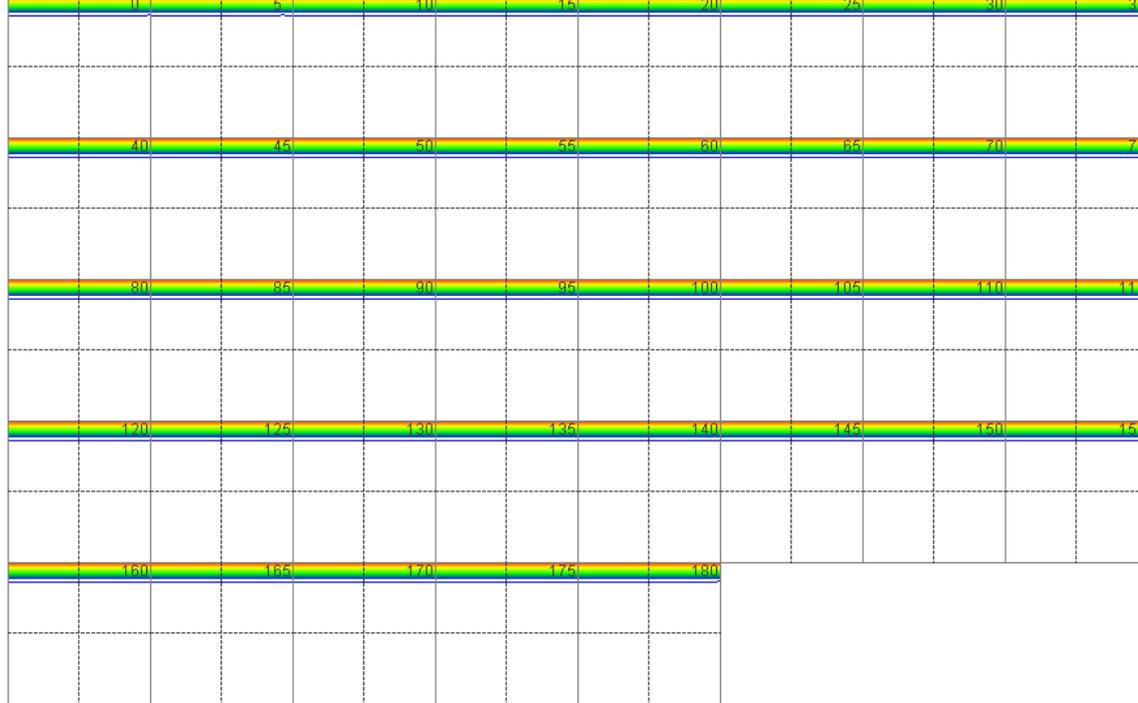


Max=188
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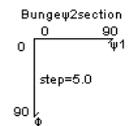
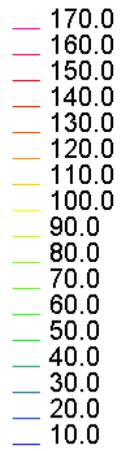


