

2種類の β -P o l y p r o p y l e n e

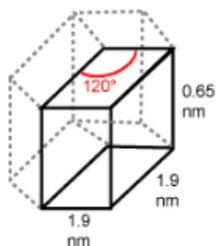
2025年10月27日

HelperTex Office

概要

β -polypropylene の文献を検索すると以下の2種類がhitする。

Beta phase



β Phase

- This phase is metastable, and the crystals are pseudo-hexagonal.
- β -phase is mainly found in block PP copolymers and can be generated by addition of specific nucleating agents.
- This form was discovered by Padden and Keith in 1953 and can be improved by crystallization between 130 and 132°C or by orientation with high shear or through addition of specific nucleating agents.
- Presence of β -phase in PP homopolymer generally increase ductility in the finished parts. Maximum effect is observed at 65% of β -phase.

until 1994 that Meille [9] and Lotz [10] independently established that the β -crystal was a rhombohedral crystal structure, and that the unit cell parameters were $a = b = 11.01 \text{ \AA}$, $c = 6.5 \text{ \AA}$, $\alpha = \beta = 90^\circ$, $\gamma = 60^\circ$, and a density of 0.921 g/cm^3 . Due to their unique molecular

(1 9 , 1 9 , 6 . 5 , 9 0 , 9 0 , 1 2 0)

(1 1 . 0 1 , 1 1 . 0 1 , 6 . 5 , 9 0 , 9 0 , 1 2 0)

1 9 と 1 1 . 0 1 は

$\sin 60^\circ * 11.01 * 2 = 19$ の関係が成り立つ

11.01

11.01

6.5

90.0

90.0

120.0

1.541838

3

0	0	1	1.84	6.5	13.612
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1	1	0	37.03	2.8868	16.087
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1	1	1	1.84	4.1919	21.131
---	---	---	------	--------	--------

19

19

6.5

90.0

90.0

120.0

1.541838

3

2	1	0	1.0	6.2192	14.229
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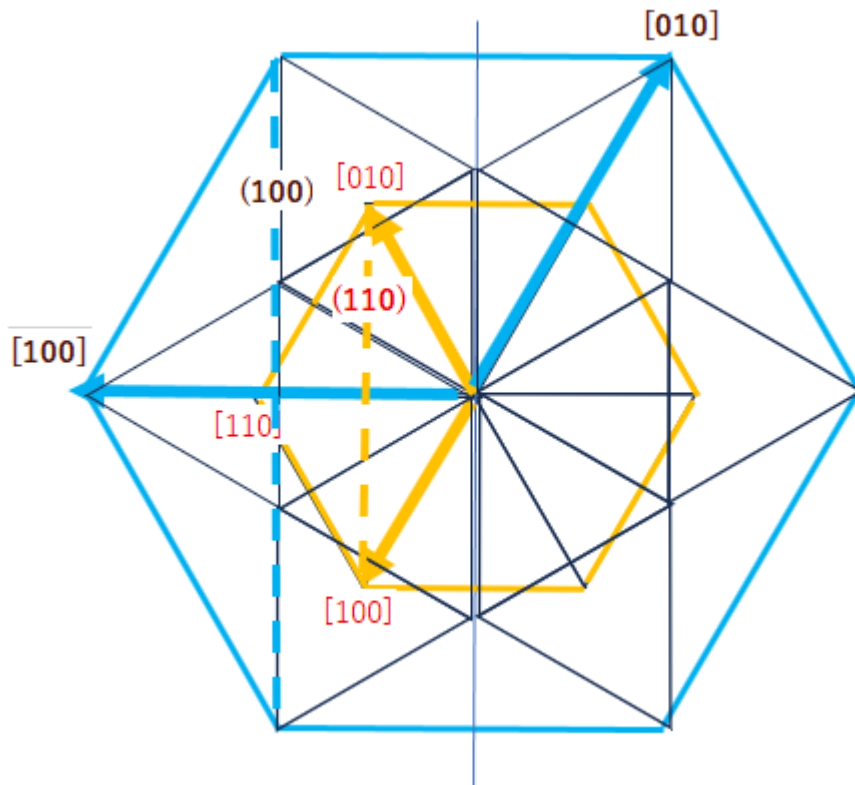
3	0	0	37.03	5.4848	16.146
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3	0	1	1.84	4.1919	21.177
---	---	---	------	--------	--------

