

## P o l y p r o p y l e n の O D F 解析例

Monoclinic の ODF 解析は L a b o T e x、T e x T o o l s で行えるが、基本軸の扱い、極点図の回転方向の考えが異なるため、ややこしくなっています。

T e x T o o l s

TD方向は極点図の左側 (CCW)

結晶系は、b a x i s - S e t t i n g

L a b o T e x

TD方向は極点図の左側 (CW)

結晶系は、c a x i s - S e t t i n g

B → C - a x i s 変換の場合、{ 1 - h k } とすべきである。

2013年12月12日

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テストデータ

LaboTexで  $\{1\ 2\ 1\} \langle 1\ -1\ 1 \rangle$  非対称ODF図から  
 $\{1\ 2\ 1\}$ 、 $\{0\ -1\ 1\}$ 、 $\{1\ -1\ 1\}$  極点図を作成する

**Model ODF**

Crystal Symmetry:  $C_2$  (Monoclinic) | Sample Symmetry: Triclinic | Grid Cells for Output ODF: 5.0\*5.0 | Step: 0.50 | Diagram Range +/-: 45.0

Centre of Orientation (3 plots) | FWHM  $\phi_1 = 10.0$  | FWHM  $\Phi = 10.0$  | FWHM  $\phi_2 = 10.0$

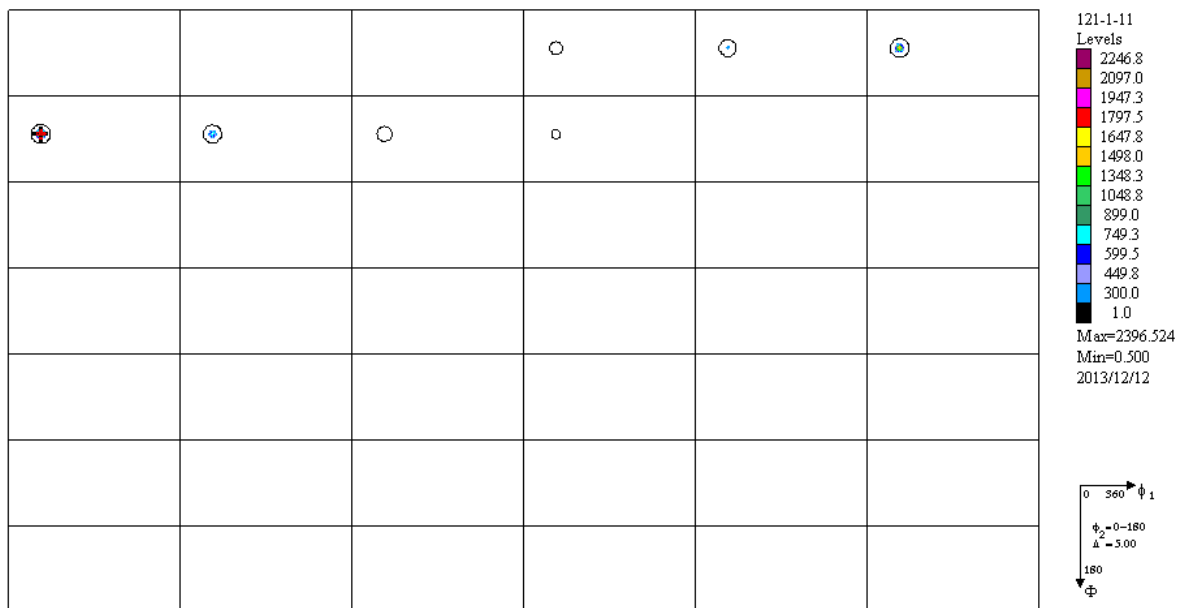
No	Texture Component	On	Distribution	FWHM $\phi_1$	FWHM $\Phi$	FWHM $\phi_2$	Volume Fraction
1	$\{1\ 2\ 1\} \langle 1\ -1\ 1 \rangle$	<input checked="" type="checkbox"/>	Gauss	10.0	10.0	10.0	50 %
2	( 54.74, 90.0, 45.) brass	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
3	( 39.23, 65.91, 26.5) copper	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
4	( 0.0, 45., 0.) goss	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
5	( 45., 90., 0.)	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
6	( 35.26, 90., 45.)	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
7	( 35.26, 90., 45.)	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
8	( 90., 54.74, 45.)	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
9	( 74.21, 45., 90.)	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %
10	( 15.23, 47.12, 68.20)	<input type="checkbox"/>	Gauss	10.0	10.0	10.0	10 %

