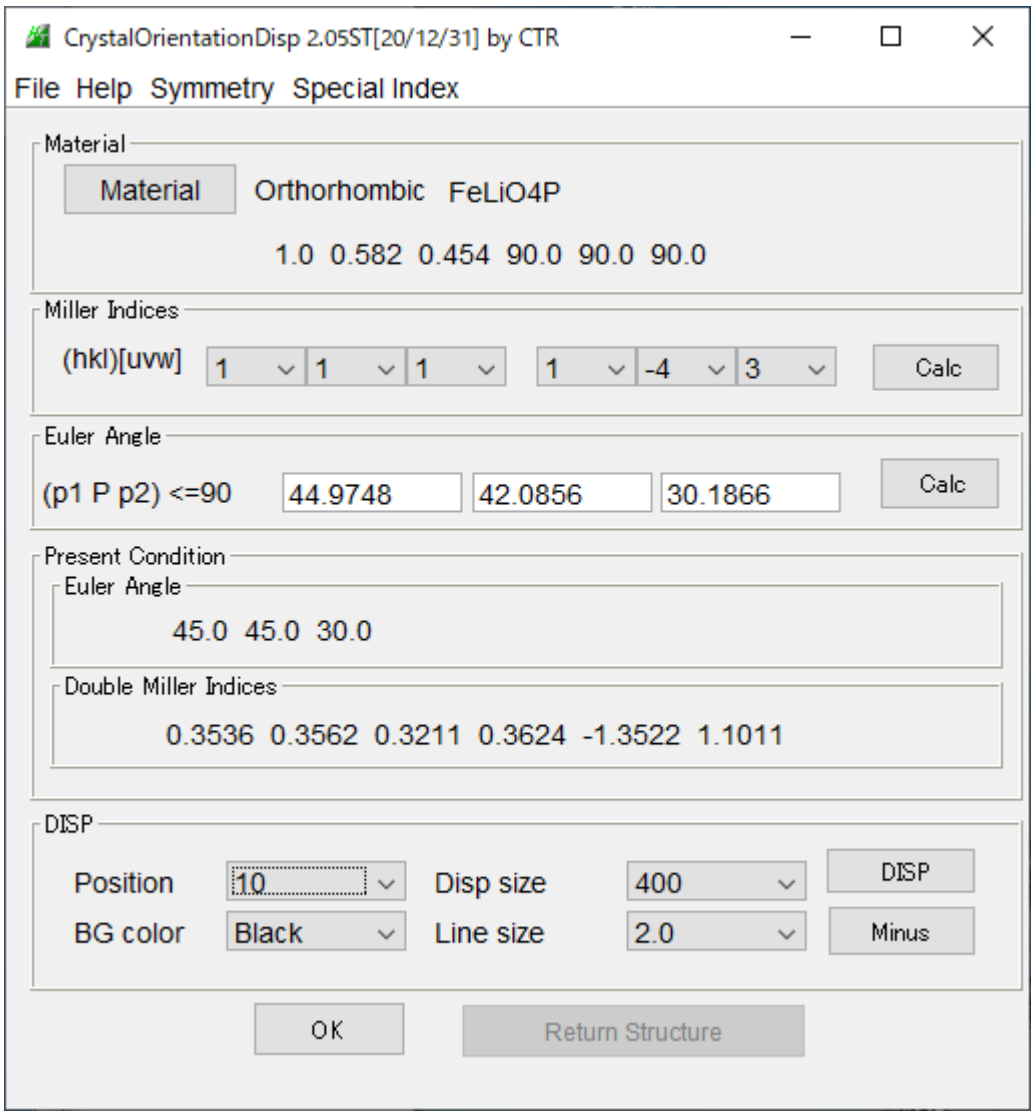
リチウム電池関係の正極材ＬｉＦｅＰＯ４をＭＴＥＸでシュミレーション

２０２０年１０月３１日

HelperTex Office

概要

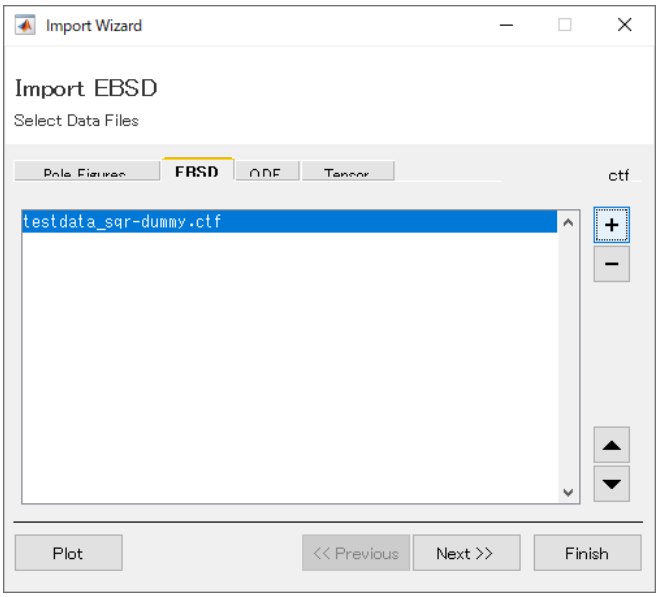
Ｏｒｔｈｏｒｈｏｍｂｉｃ材として、ＬｉＦｅＰＯ４を対象とし、ダミーのファイルを指定しＣＩＦファイルに、ＬｉＦｅＰＯ４を指定、内部で(１１１)[1 -4 3]を与え、ＯＤＦ図と逆極点の評価を行ってみます。