(19, 19, 6.5, 90, 90, 120) を **B-PPL**

(11.01, 11.01, 6.5, 90, 90, 120) を **B-PPS** とする。

B-PPL と **B-PPS** の関係は



B-PPL

B-PPS

(300)

(110)

(301)

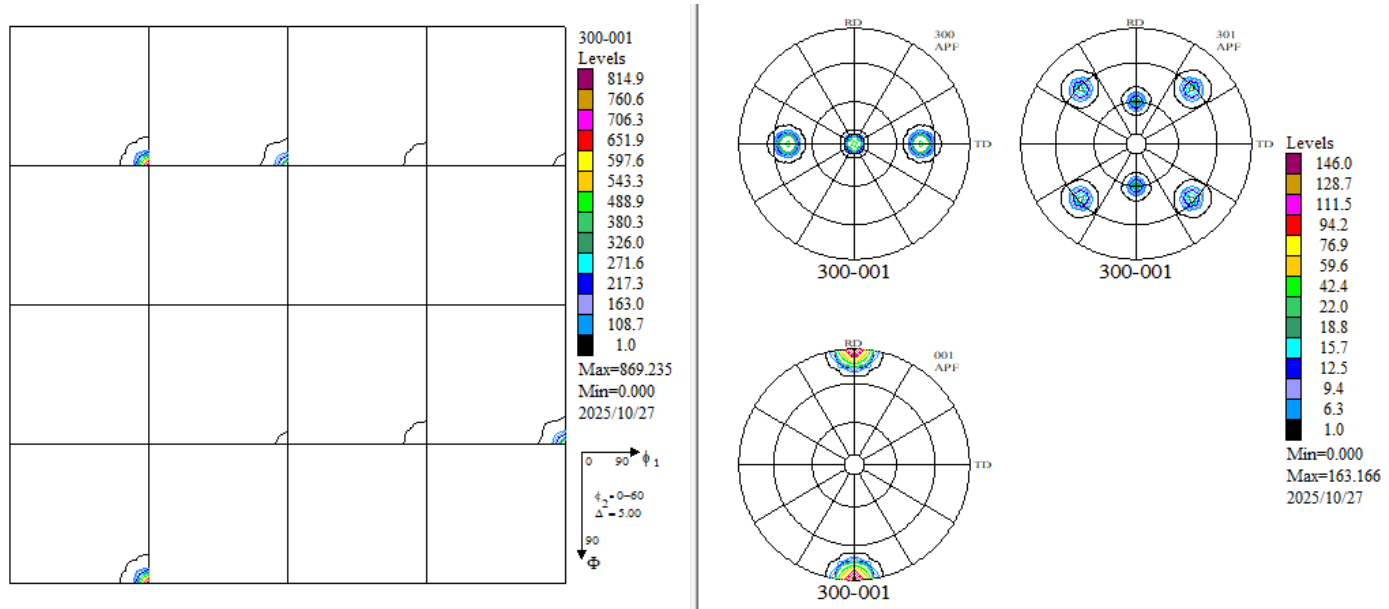
(111)