MTEX 1.0 1.941 2.913 90.0 90.0 90.0

filename: C:\CTR\DATA\1-axis-polyethylene\laboabc\MTEX\mtexodfabo.bt

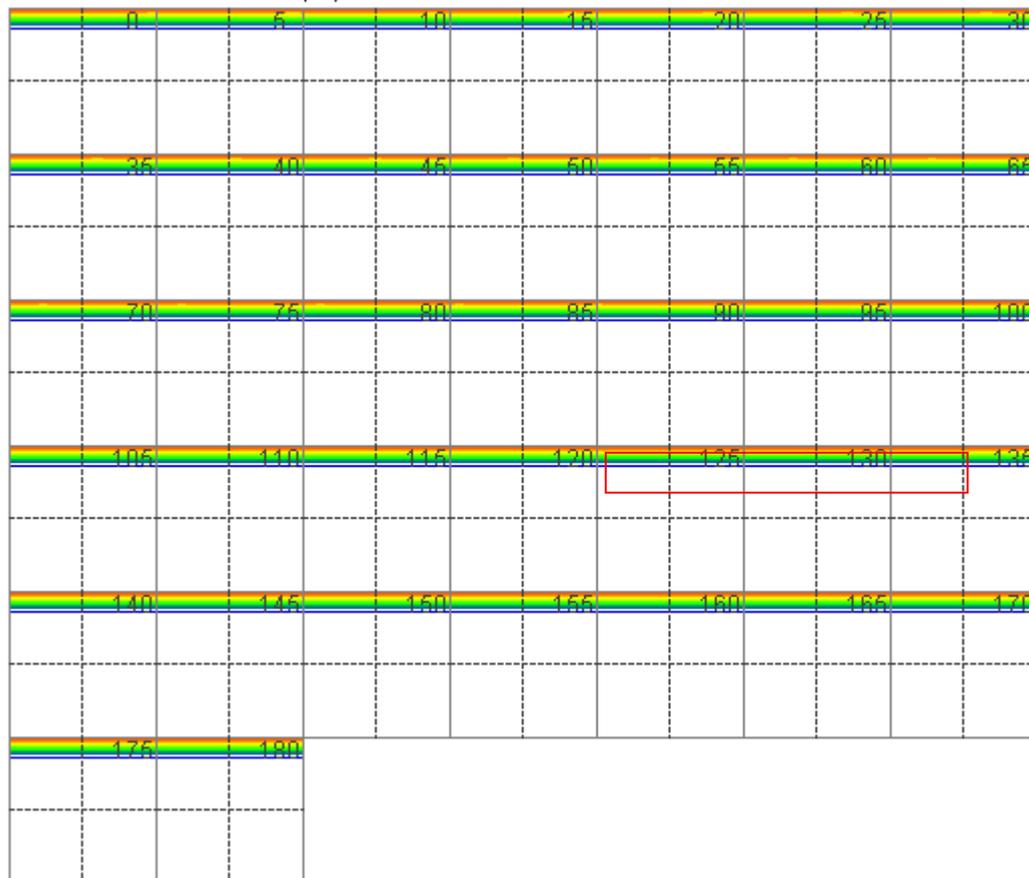


Max=136.0
Min=0.0

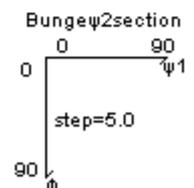


GPODFDisplay にて Orthorhombic 化

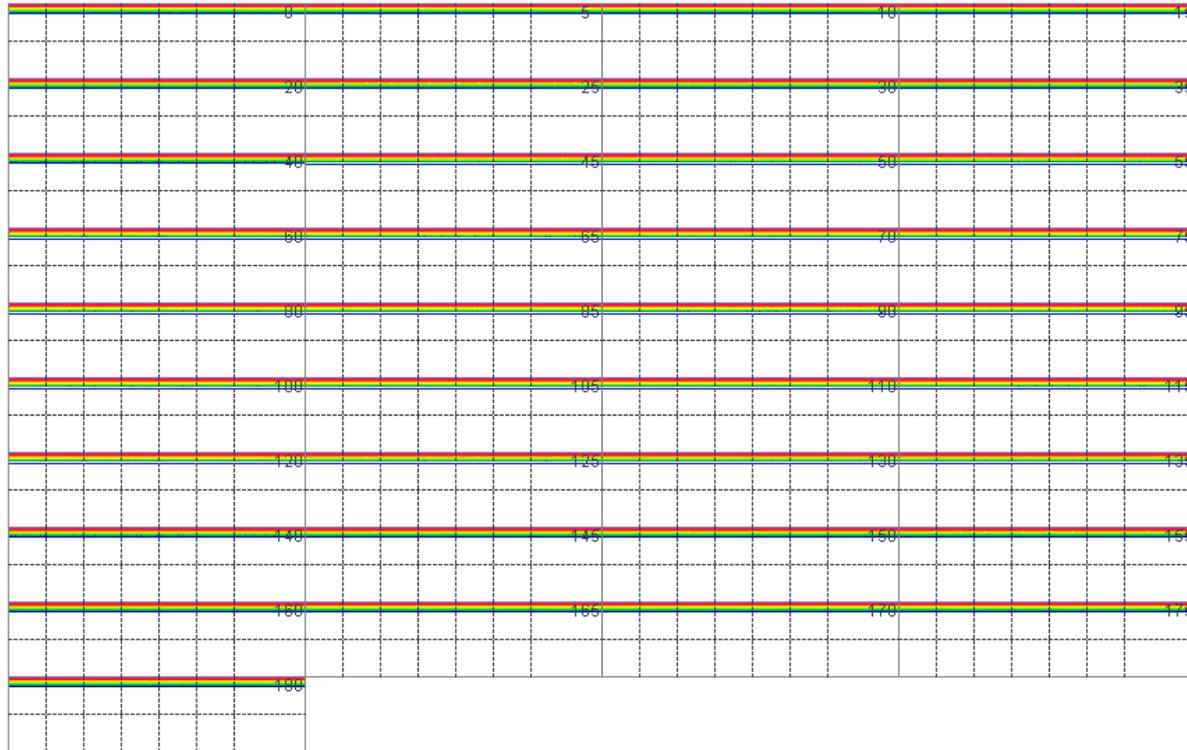
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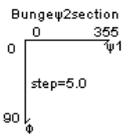
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Min=0.0



