ＭＴＥＸによるＭｇのＴＤ－ｓｐｉｌｔシュミレーション

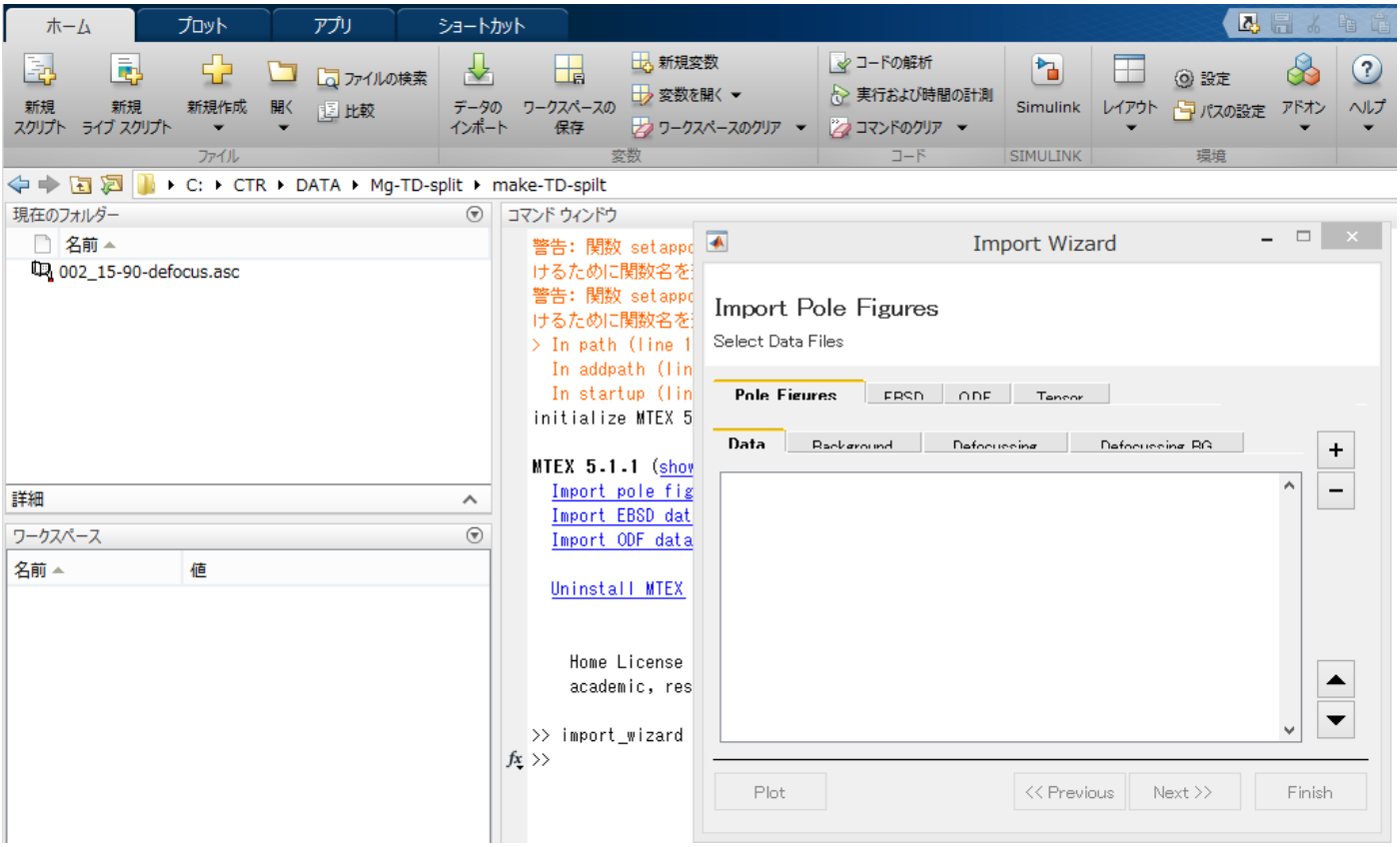
２０１９年０１月２７日

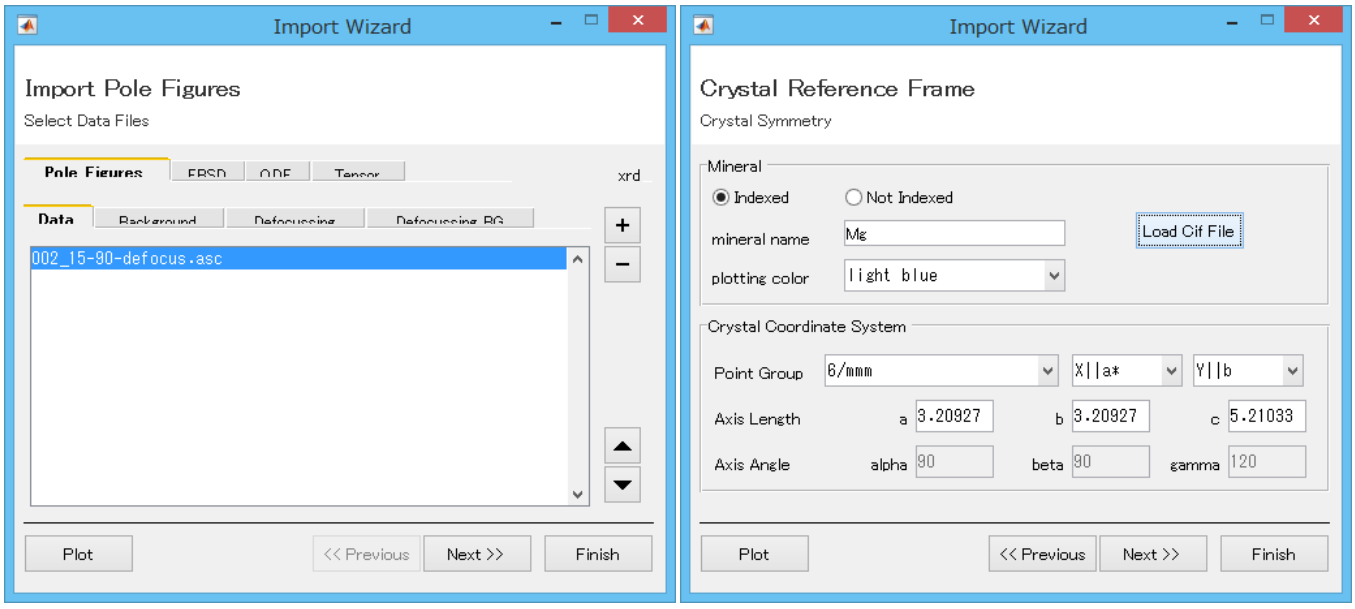