の 2θ 角度が一致している。

B-PPL (300) [001] とB-PPS (110) [001] の関係を調べる。

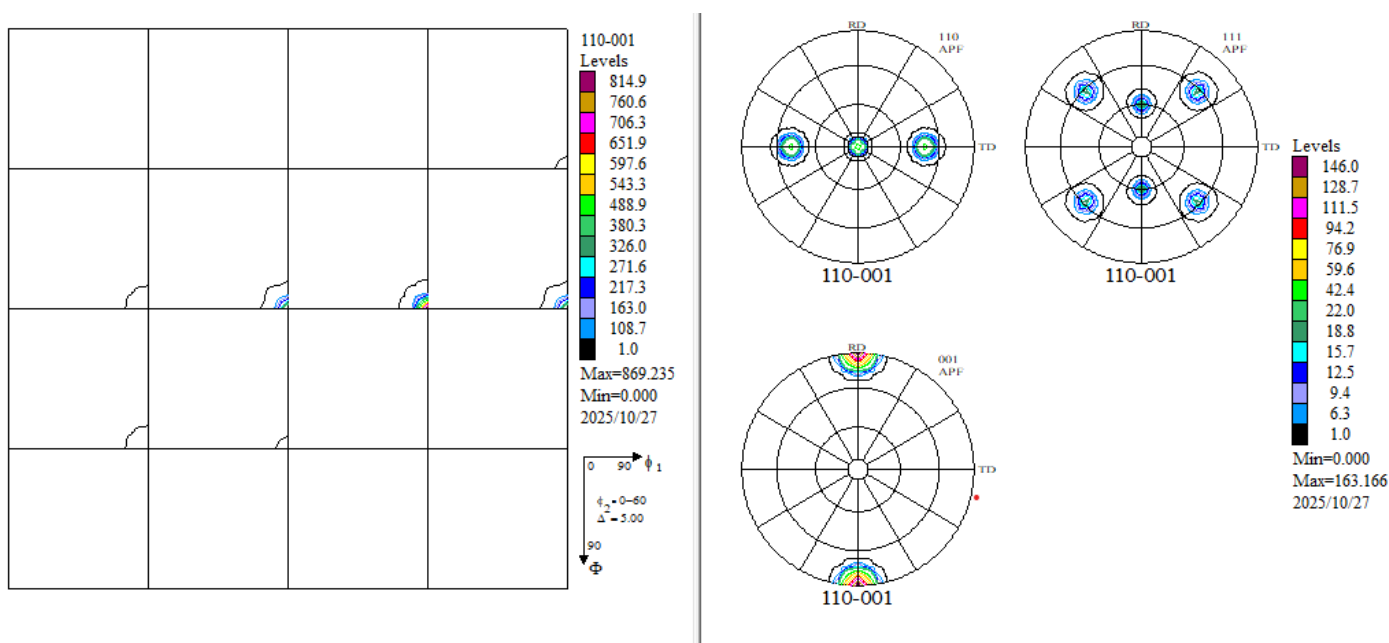
B-PPL

(300), (301), (001)



B-PPS

(110), (111), (001)