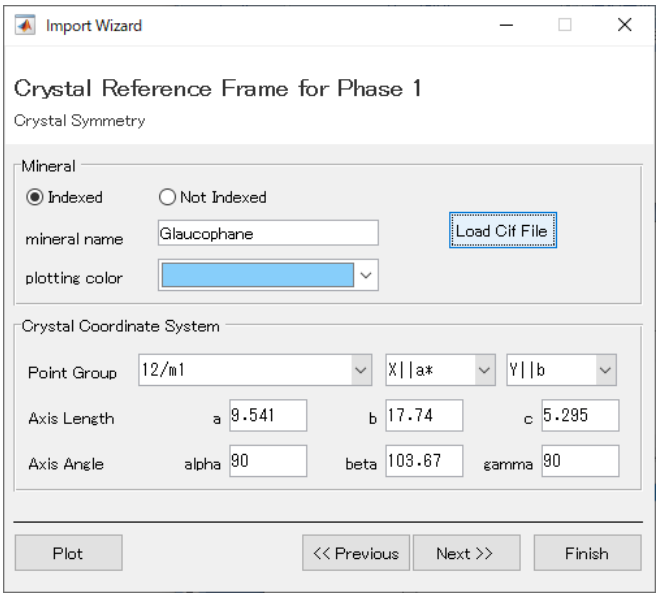


Ｉｎｖｅｒｓｅ表示プログラムにて、[100]のｔｏｐの場合、ｖａｌｕｅが追随していない修正

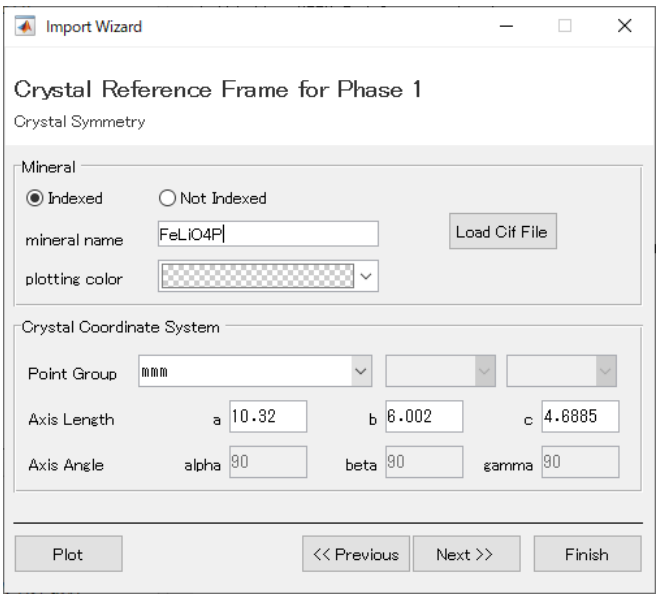
ＩｎｖｅｒｓｅＣｏｎｔｏｕｒＤｉｓｐｌａｙ(Ver1.30)にて修正

ＭＴＥＸに適当なファイルを指定

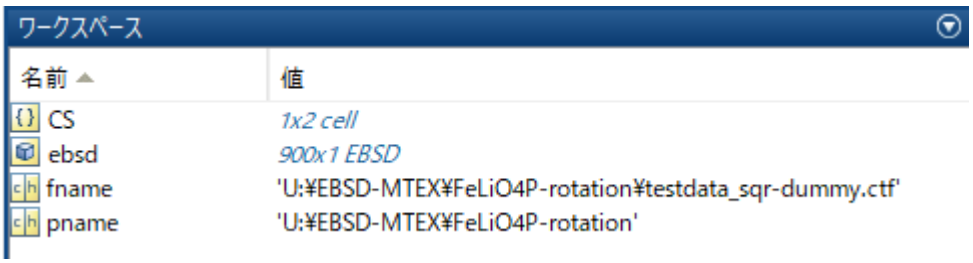




ＣＩＦファイル変更



```
% crystal symmetry
CS = {...
  'notIndexed',...
  crystalSymmetry('mmm', [10 6 4.7], 'mineral', 'FeLiO4P')};
```