Sample Name: 121-1-11 | Project Name: Demo | Cell Parameters (Relative): a: 1.0, b: 1.02, c: 1.1969,  $\alpha$ : 90.0,  $\beta$ : 90.0,  $\gamma$ : 80.5

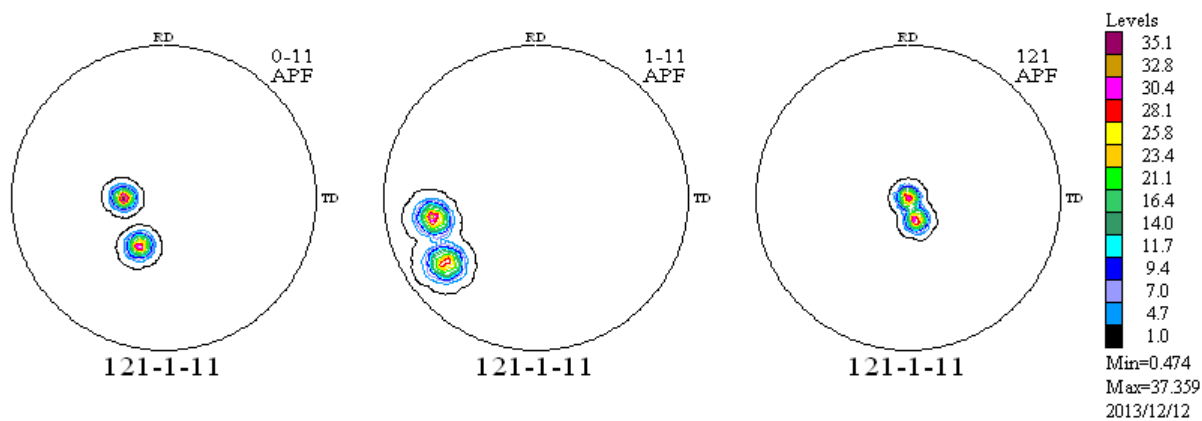
Max. Linearity:  | Background: 50 %

Creation of Model ODF | Exit

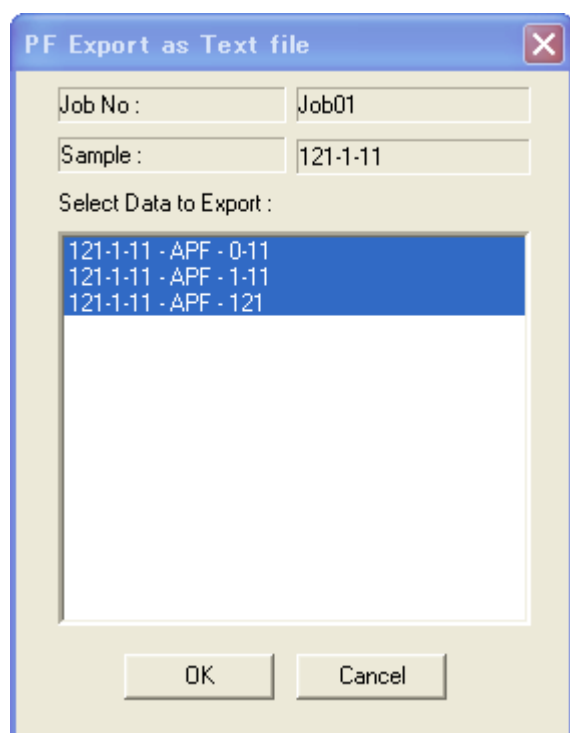
Step 5.00 |  $\phi_1 = 69.43$  |  $\Phi = 81.44$  |  $\phi_2 = 28.78$  | HKL ( 1 2 1 ) | Uvw [ 1 -1 1 ]