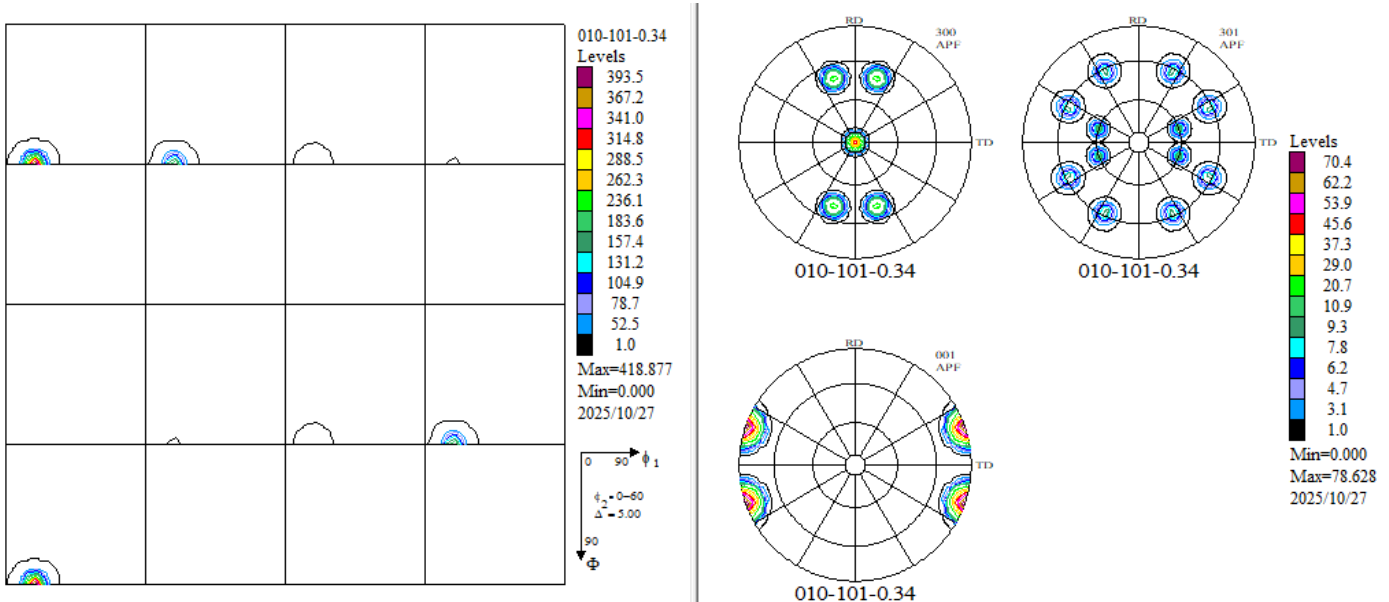
B-PPLのODF (90, 90, 0)

B-PPSのODF (90, 90, 30)