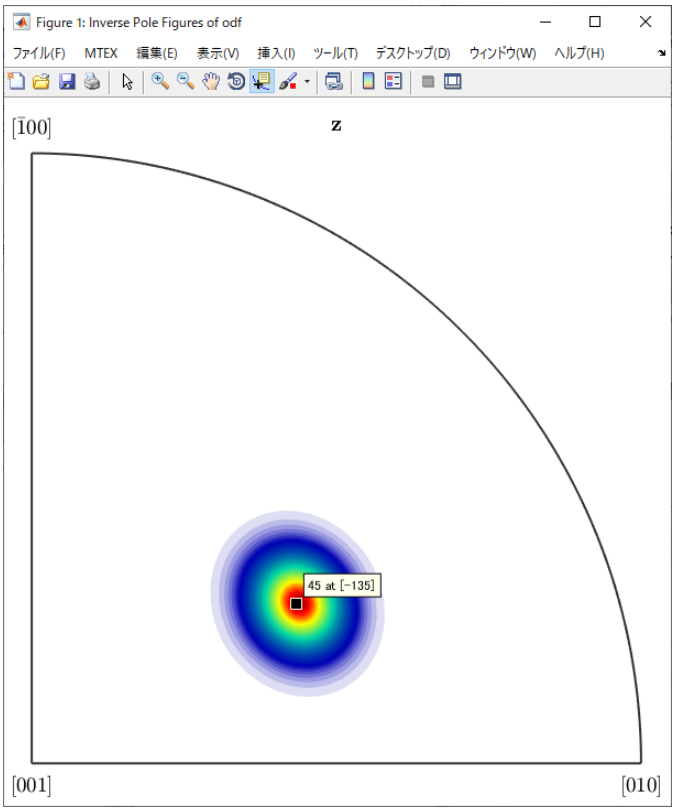


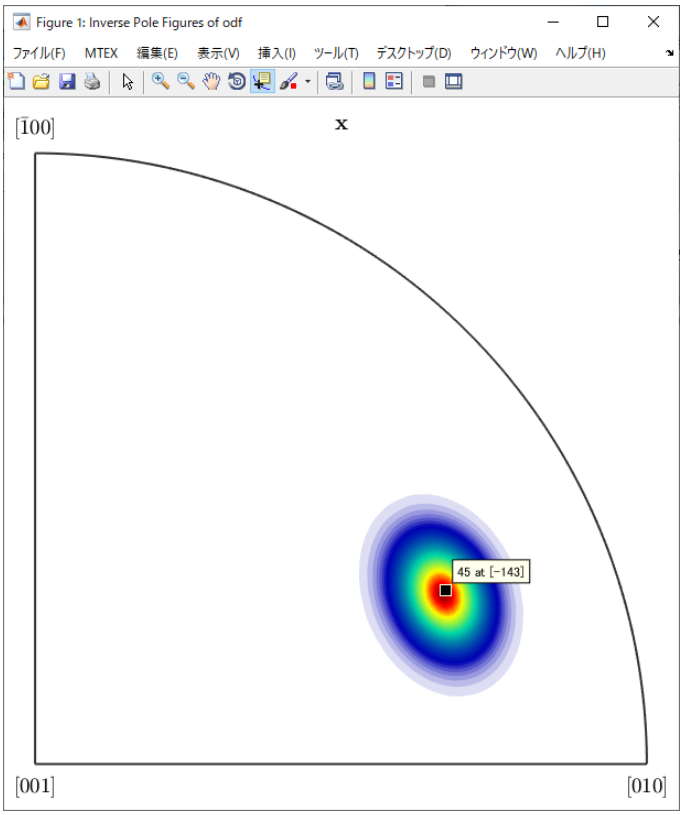
ＦｅＬｉＯ４Ｐの方位を作成

```
>> cs=ebsd('FeLiO4P').CS

cs = crystalSymmetry (show methods, plot)
  mineral : FeLiO4P
    color     : LightSkyBlue
symmetry: mmm
elements: 8
a, b, c : 10, 6, 4.7

>> ori = orientation.byMiller([1 1 1],[1 -4 3],cs)

ori = orientation (show methods, plot)
size: 1 x 1
rystal symmetry : FeLiO4P (mmm)
specimen symmetry: 1
Bunge Euler angles in degree
hi1        Phi        phi2        Inv.
44.9764 42.4122 30.9638            0

psi = vonMisesFisherKernel('HALFWIDTH',5*degree)
odf= unimodalODF(ori,psi)
```