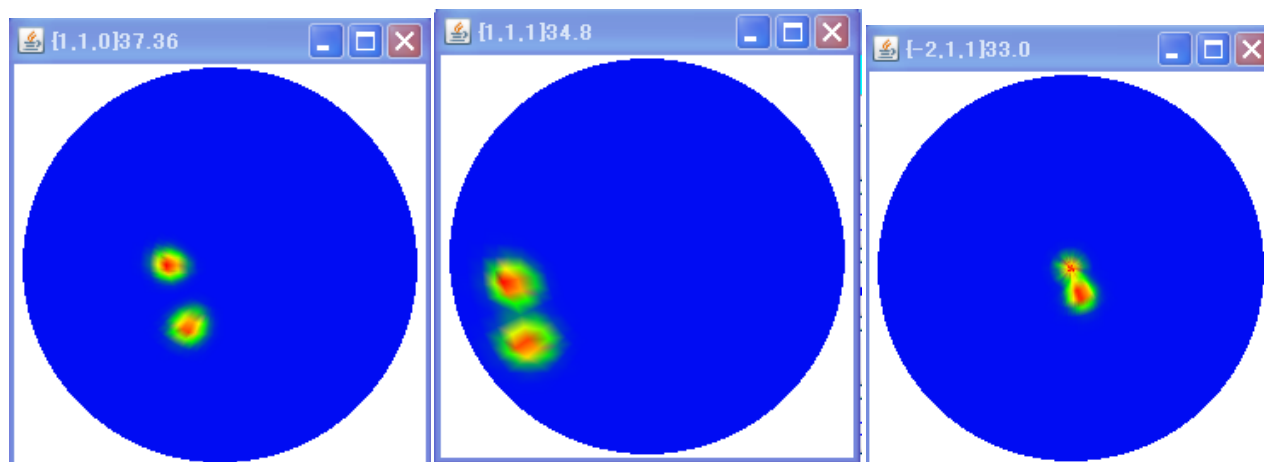
再計算極点図



PF-Export



c-Axis → B-Axis 変換



このB-axis極点図からTextoolsで解析を行う。

Lattice constant

Material  $\alpha$ -Polypropylene.txt

Structure Code(Symmetries after Schoenfiles) 2 - C2 (monoclinic)

a 1.0 <=b 3.1342 <=c 0.9804 alfa 90.0 beta 99.5 gamm 90.0

Initialize Start

getHKL<-Filename AllFileSelect

PF Data

SelectFile(TXT(b,intens),TXT2(a,b,intens.))	h,k,l	2Theta	Alfa Area	AlfaS	AlfaE	Select
-211_labotex-rp_2.TXT	-2,1,1	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>
110_labotex-rp_2.TXT	1,1,0	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>
111_labotex-rp_2.TXT	1,1,1	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>

L a b o t e x の場合

Lattice constant

Material  $\alpha$ -Polypropylene.txt

Structure Code(Symmetries after Schoenfiles) 2 - C2 (monoclinic)

