

LaboTexによる結晶軸回転1

cube方位を [100] 軸45度回転でgoss方位を得る

を評価

2018年08月25日

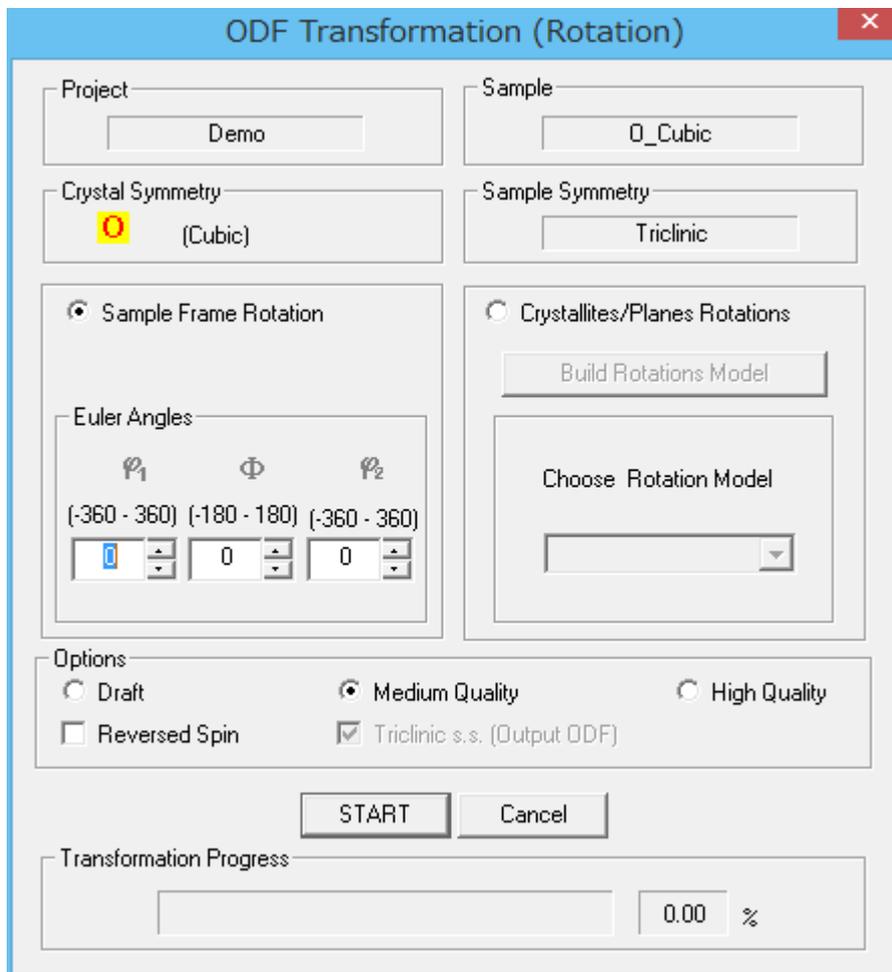
HelperTex Office

概要

LaboTexでは、Euler角度指定によるODF TransformationでTD方向の測定ODF図をND方向のODF図に変換し、材料の深さ方向の方位分布解析を行っていた。

今回は、特定の結晶方位を指定した方向を軸に回転する事を試してみます。

例として、cube {001} <100>を回転し、goss {011} <100>を作成します。



LaboTexのRotation画面

ODF図モデリングで cube 方位50%を作成

Crystal Symmetry: **C** (Cubic)
 Sample Symmetry: Orthorhombic
 Grid Cells for Output ODF: 5.0*5.0
 Step: 0.50
 Diagram Range +/-: 45.0