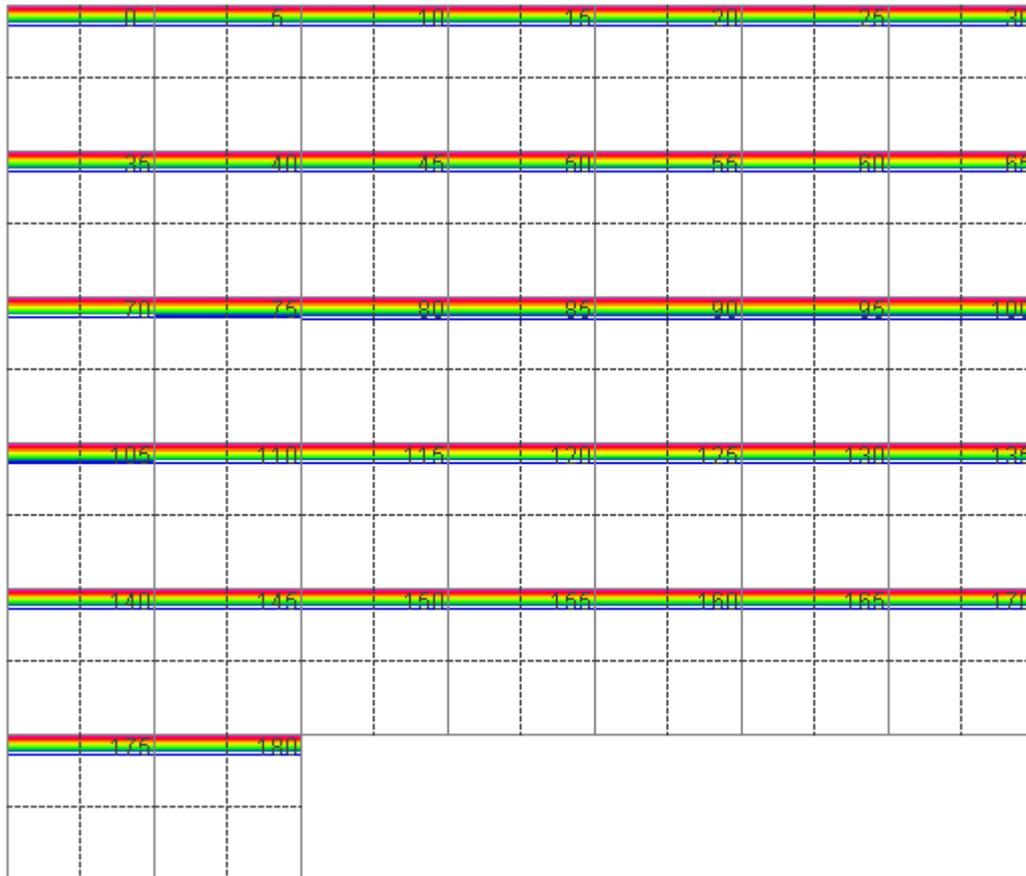
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Max=171
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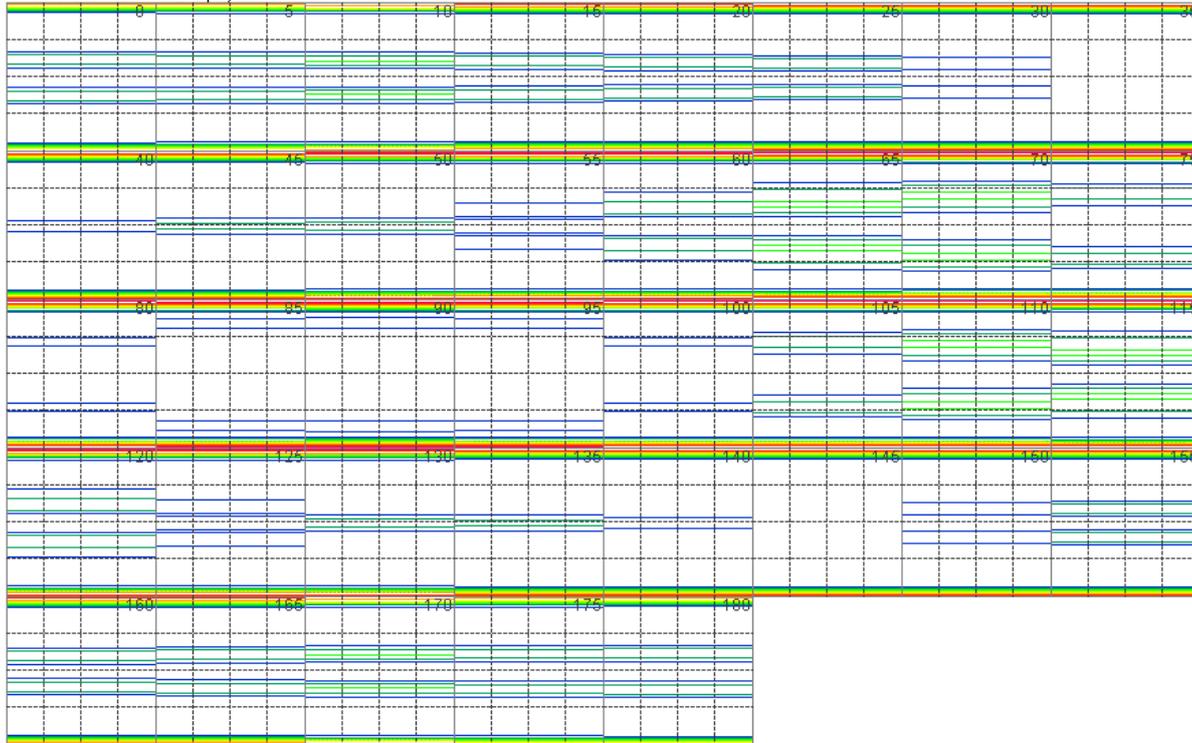
filename: C:\CTR\DATA\1-axis-polyethylene\laboabc\newODF\ODF-Ortho.bt