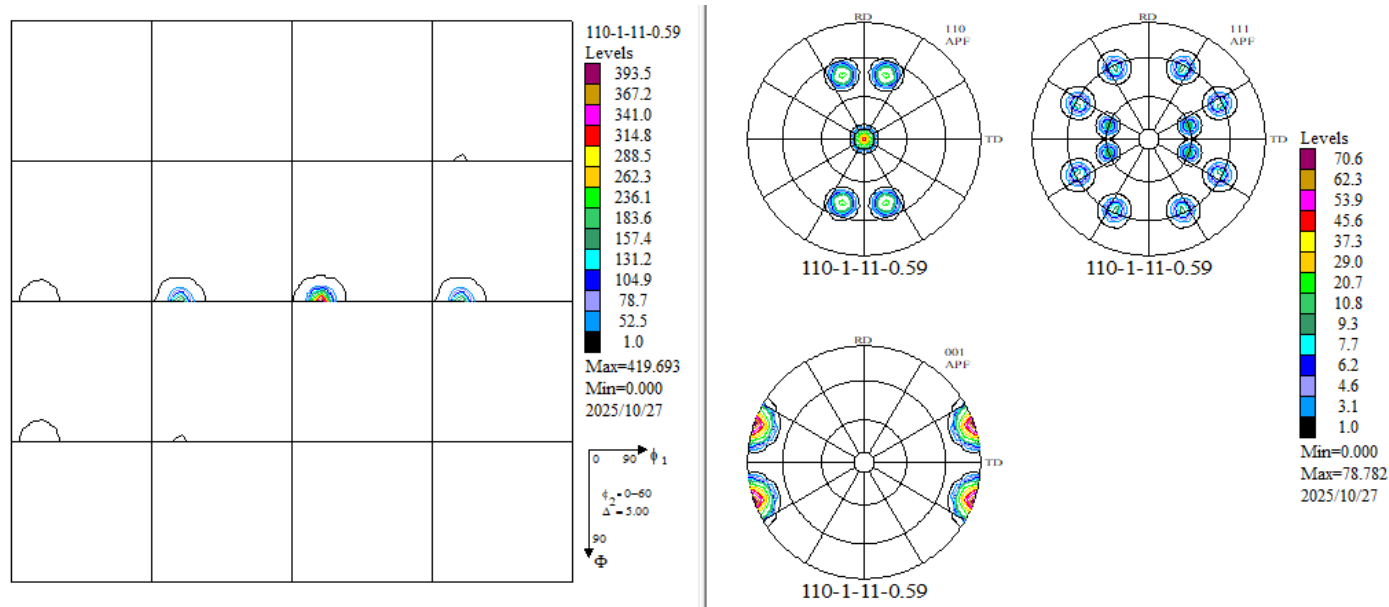
極点図は同一

B-PPL (010) [101] とB-PPS (110) [1-11] の関係を調べる。

B-PPL (300), (301), (001)



B-PPS (110), (111), (001)



B-PPLのODF { 0 1 0 } < 1 0 1 > { 18.78, 90.00, 0.00 }

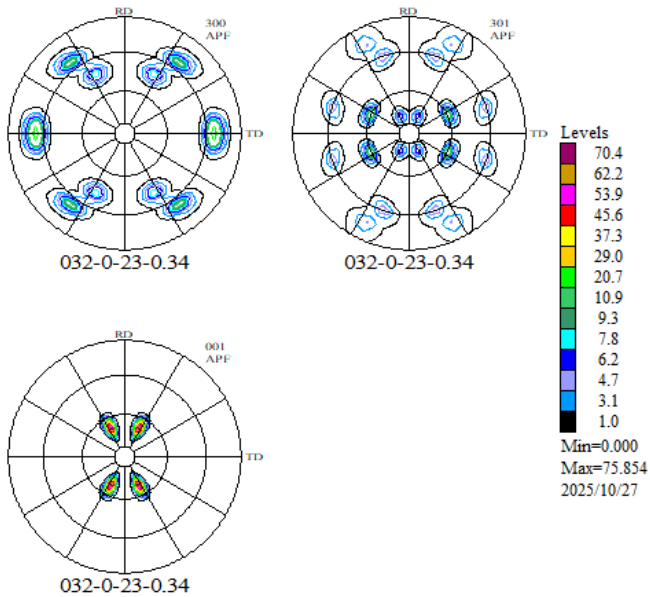
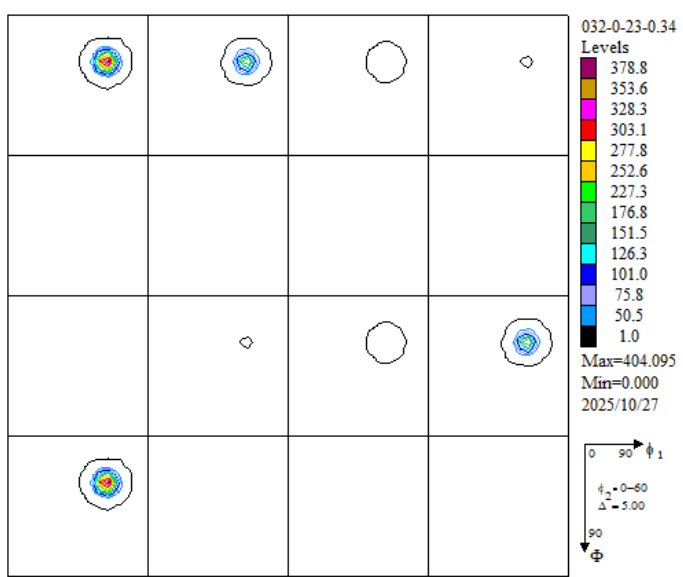
B-PPSのODF { 1 1 0 } < 1 -1 1 > { 18.81, 90.00, 30.00 }