作成されたＯＤＦ図

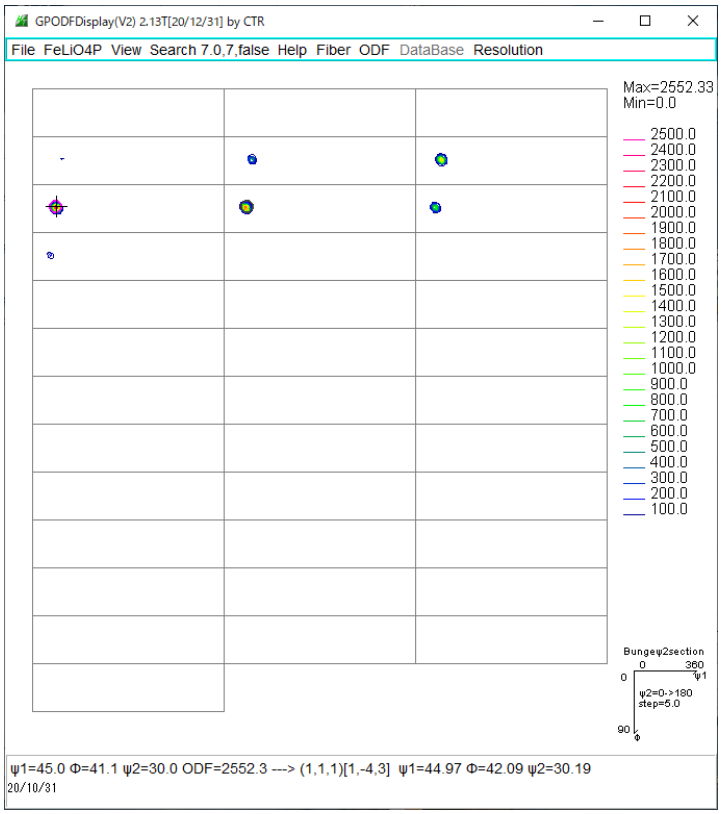
plot(odf)