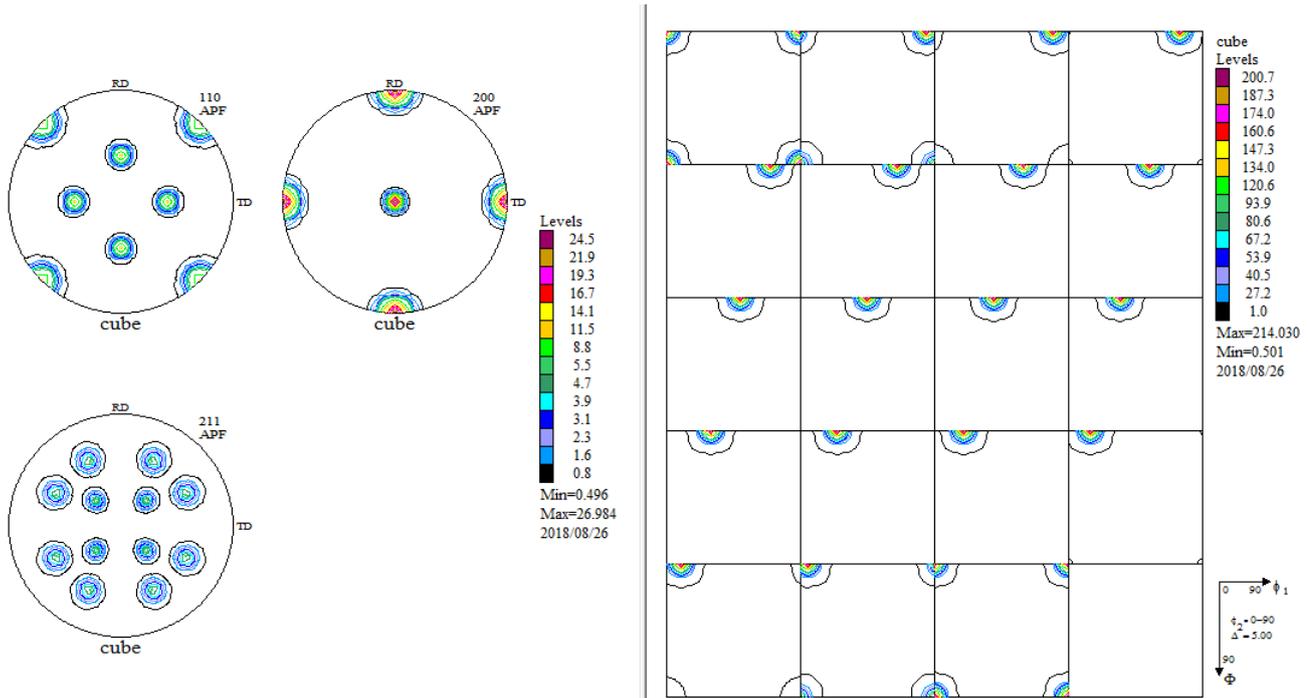
Component No. 1: 100.0%
 FWHM Φ_1 = 10.0
 FWHM Φ_2 = 10.0
 FWHM Φ_3 = 10.0

No	Texture Component	On	Distribution	FWHM Φ_1	FWHM Φ_2	FWHM Φ_3	Volume Fraction
1	{ 0 0 1 } < 1 0 0 > cube	<input checked="" type="checkbox"/>	Gauss	10.0	10.0	10.0	50 %
2	{ 1 1 2 } < 1 1 -1 > copper	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
3	{ 0 0 1 } < 1 0 0 > cube	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
4	{ 1 1 0 } < 0 0 1 > goss	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
5	{ 0 0 1 } < 1 1 0 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
6	{ 1 1 0 } < 1 -1 1 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
7	{ 1 1 1 } < -1 -1 2 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
8	{ 1 0 1 } < 5 2 5 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
9	{ 5 2 5 } < 1 -5 1 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
10	{ 0 1 3 } < 1 0 0 >	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %

Sample Name: cube
 Project Name: Demo
 Cell Parameters (Relative): a=1.0, b=1.0, c=1.0
 α =90.0, β =90.0, γ =90.0
 Max. Linearity:
 Background: 50 %