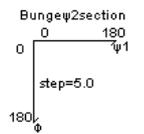
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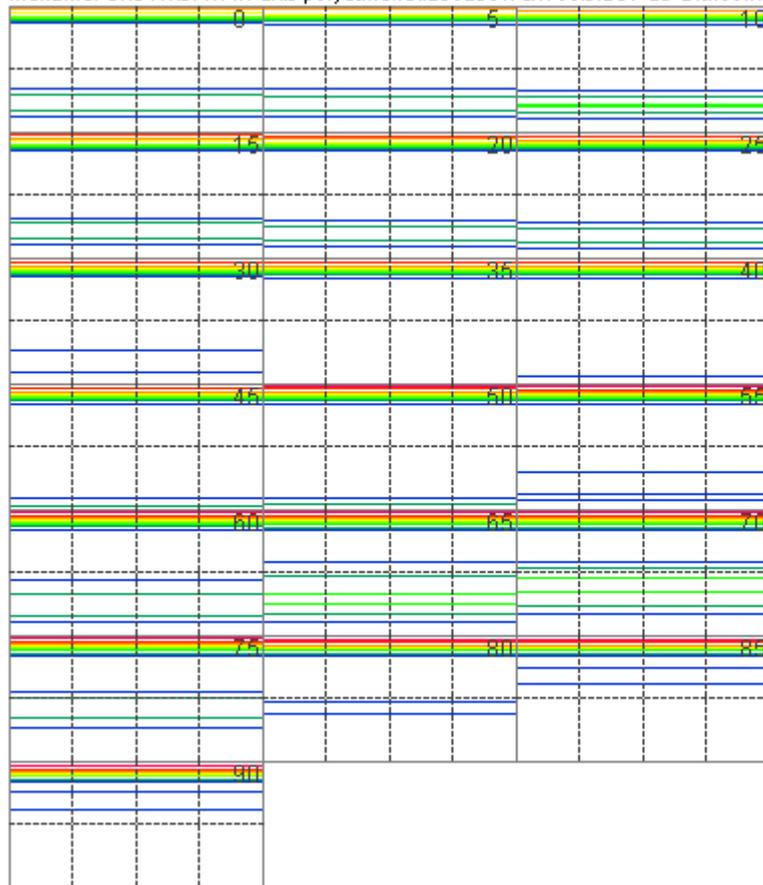
filename: C:\CTR\DATA\1-axis-polyethylene\laboabc\TexTools\ODF-abc.HODF



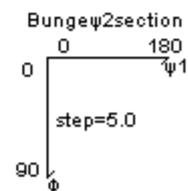
Max=8.79
Min=0.01



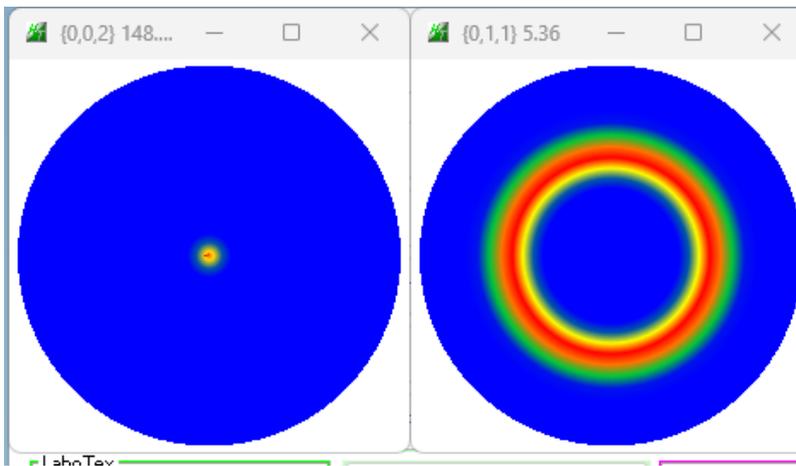
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Max=8.79
Min=0.01