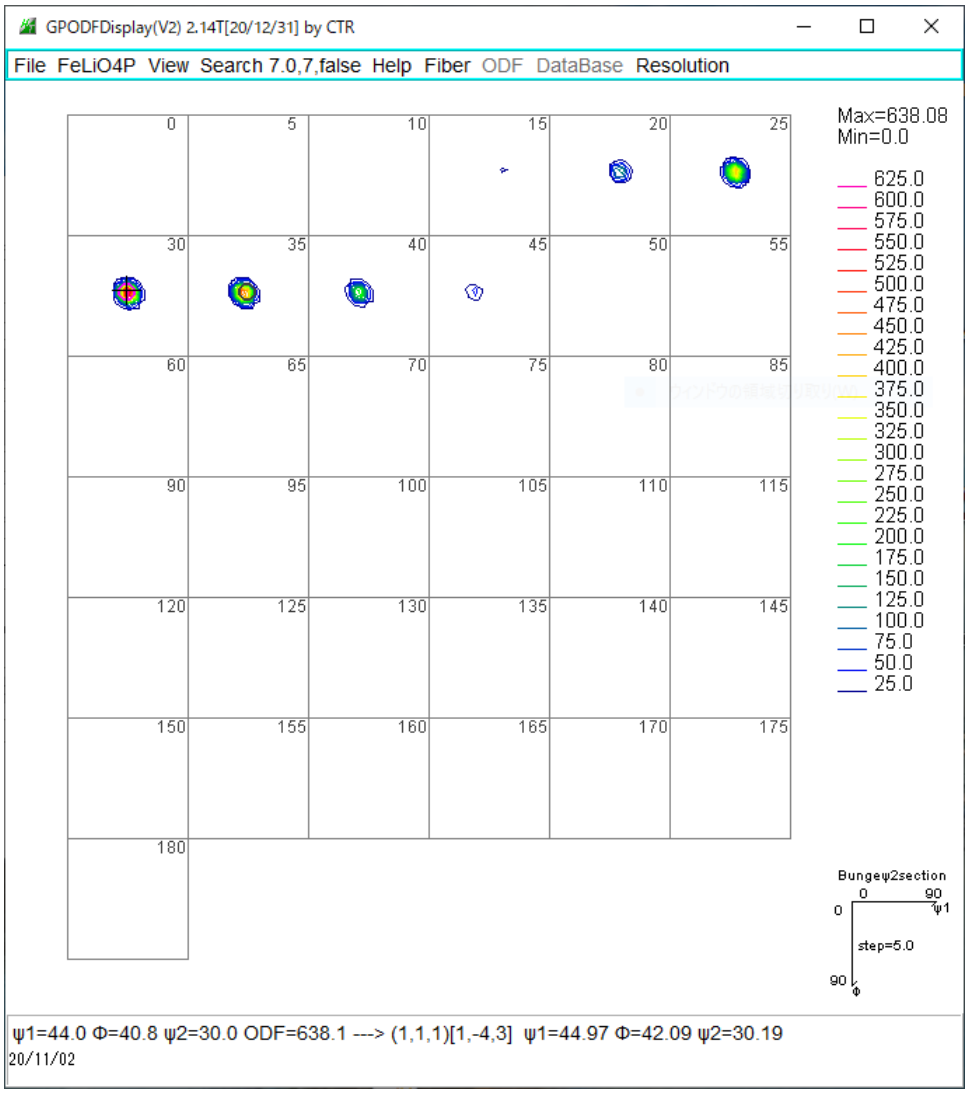




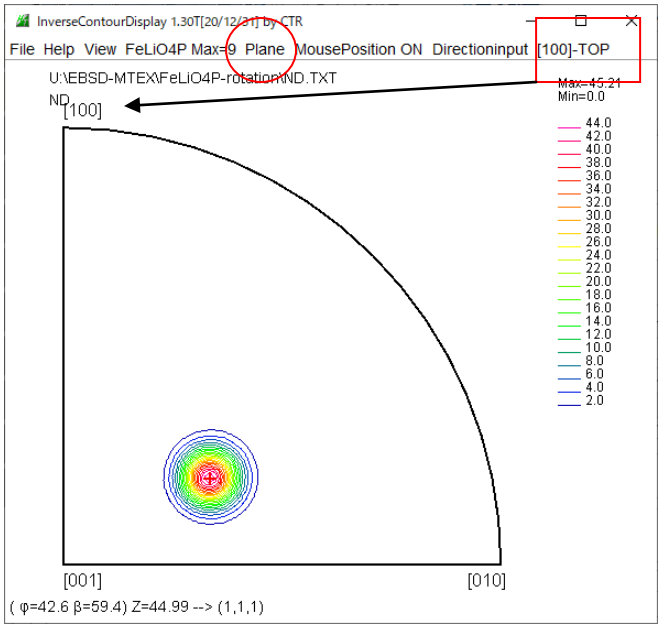
ＯＤＦ図と逆極点図をＥｘｐｏｒｔし評価

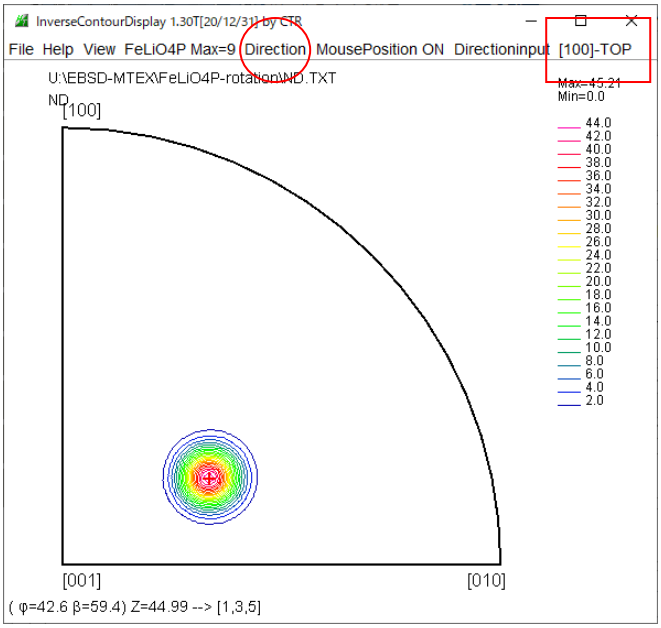
ＯＤＦ図

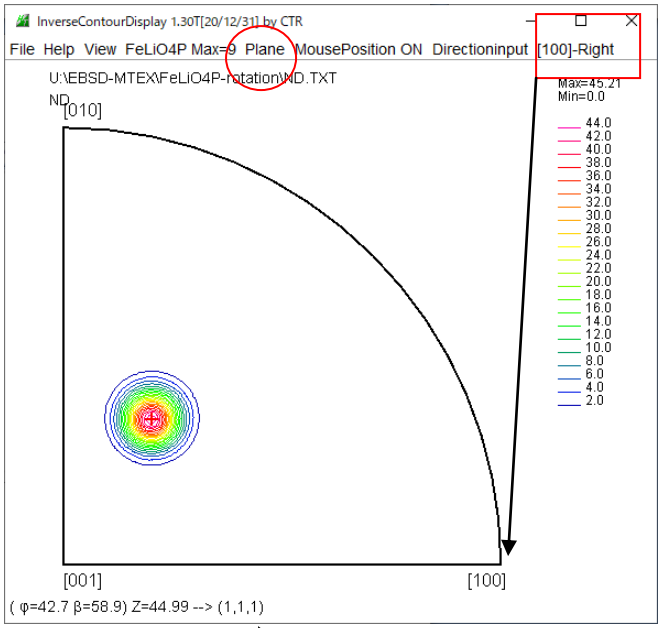

GPODFDisplay(V2) 2.13T[20/12/31] by CTR
File FeLiO4P View Search 7.0,7,false Help Fiber ODF DataBase Resolution
Max=2552.33
Min=0.0
2500.0
2400.0
2300.0
2200.0
2100.0
2000.0
1900.0
1800.0
1700.0
1600.0
1500.0
1400.0
1300.0
1200.0
1100.0
1000.0
900.0
800.0
700.0
600.0
500.0
400.0
300.0
200.0
100.0
Bungeψ2section
0
360
ψ1
ψ2=0->180
step=5.0
90
Φ
ψ1=45.0 Φ=41.1 ψ2=30.0 ODF=2552.3 ---> (1,1,1)[1,-4,3] ψ1=44.97 Φ=42.09 ψ2=30.19
20/10/31