Creation of Model ODF Exit

gauss分布で半幅幅を10degとし、Volume Fractionを50%とする。
 作成されたODF図と極点図



このcube ODF図からgossを 軸回転で作成する。

c u b e 方位の軸回転 (材料系)

Build Crystallites (Planes) Rotations Model

Builded Models: Models Step: 0.50 Diagram Range +/-: 45.0 CP

ODF(max) 100.0% Static ODF(max) 100.0% Static ODF(max) 100.0% Static

0.50 $\Delta\varphi_1 = 15.00$ 45.0 0.50 $\Delta\Phi = 15.00$ 45.0 0.50 $\Delta\varphi_2 = 15.00$ 45.0

Rotations Parameters

No	Texture Component	On	Range of Euler Angles			Rotation Vector			Rotation Angle	% of Upturned Planes
			$\Delta\varphi_1$	$\Delta\Phi$	$\Delta\varphi_2$	h	k	l		
1	{ 0 0 1 } < 1 0 0 > cube	<input checked="" type="checkbox"/>	15.00	15.00	15.00	1	0	0	45	100 %
2	{ 0 1 3 } < 1 0 0 >	<input type="checkbox"/>	10.0	10.0	10.0	1	1	1	30	100 %
3	{ 1 1 0 } < 1 -1 2 > brass	<input type="checkbox"/>	10.0	10.0	10.0	1	1	1	30	100 %
4	{ 1 1 2 } < 1 1 -1 > copper	<input type="checkbox"/>	10.0	10.0	10.0	1	1	1	30	100 %
5	{ 1 1 0 } < 0 0 1 > goss	<input type="checkbox"/>	10.0	10.0	10.0	1	1	1	30	100 %
6	{ 0 0 1 } < 1 1 0 >	<input type="checkbox"/>	10.0	10.0	10.0	1	1	1	30	100 %
7	{ 1 1 0 } < 1 -1 1 >	<input type="checkbox"/>	10.0	10.0	10.0	1	1	1	30	100 %
8	{ 1 1 1 } < -1 -1 2 >	<input type="checkbox"/>	10.0	10.0	10.0	1	1	1	30	100 %
9	{ 1 0 1 } < 5 2 -5 >	<input type="checkbox"/>	10.0	10.0	10.0	1	1	1	30	100 %
10	{ 5 2 5 } < 1 -5 1 >	<input type="checkbox"/>	10.0	10.0	10.0	1	1	1	30	100 %

Warning: Only Crystallites/Planes Inside Region Around Chosen Texture Component and its Symmetrical Equivalent Positions are Rotated.

Save Transformation Model Close

軸回転は最大 10 個、今回は c u b e を 100%[100]軸に 45 度回転

ODF Transformation (Rotation)