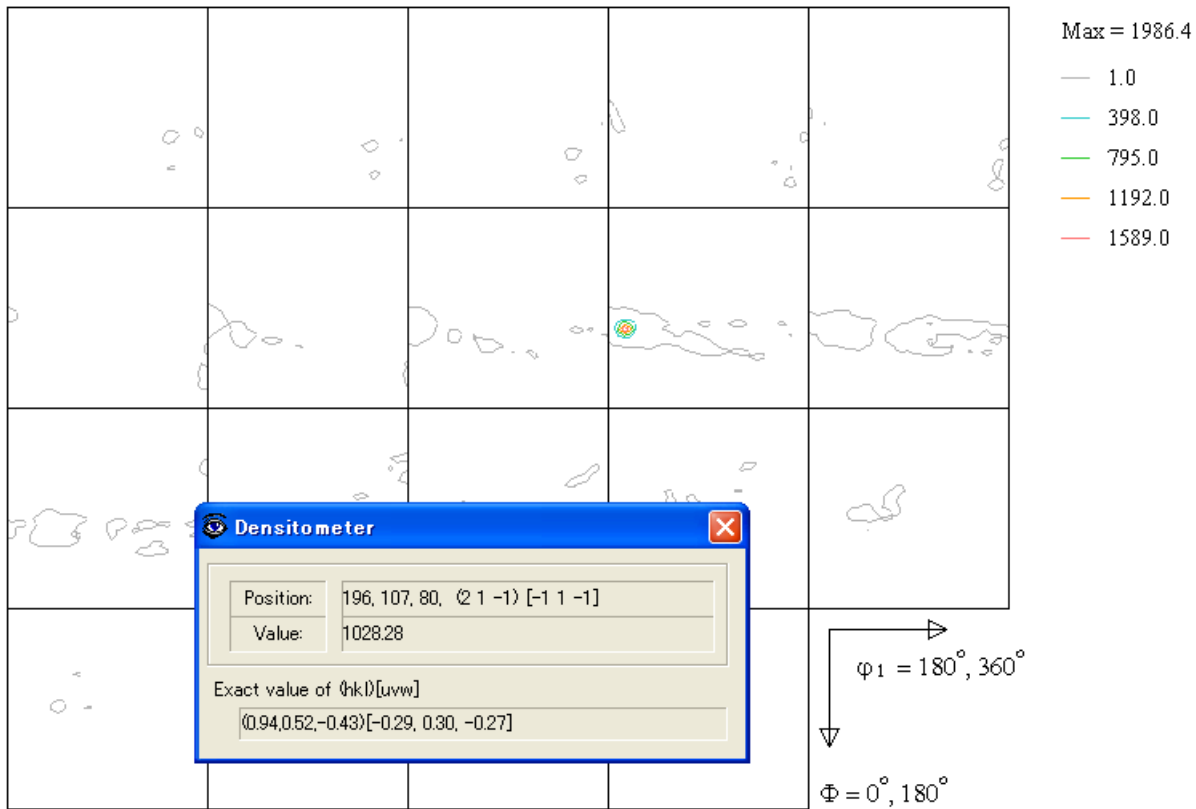
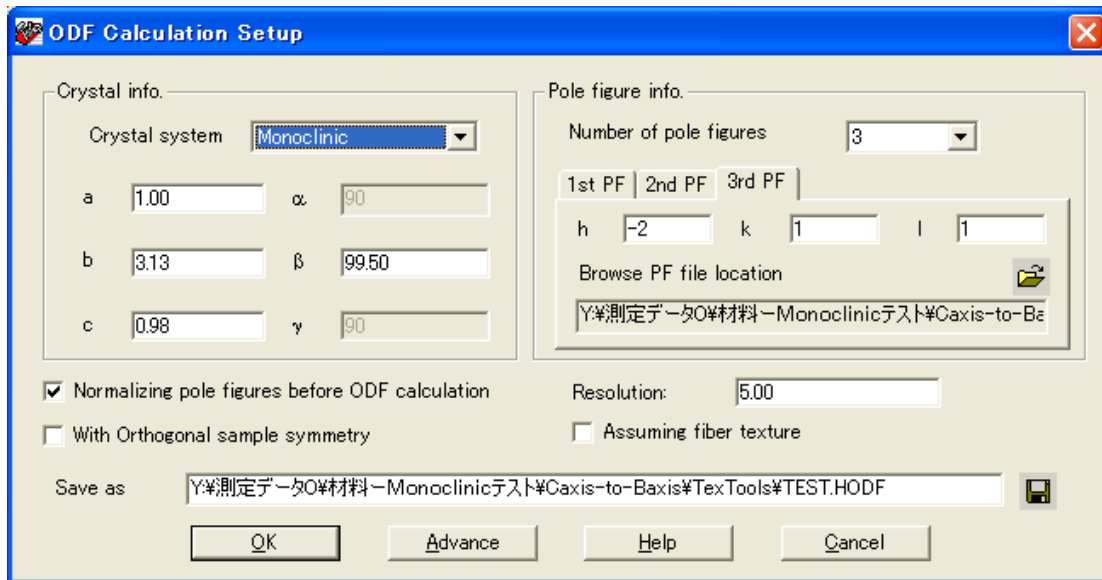
a 1.0 <=b 1.02 <=c 3.1969 alfa 90.0 beta 90.0 gamm 80.5