軸回回転



PFRotation 1.19T[23/04/30] by CTR

File Help Polefigure(3D)

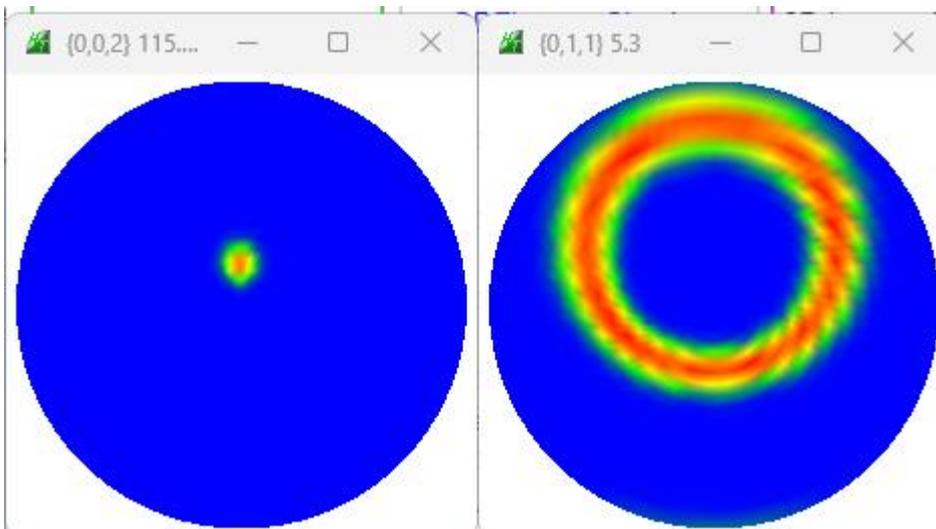
TXT2 files select
Path: C:\CTR\DATA\1-axis-polyethylene\laboabc
File: 002_labotexCCW-rp_2.TXT 011_labotexCCW-rp_2.TXT

Rotation(-360 <= degrees <= 360) of vector machine axis
AlongRD(X) 1 10 AlongTD(Y) 2 20 AlongND(Z) 3 30 4 0 toOrthorhombic Rotate PoleFigure

Check
Previous Next 002_labotexCCW-rpR10T20N30.TXT Alfa angle check

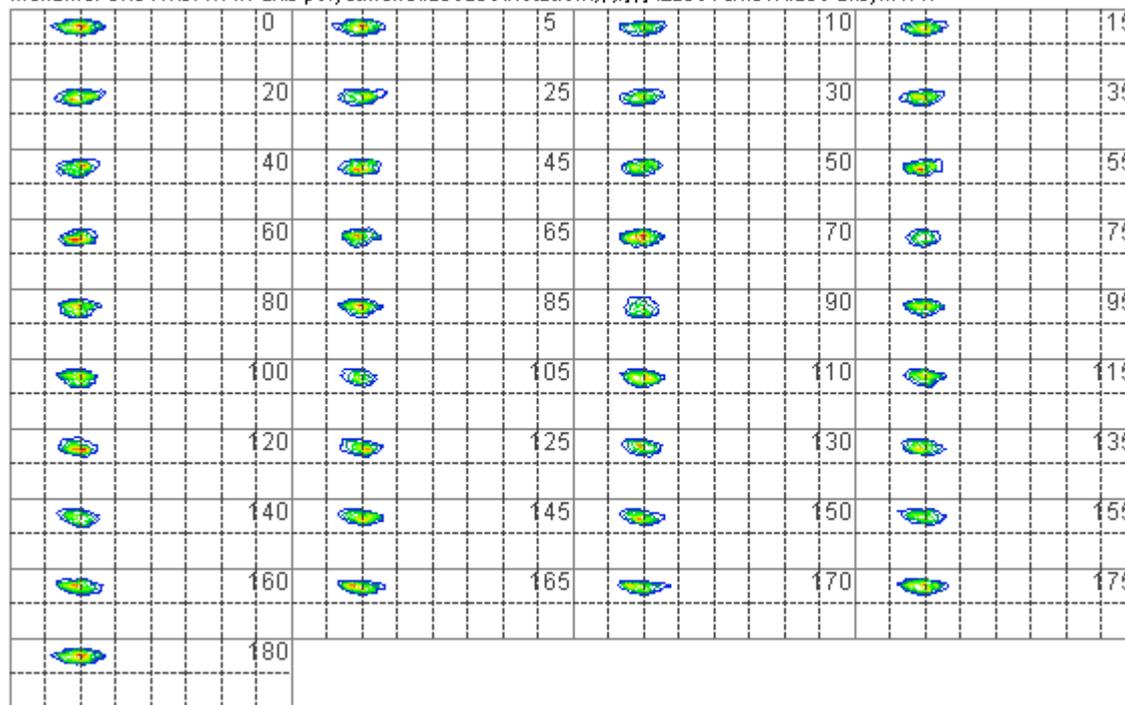
Save
 Normalization TXT(Pole) ASC(Pole) Ras(Pole) TXT2(Pole) Save