極点図は同一

B-PPL (032) [0-23] とB-PPS (-122) [2-23] の関係調べる。

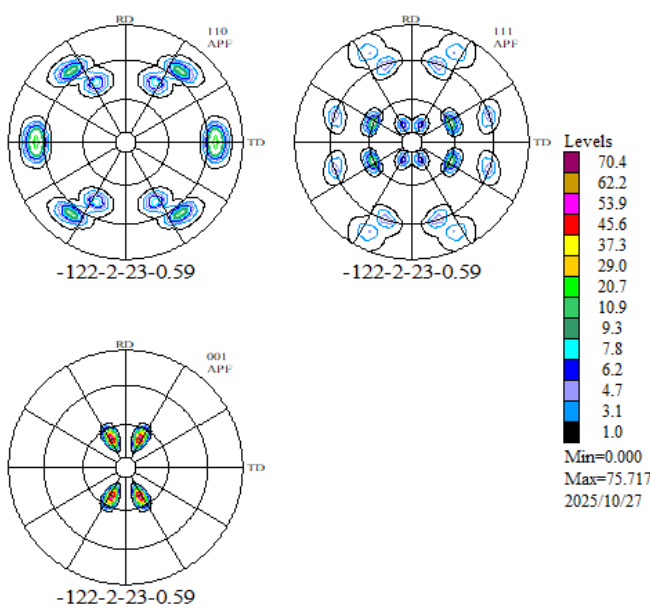
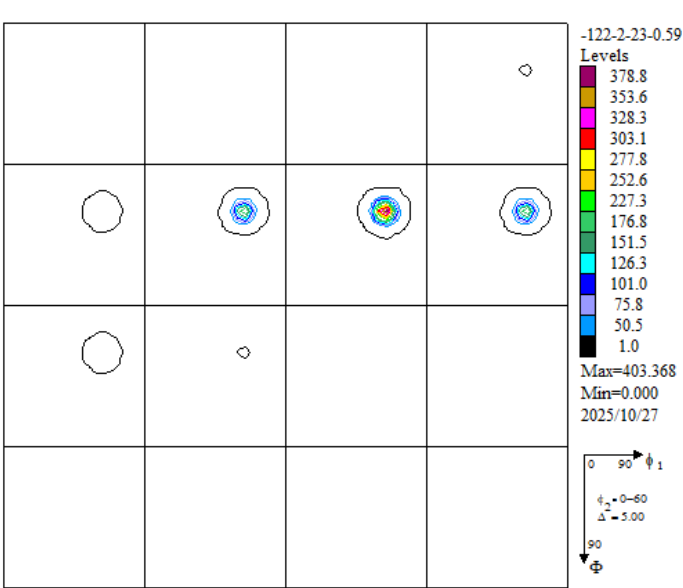
B-PPL

(300), (301), (001)



B-PPS

(110), (111), (001)



B-PPLのODF { 0 3 2 } < 0 -2 3 > { 63.55, 30.49, 0.00 }

B-PPSのODF { -1 2 2 } < 2 -2 3 > { 63.56, 30.54, 330.00 }

極点図は同一

シュミレーション

今回のシュミレーションはL a b o T e xを使用しているが

同一のシュミレーションをH e x a C o n v e r tやs t e r e o G Pでも可能

B-P P L

HexaConvert 1.14S by CTR PDuser HelperTex CTR

File Step Help random Dispfile

A ☒ X-Axis[100] ([2-1-10]) .. B ☐ X-Axis[210] ([10-10])

Miller Notation (3Axis Notation)

☒ 0 3 0 0 0 1 hkl uvw

Miller Bravais Notation (4 Axis Notation)

☐ 0 3 -3 0 0 0 1 hkil uvxw

Euler(p1Fp2)