Initialize Start

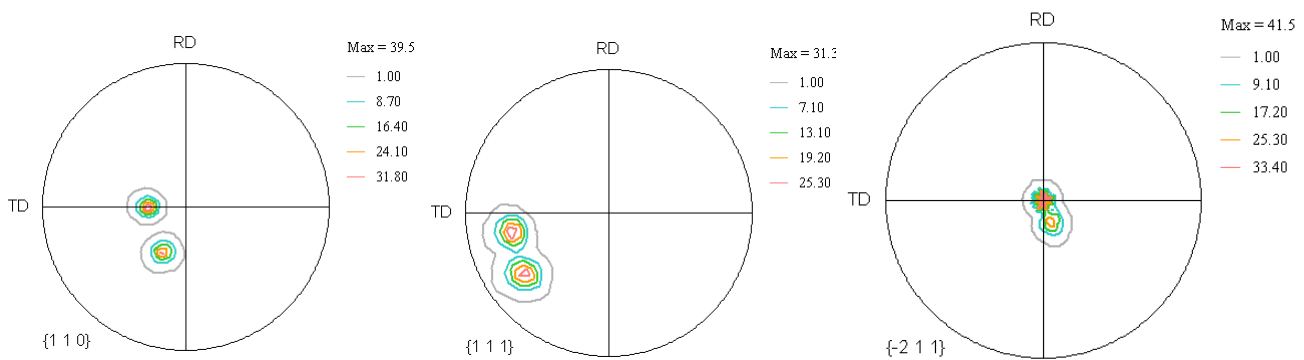
getHKL<-Filename AllFileSelect

PF Data

SelectFile(TXT(b,intens),TXT2(a,b,intens.))	h,k,l	2Theta	Alfa Area	AlfaS	AlfaE	Select
-211_labotex-rp_2.TXT	1,2,1	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>
110_labotex-rp_2.TXT	0,-1,1	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>
111_labotex-rp_2.TXT	1,-1,1	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>

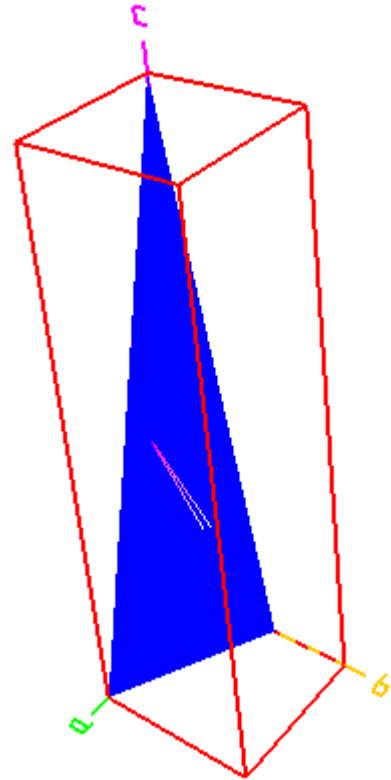
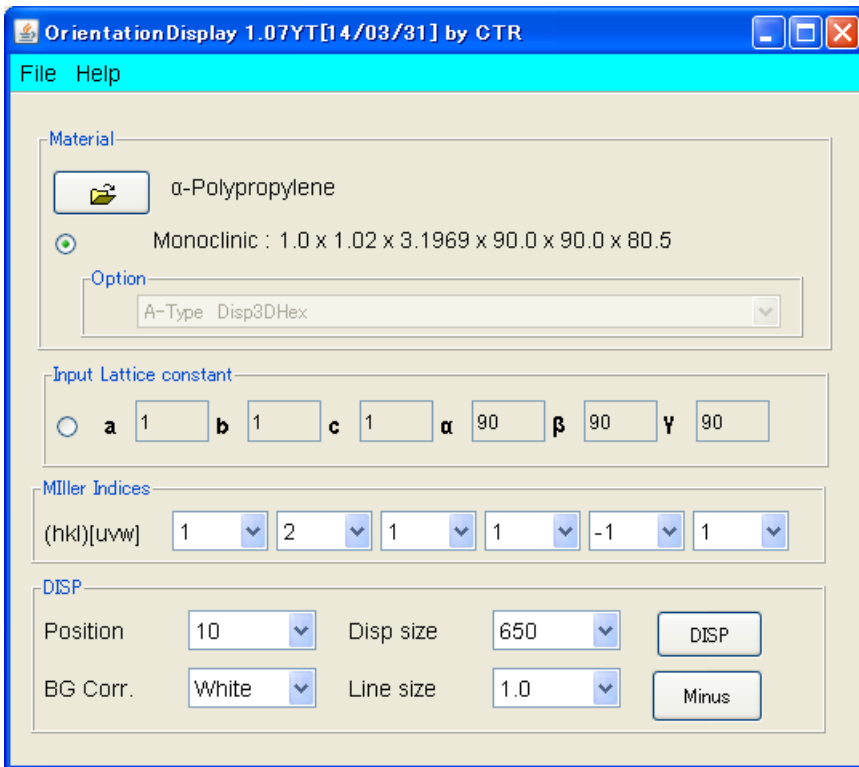