Create success !! PoleFigureStepChenger



LaboTex 非对称 1.0 1.941 2.913 90.0 90.0 90.0

filename: C:\CTR\DATA\1-axis-polyethylene\Laboabc\Rotation\非对称\LaboTex\CW\Labo-ansyn.TXT

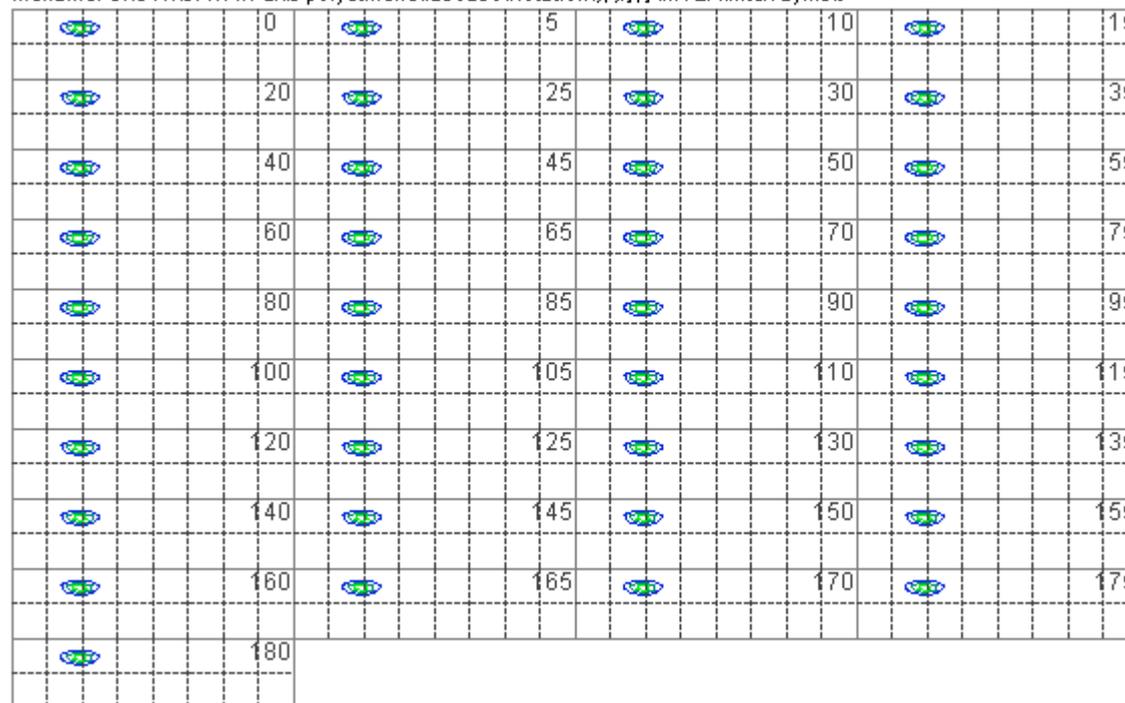


Max=182
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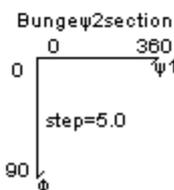
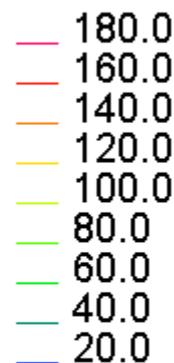


MTEX 1.0 1.941 2.913 90.0 90.0 90.0

filename: C:\CTR\DATA\1-axis-polyethylene\Laboabc\Rotation\非对称\MTEX\mtex-ansyn.bt