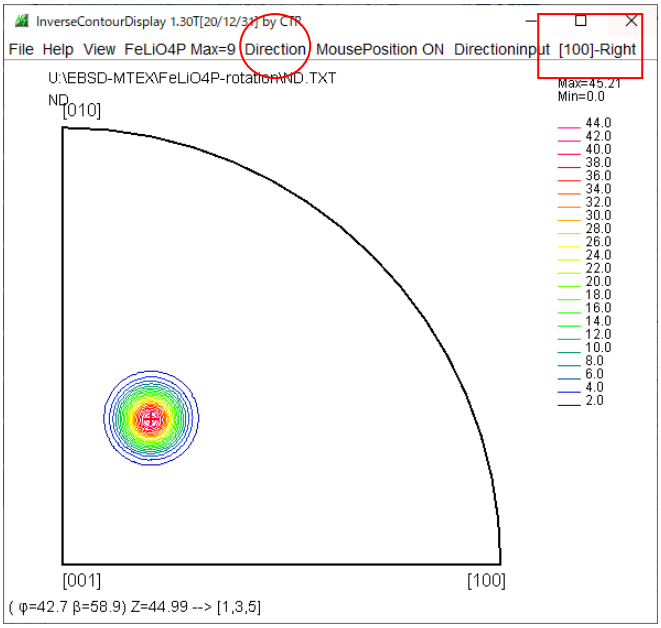

GPODFDisplay(V2) 2.14T[20/12/31] by CTR
File FeLiO4P View Search 7.0,7,false Help Fiber ODF DataBase Resolution
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
85
90
95
100
105
110
115
120
125
130
135
140
145
150
155
160
165
170
175
180
Max=638.08
Min=0.0
625.0
600.0
575.0
550.0
525.0
500.0
475.0
450.0
425.0
400.0
375.0
350.0
325.0
300.0
275.0
250.0
225.0
200.0
175.0
150.0
125.0
100.0
75.0
50.0
25.0
Bungeψ2section
0
90
ψ1
step=5.0
90
Φ
ψ1=44.0 Φ=40.8 ψ2=30.0 ODF=638.1 ---> (1,1,1)[1,-4,3] ψ1=44.97 Φ=42.09 ψ2=30.19
20/11/02

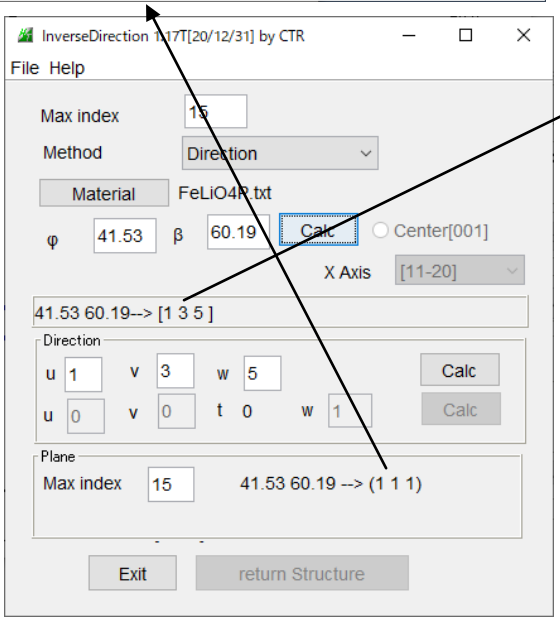
逆極点図（ND）


InverseContourDisplay 1.30T[20/12/31] by CTR
File Help View FeLiO4P Max=9 Plane MousePosition ON Directioninput [100]-TOP
U:\EBSD-MTEX\FeLiO4P-rotation\ND.TXT
ND
[100]
Max=45.21
Min=0.0
44.0
42.0
40.0
38.0
36.0
34.0
32.0
30.0
28.0
26.0
24.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
[001]
[010]
(φ=42.6 β=59.4) Z=44.99 --> (1,1,1)

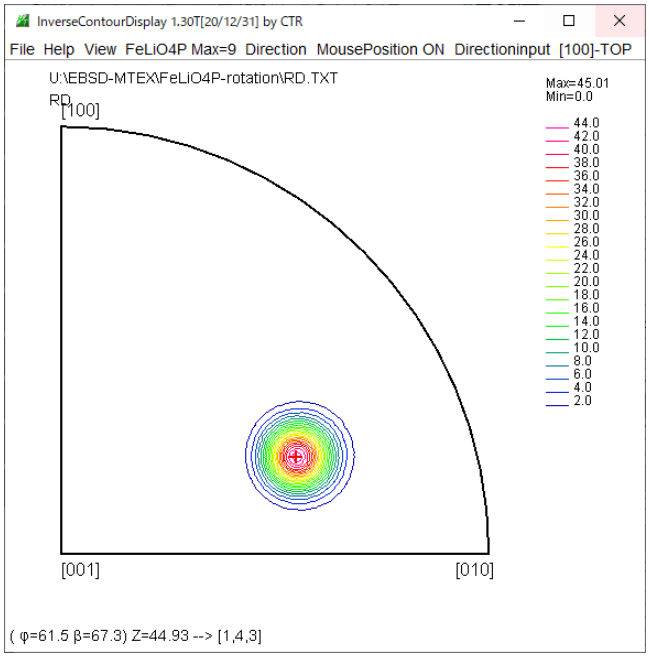

InverseContourDisplay 1.30T[20/12/31] by CTR
File Help View FeLiO4P Max=9 Direction MousePosition ON Directioninput [100]-TOP
U:\EBSD-MTEX\FeLiO4P-rotation\ND.TXT
ND
[100]
Max=45.21
Min=0.0
44.0
42.0
40.0
38.0
36.0
34.0
32.0
30.0
28.0
26.0
24.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
[001]
[010]
(φ=42.6 β=59.4) Z=44.99 --> [1,3,5]