1



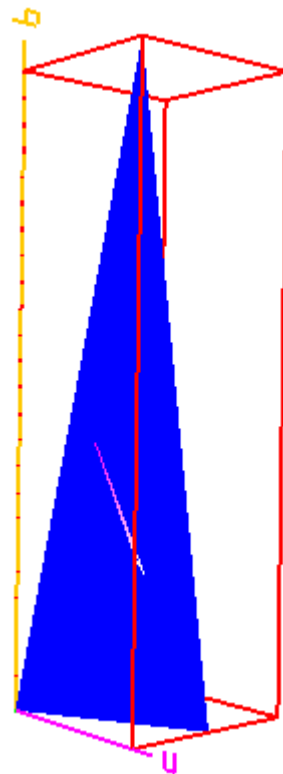
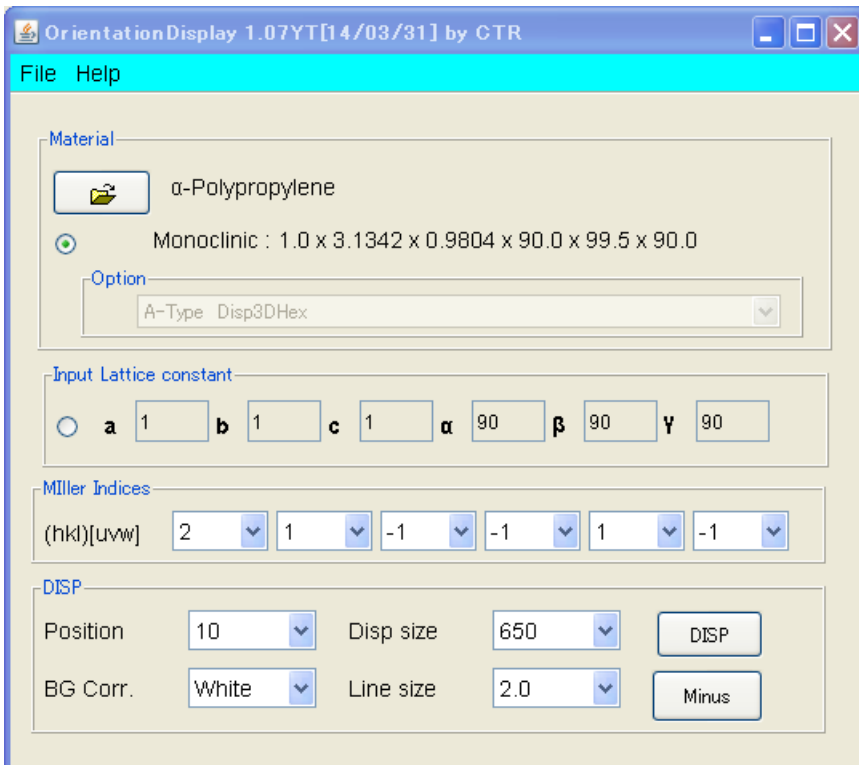
LaTeXでは