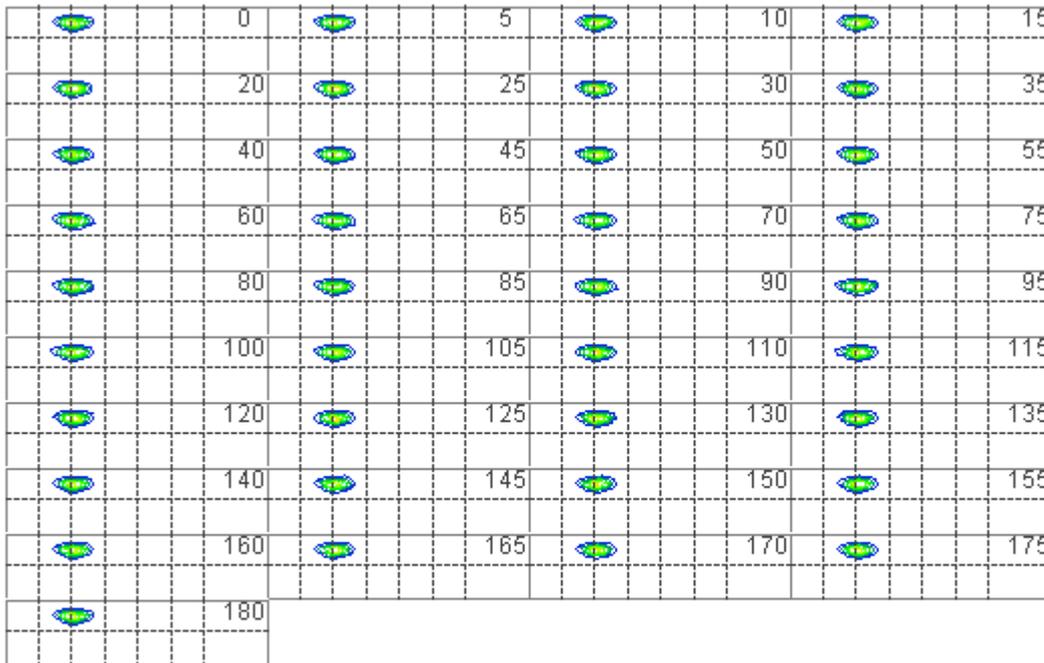


Max=73.1
Min=0.02

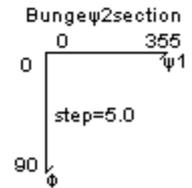
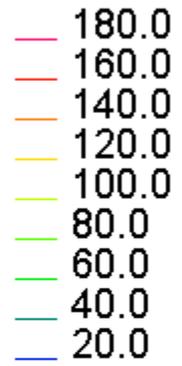


SmartLab 1.0 1.941 2.913 90.0 90.0 90.0

filename: C:\CTR\DATA\1-axis-polyethylene\Laboabc\Rotation\非对称\newODF\ODF-ortho.bt

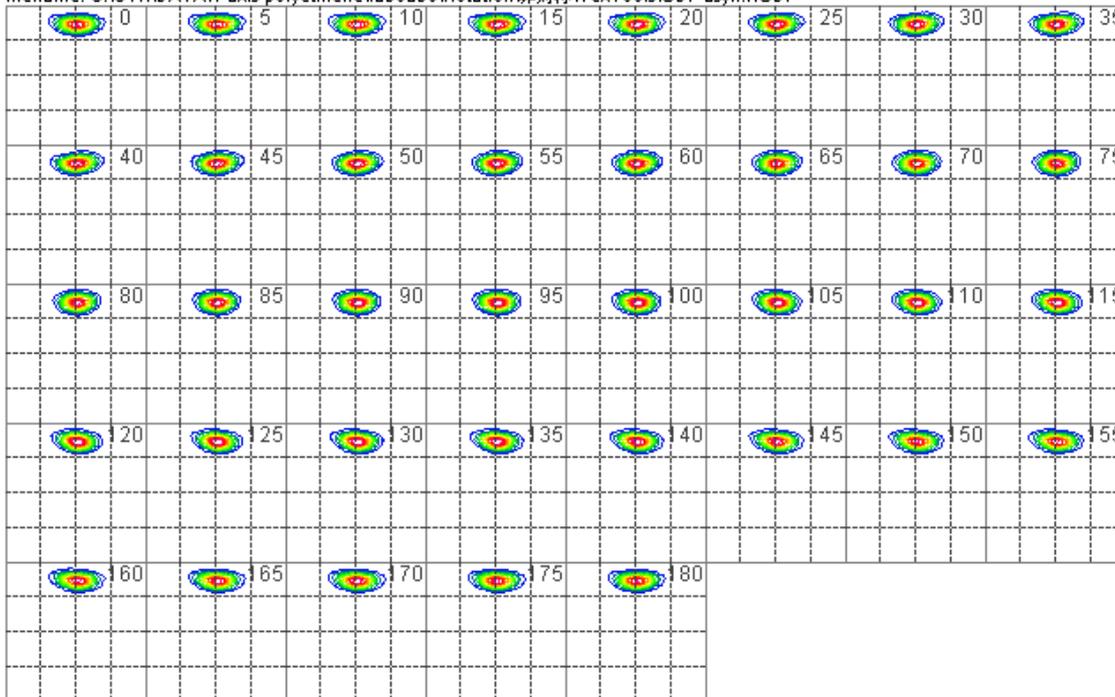


Max=134
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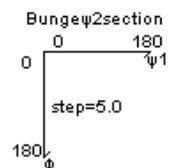
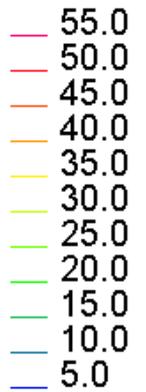