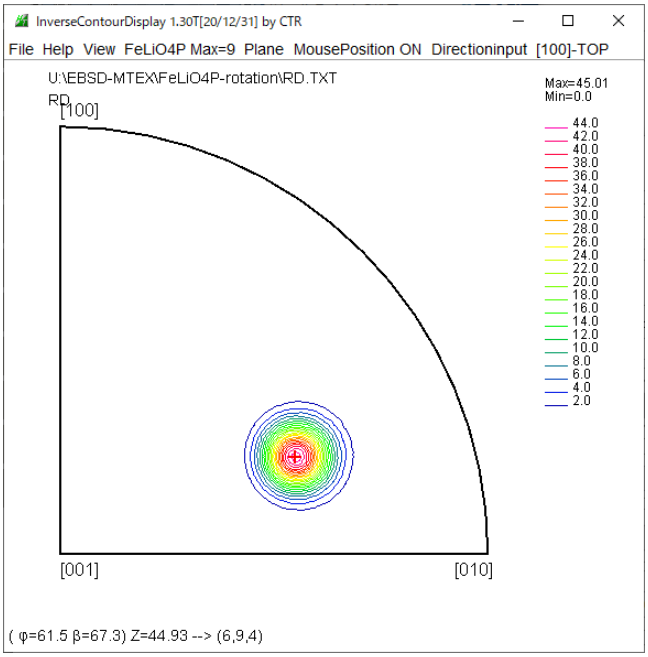

InverseContourDisplay 1.30T[20/12/31] by CTR
File Help View FeLiO4P Max=9 Plane MousePosition ON Directioninput [100]-Right
U:\EBSD-MTEX\FeLiO4P-rotation\ND.TXT
ND
[010]
Max=45.21
Min=0.0
44.0
42.0
40.0
38.0
36.0
34.0
32.0
30.0
28.0
26.0
24.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
[001]
[100]
(φ=42.7 β=58.9) Z=44.99 --> (1,1,1)

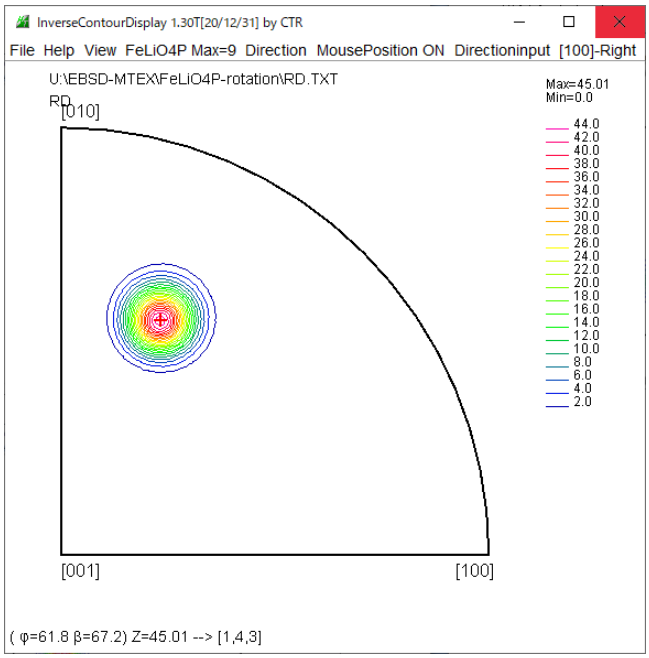

InverseContourDisplay 1.30T[20/12/31] by CTR
File Help View FeLiO4P Max=9 Direction MousePosition ON Directioninput [100]-Right
U:\EBSD-MTEX\FeLiO4P-rotation\ND.TXT
ND
[010]
Max=45.21
Min=0.0
44.0
42.0
40.0
38.0
36.0
34.0
32.0
30.0
28.0
26.0
24.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
[001]
[100]
(φ=42.7 β=58.9) Z=44.99 --> [1,3,5]