$$\{121\} \langle 1-11 \rangle$$



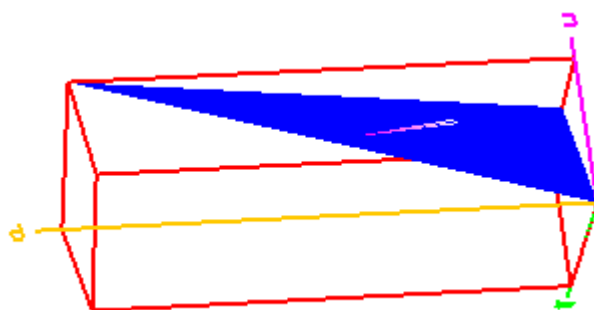
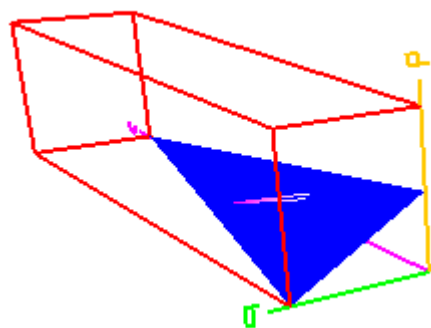
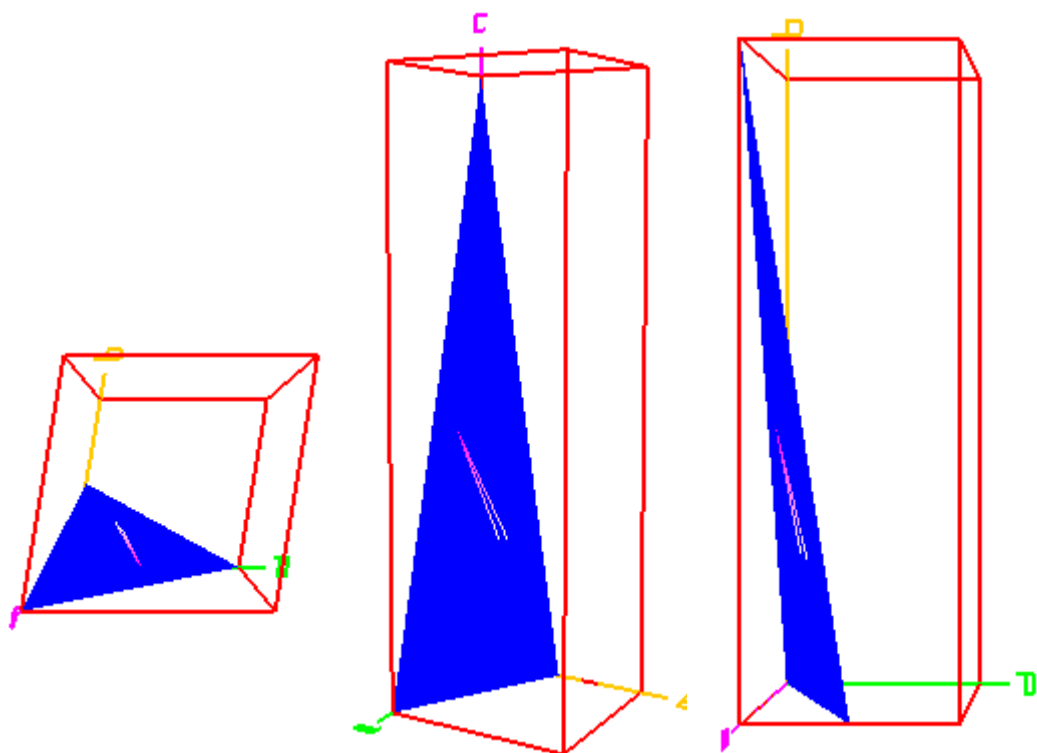
TeXToolsでは

$$\{21-1\} \langle -11-1 \rangle$$



LaTeX表示

TeXTools表示



LaTeXでは、 $\{h k l\} \longrightarrow \{1 - h k\}$  と変換するが、 $\{1 h k\}$  とした場合

Lattice constant

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Initialize

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AllFileSelect

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SelectFile(TXT(b,intens),TXT2(a,b,intens.))	h,k,l	2Theta	Alfa Area	AlfaS	AlfaE	Select
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110_labotex-rp_2.TXT	0,1,1	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>
111_labotex-rp_2.TXT	1,1,1	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>

ODF Calculation (Finished)

Rp

dRp

Calculation Progress (100.0%)

Cycle	Iteration(Max. = 30)	Iteration (total)	Rp%](Lim. = 1.00)	dRp%](Lim. = 1.00)
3	3	37	37.67	0.95