Project: Demo Sample: cube

Crystal Symmetry: **C** (Cubic) Sample Symmetry: Orthorhombic

Sample Frame Rotation Crystallites/Planes Rotations

Euler Angles: φ_1 Φ φ_2
 (-360 - 360) (-180 - 180) (-360 - 360)
 0 0 0

Build Rotations Model

Choose Rotation Model: cube-R100-45

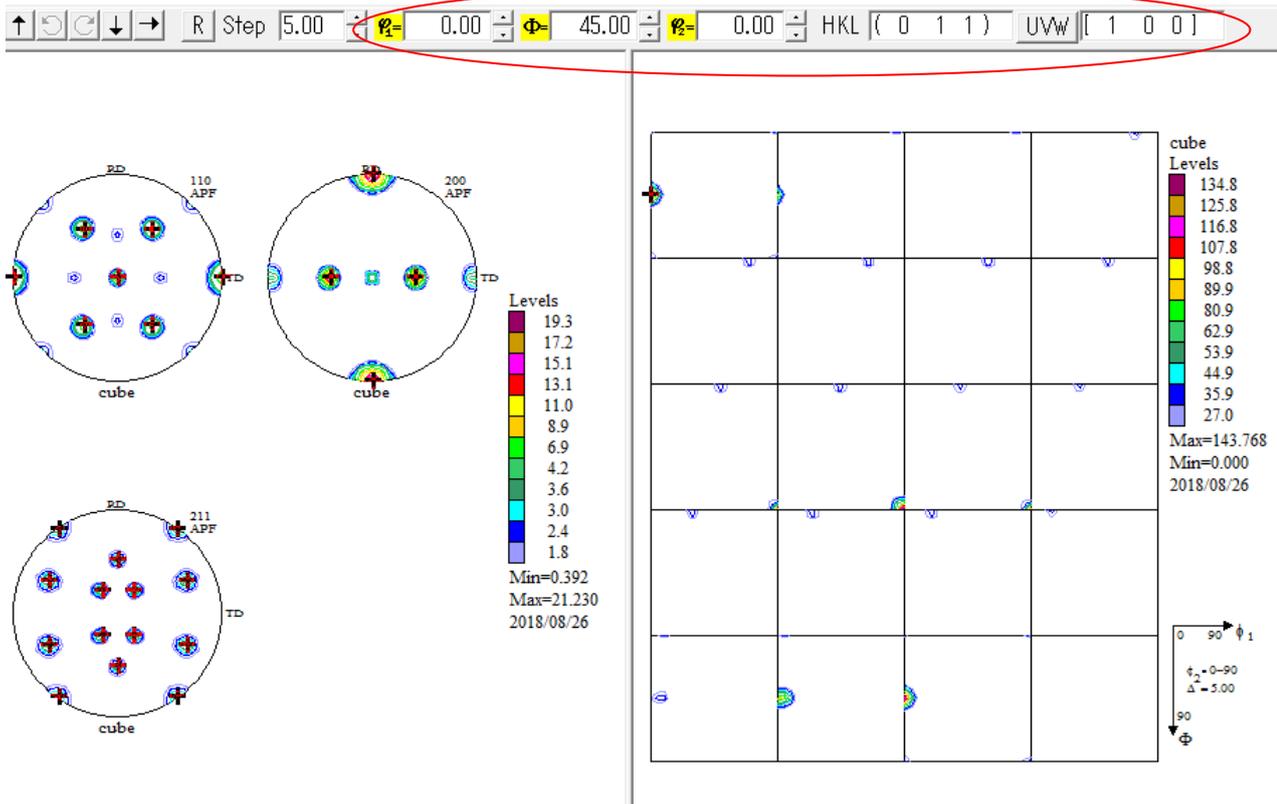
Options: Draft Medium Quality High Quality
 Reversed Spin Triclinic s.s. (Output ODF)