TexTools 1.0 1.941 2.913 90.0 90.0 90.0

filename: C:\CTR\DATA\1-axis-polyethylene\Laboabc\Rotation\非对称\TexTools\ODF-asyn.HODF

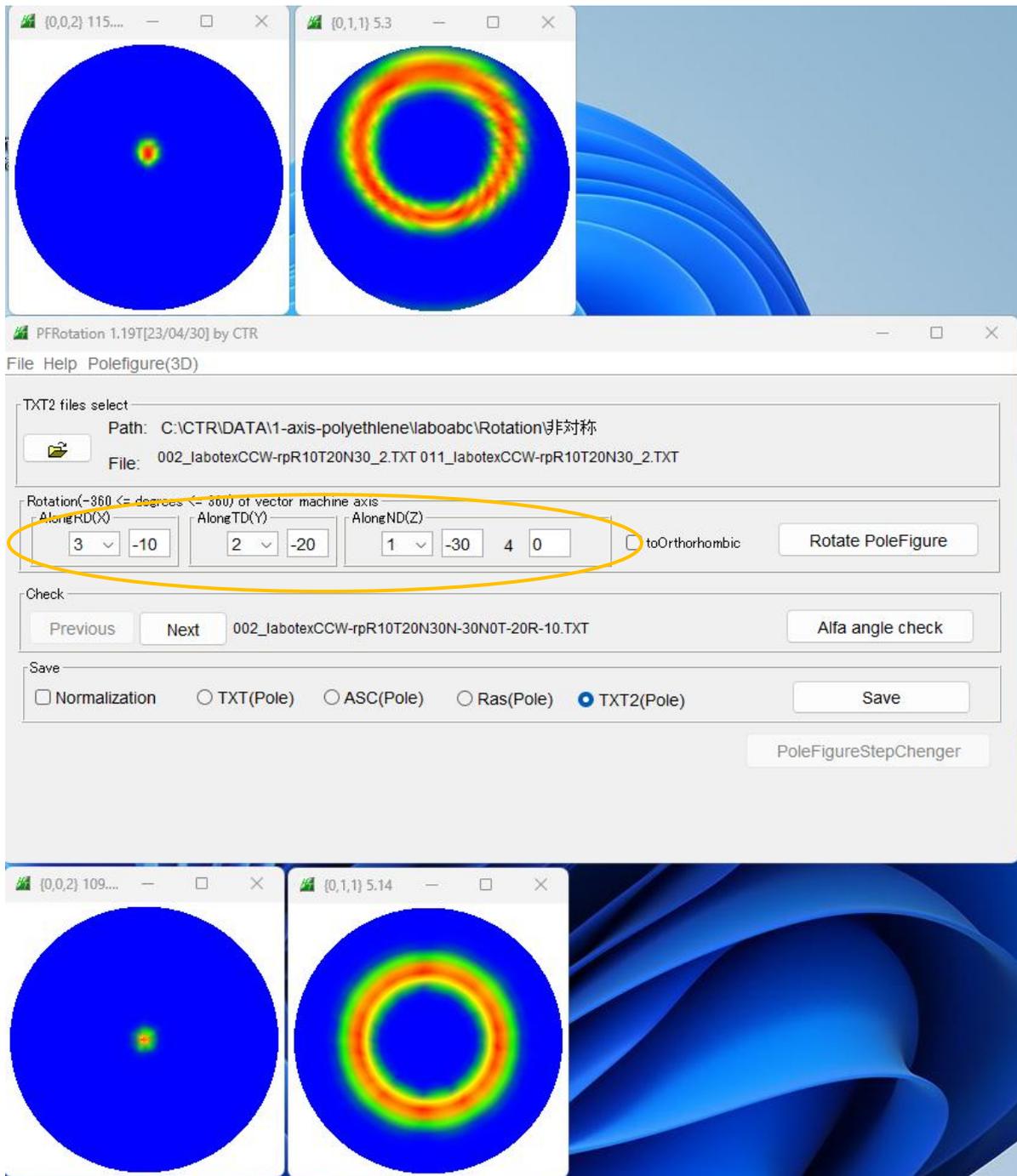


Max=63.3
Min=0.0



非対称極点図の定量

非対称のままでは解析が出来ないので、極点図、或いはODF後の再計算極点図から逆回転を行う。
回転には完全極点図が必要になります。



回転順を調整し、 $\{001\}$ - Fiberに回転を行い、Volume Fractionを計算す