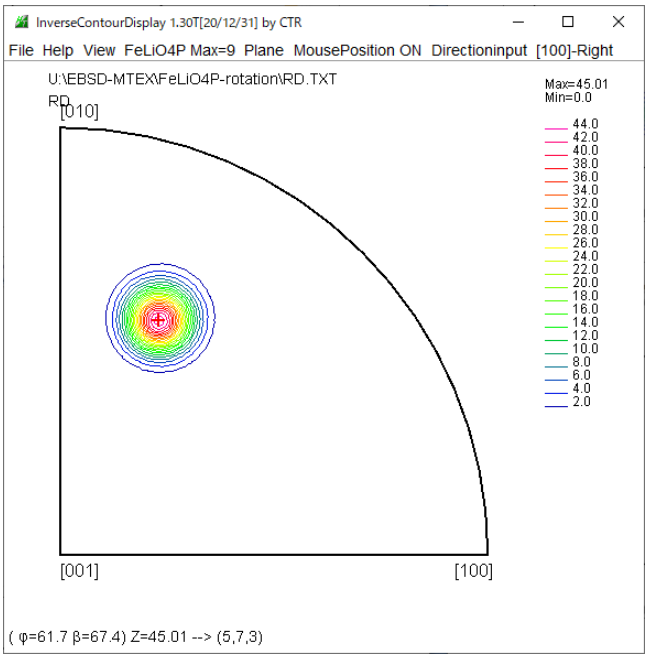

InverseDirection 1.17T[20/12/31] by CTR
File Help
Max index
15
Method
Direction
Material
FeLiO4P.txt
φ
41.53
β
60.19
Calc
Center[001]
X Axis
[11-20]
41.53 60.19--> [1 3 5]
Direction
u 1
v 3
w 5
Calc
u 0
v 0
t 0
w 1
Calc
Plane
Max index
15
41.53 60.19 --> (1 1 1)
Exit
return Structure

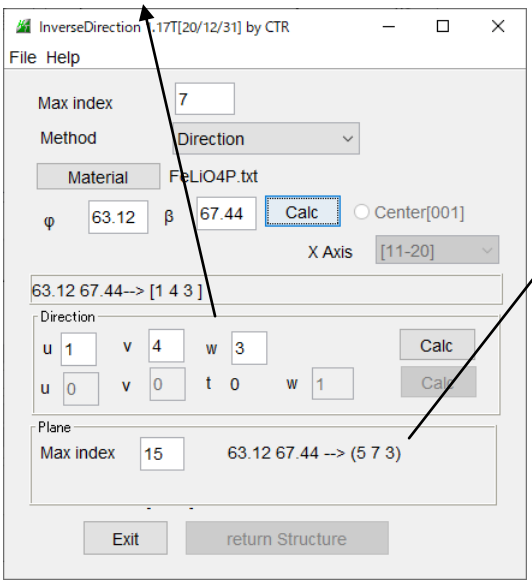
逆極点図（RD）


InverseContourDisplay 1.30T[20/12/31] by CTR
File Help View FeLiO4P Max=9 Direction MousePosition ON Directioninput [100]-TOP
U:\EBSD-MTEX\FeLiO4P-rotation\RD.TXT
RD
[100]
Max=45.01
Min=0.0
44.0
42.0
40.0
38.0
36.0
34.0
32.0
30.0
28.0
26.0
24.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
[001]
[010]
(φ=61.5 β=67.3) Z=44.93 --> [1,4,3]


InverseContourDisplay 1.30T[20/12/31] by CTR
File Help View FeLiO4P Max=9 Plane MousePosition ON Directioninput [100]-TOP
U:\EBSD-MTEX\FeLiO4P-rotation\RD.TXT
RD
[100]
Max=45.01
Min=0.0
44.0
42.0
40.0
38.0
36.0
34.0
32.0
30.0
28.0
26.0
24.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
[001]
[010]
(φ=61.5 β=67.3) Z=44.93 --> (6,9,4)


InverseContourDisplay 1.30T[20/12/31] by CTR
File Help View FeLiO4P Max=9 Direction MousePosition ON Directioninput [100]-Right
U:\EBSD-MTEX\FeLiO4P-rotation\RD.TXT
RD
[010]
Max=45.01
Min=0.0
44.0
42.0
40.0
38.0
36.0
34.0
32.0
30.0
28.0
26.0
24.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
[001]
[100]
(φ=61.8 β=67.2) Z=45.01 --> [1,4,3]


InverseContourDisplay 1.30T[20/12/31] by CTR
File Help View FeLiO4P Max=9 Plane MousePosition ON Directioninput [100]-Right
U:\EBSD-MTEX\FeLiO4P-rotation\RD.TXT
RD
[010]
Max=45.01
Min=0.0
44.0
42.0
40.0
38.0
36.0
34.0
32.0
30.0
28.0
26.0
24.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
[001]
[100]
(φ=61.7 β=67.4) Z=45.01 --> (5,7,3)


InverseDirection 1.17T[20/12/31] by CTR
File Help
Max index
7
Method
Direction
Material
FeLiO4P.txt
φ
63.12
β
67.44
Calc
Center[001]
X Axis
[11-20]
63.12 67.44--> [1 4 3]
Direction
u 1
v 4
w 3
Calc
u 0
v 0
t 0
w 1
Plane
Max index
15
63.12 67.44 --> (5 7 3)
Exit
return Structure