☐ 90.0 90.0 0.0

Material select

β -Polypropylene.TXT

c/a 0.59 Input ψ 2 Angles 0.0 Calc

DISP

Position 10 Disp size 200 DISP

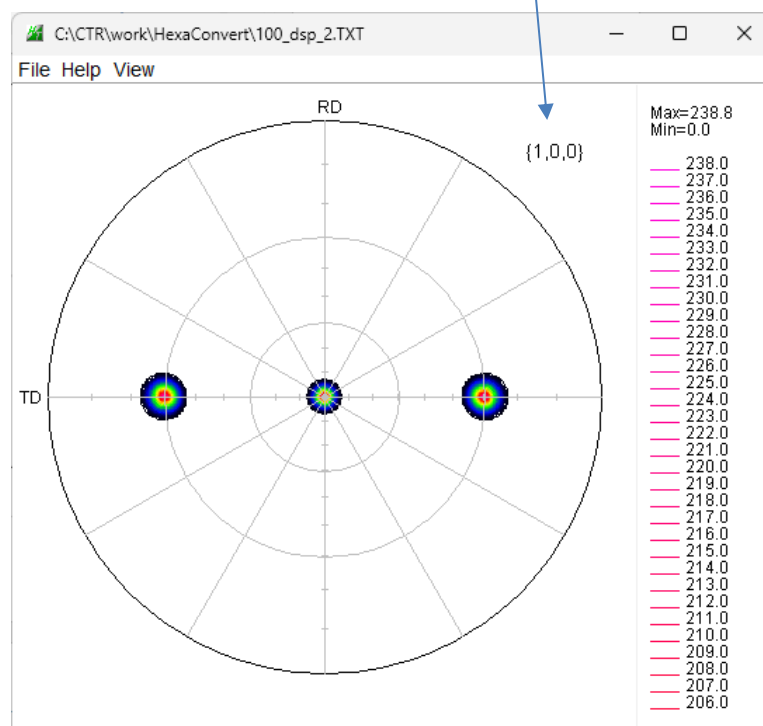
BG Corr Black Line size 1.0 MINUS

Polefigure

FWHM 5 degree Step 1 Polefigure 3,0,0 ☒ Orthorhombic Disp

Gratio 1.0 ☒ Lorentzcut(max/20) Holder C:\CTR\work\HexaConvert

OK Return Structure



HexaConvert 1.14S by CTR PDuser HelperTex CTR

File Step Help random Dispfile

A ☒ X-Axis[100] ([2-1-10]) B ☐ X-Axis[210] ([10-10])

Miller Notation (3Axis Notation)

☒ 1 1 0 0 0 1 hkl uvw

Miller Bravais Notation (4 Axis Notation)

☐ 1 1 -2 0 0 0 0 1 hkil uvxw

Euler(p1Pp2)