Creation of pole figures files NPF and RPF

Creation of orientation distribution file ODF

Creation of inverse figures file INV

END OF ODF CALCULATION

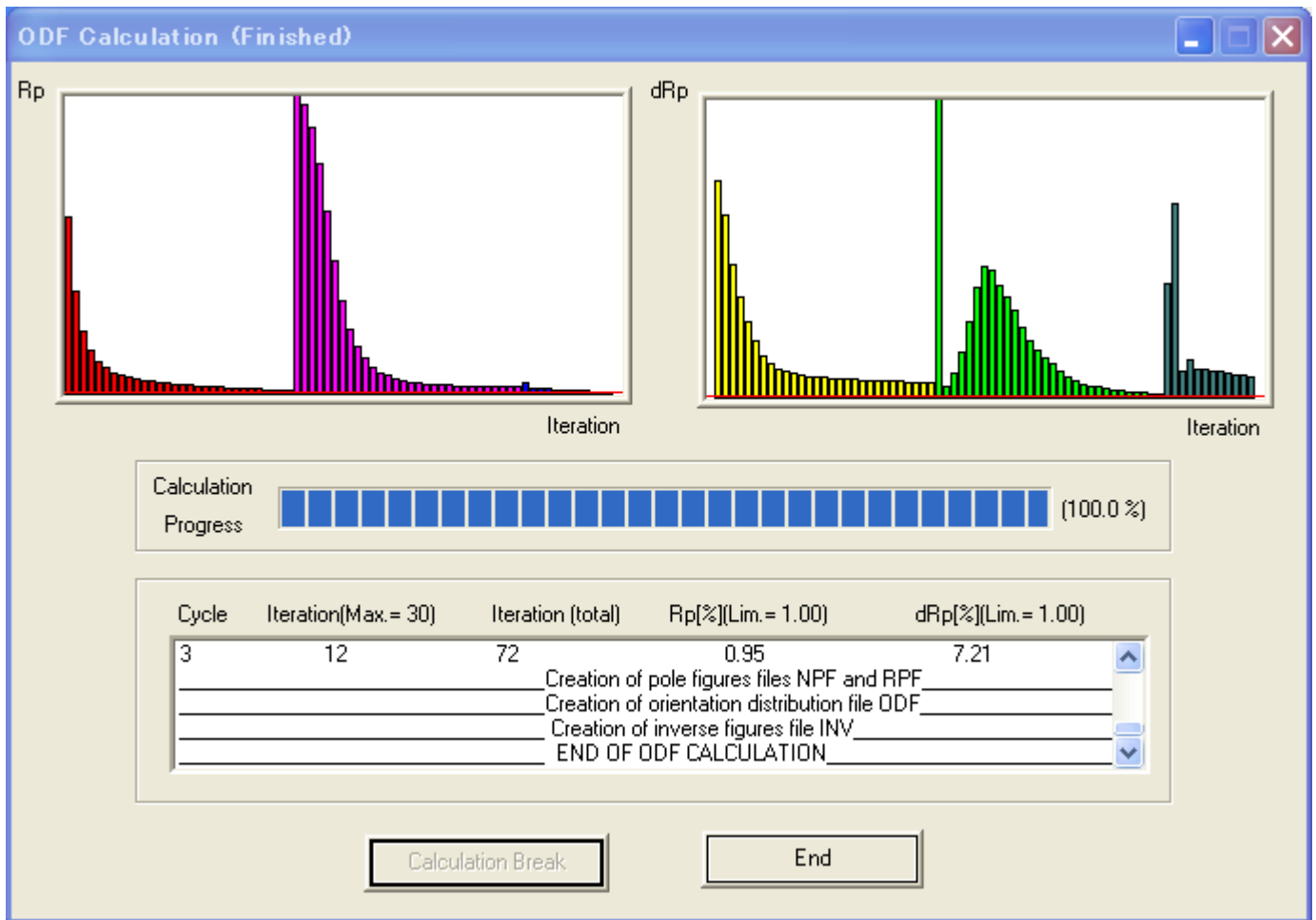
Calculation Break

End

Errorが大きい



LaboTexでは、 $\{hk1\} \longrightarrow \{1-hk\}$  とした場合



Errorは小さい

やはり、C-Axisの場合、 $\{1-hk\}$  である。