START Cancel

Transformation Progress: 0.00 %

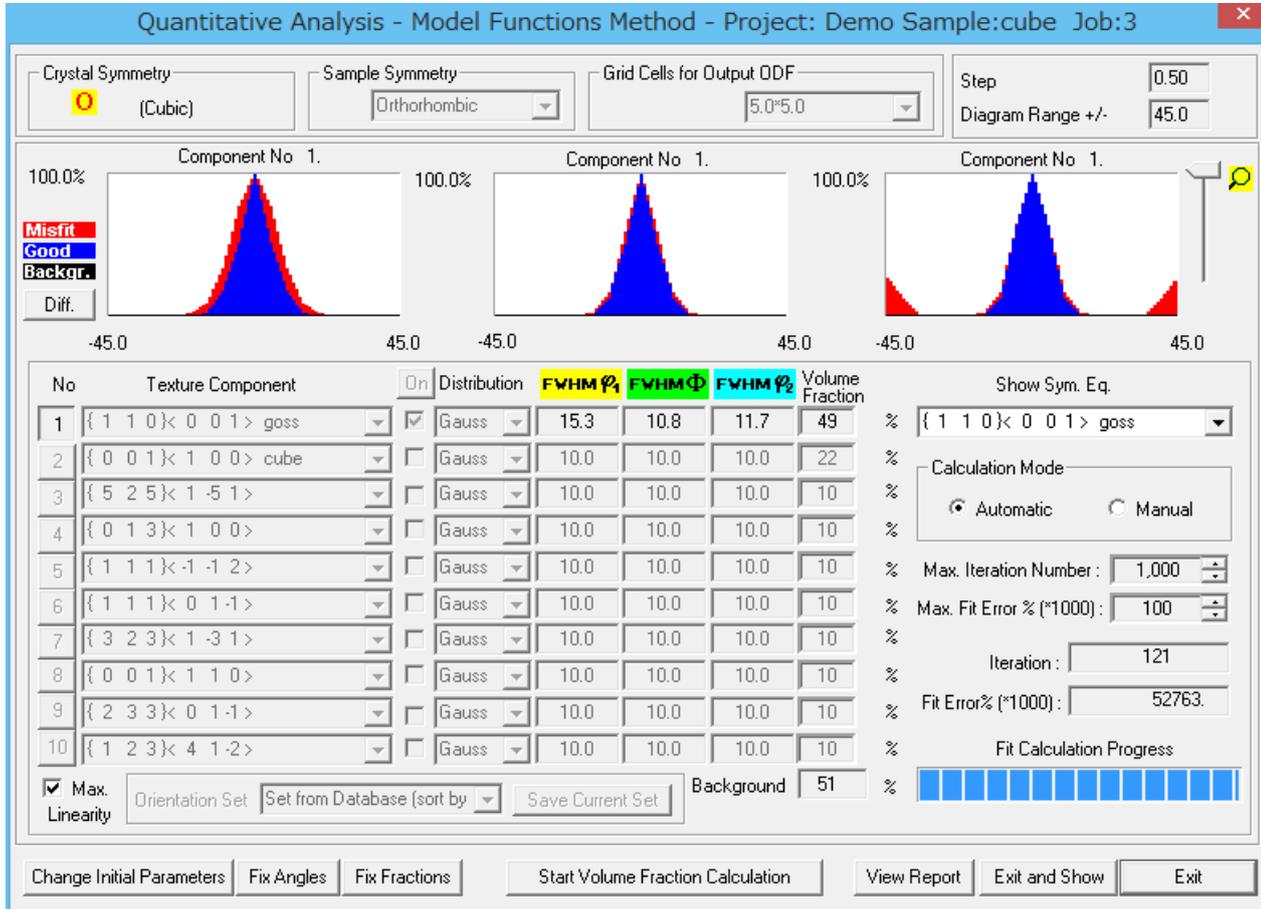
Orthorhombicで作成

cubeを[100]軸に45deg回転で{011}<100>が作成される。

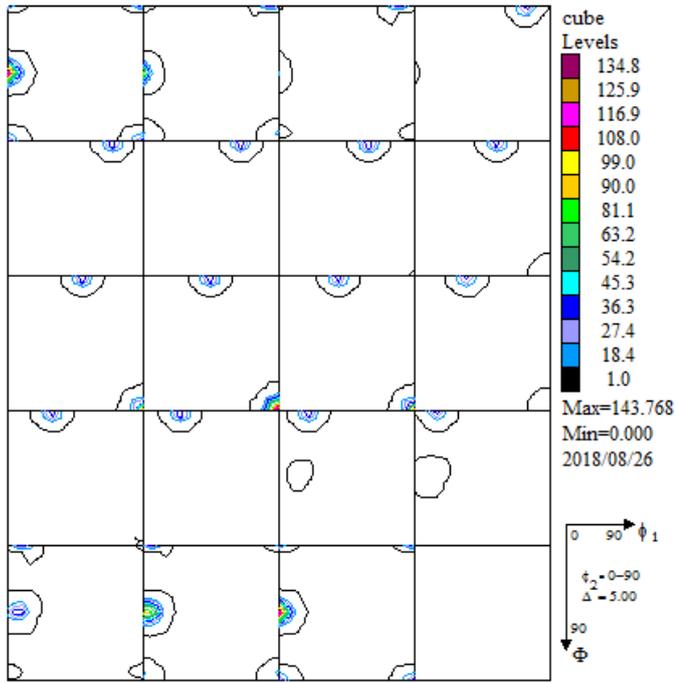


若干のcube方位が残っているがgoss方位が得られる。

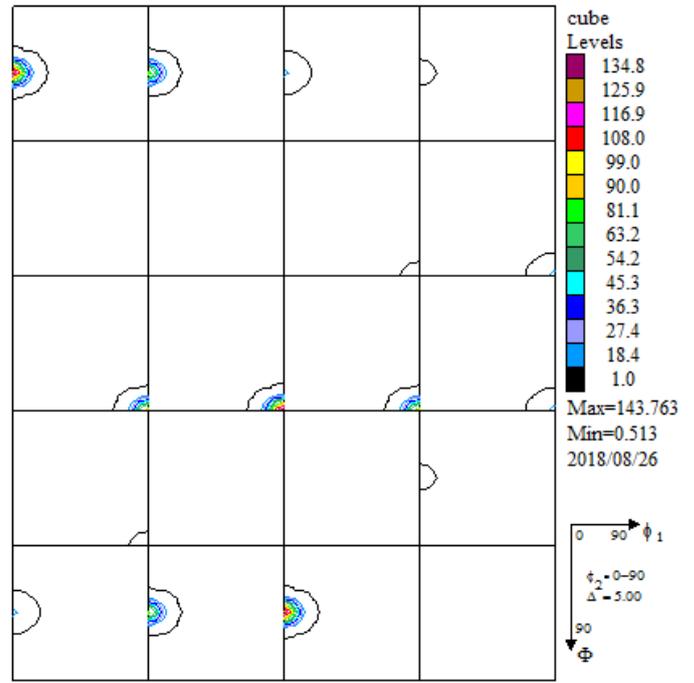
Volume Fraction計算 49%を得る。



cube を[100] 軸 45 度回転の ODF 図



VolumeFraction 4.9%から計算した ODF 図

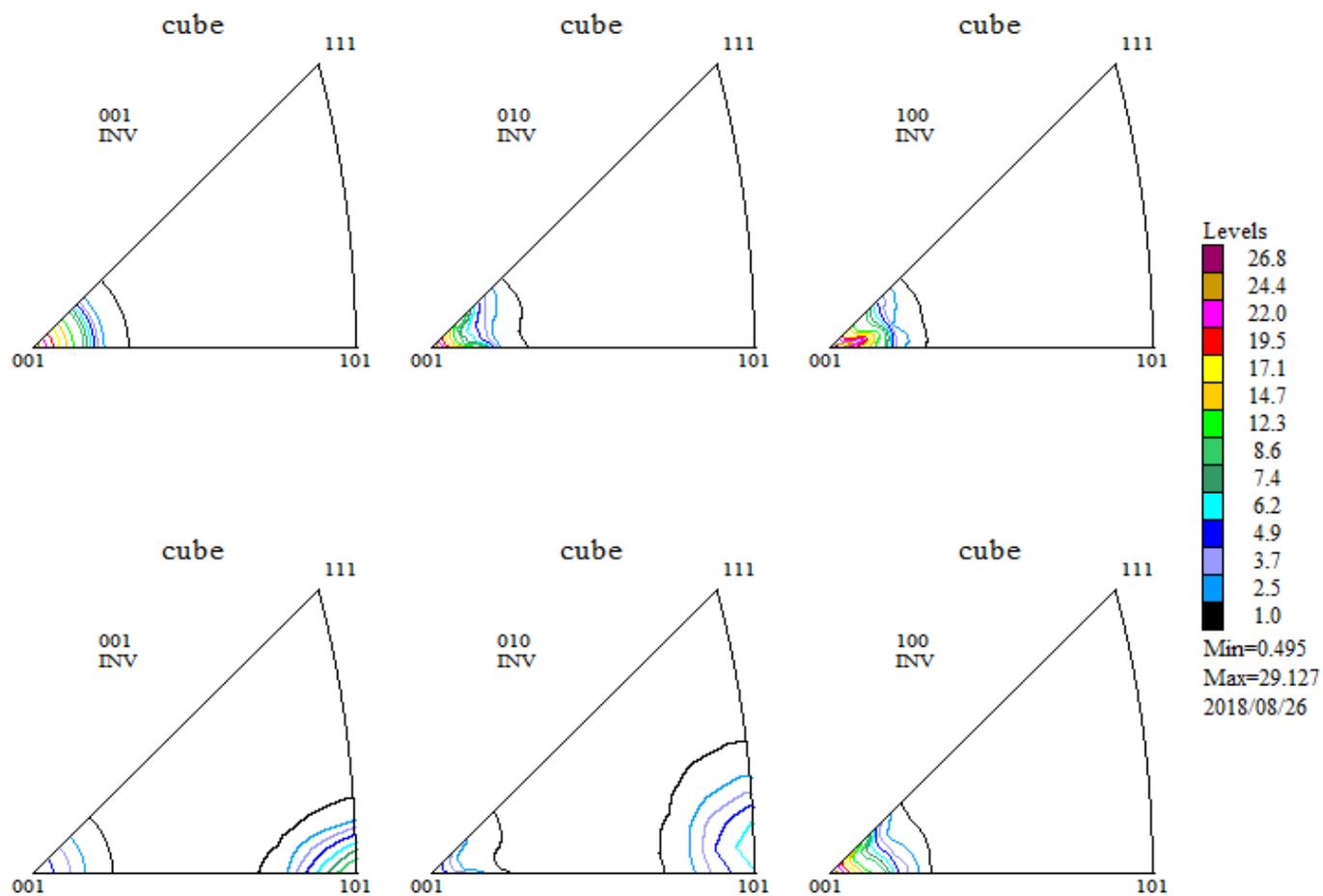


LaboTex - Texture - Quantitative Analysis Report
 User: R1
 Project: Demo
 Sample: cube
 Job: 5
 Date: 2018/08/26
 Time: 10:16:45

Volume Fraction	FWHM Phi1	FWHM Phi	FWHM Phi2	Orientation