☐ 90.0 90.0 30.0

Material select

β -Polypropylene.TXT

c/a 0.342 Input ψ 2 Angles 0 Calc

DISP

Position 10 Disp size 200 DISP

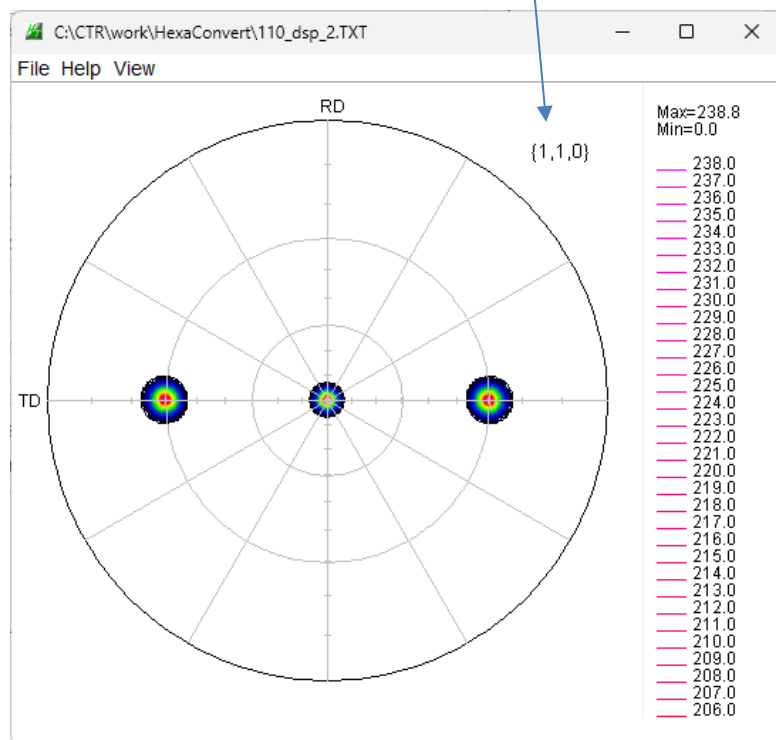
BG Corr Black Line size 1.0 MINUS

Polefigure

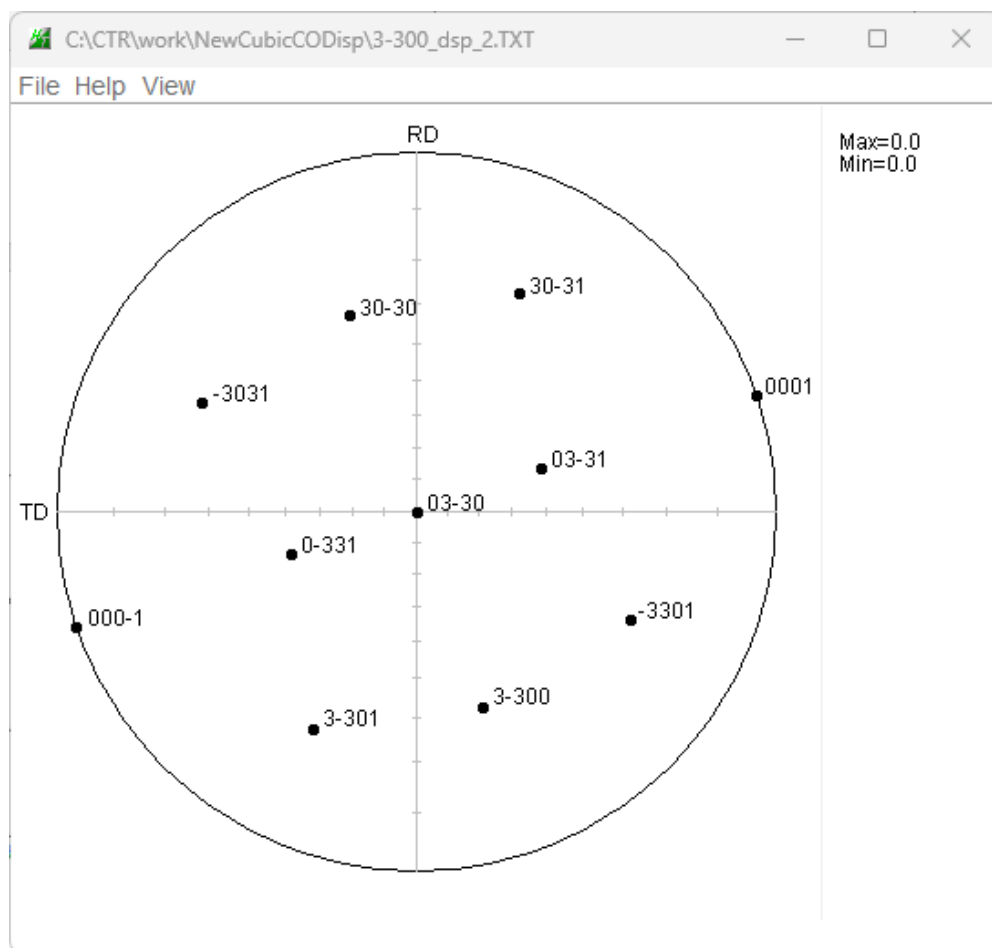
FWHM 5 degree Step 1 Polefigure 1,1,0 ☒ Orthorhombic Disp

Gratio 1.0 ☒ Lorentzcut(max/20) Holder C:\CTR\work\HexaConvert

OK Return Structure



B-PPL (030) [101]



B-PPS (110) [1-11]