Component No 1 - Distribution :Gauss 48.72	15.3	10.8	11.7	{ 1 1 0 } < 0 0 1 > goss
51.28	Background Volume Fraction			

4.9%は48.72%で、差0.28%はcube方位が残っているが、

c u b e (上段) と g o s s (下段) の逆極点図



回転軸を結晶系で計算する。

The screenshot shows the 'CrystalRotation 1.00T[19/03/31] by CTR' application window. It features a menu bar with 'File' and 'Help'. The main interface is divided into several sections:

- Input Section:** A field for Miller indices $\{hkl\} \langle uvw \rangle$ with dropdown menus set to 0, 0, 1, 1, 0, 0.
- Rotation Vector:** A field with dropdown menus set to 1, 0, 0.
- Rotation Angle:** A text input field containing '45' and a 'Calc' button.
- Result Section:** A scrollable text area displaying the following output:

```
{001}<100>      eulerangle:(0.0,0.0,0.0)
g( $\psi_1 \Phi \psi_2$ )=
  1.0   0.0   0.0
  0.0   1.0   0.0
  0.0   0.0   1.0
Rotation [100]  angle:45.0
CalcN=(1.0,0.0,0.0)
a(100),45.0=
  1.0   0.0   0.0
  0.0   0.7071  0.7071
  0.0  -0.7071  0.7071
ag=
  1.0   0.0   0.0
  0.0   0.7071  0.7071
  0.0  -0.7071  0.7071
Calc Miller indices
  {0 1 1}<1 0 0>
```