ＨｅｌｐｅｒＴｅｘ　Ｏｆｆｉｃｅ

１．概要

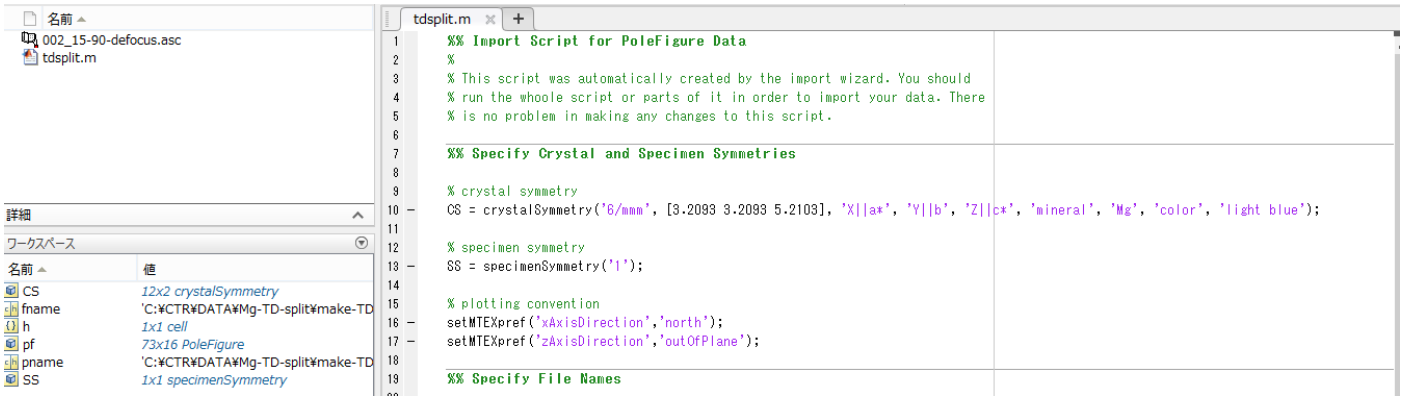
ＭＴＥＸによるシュミレーションはｃｕｂｉｃに関して
ＭＴＥＸＯＤＦのシュミレーションにおける結晶方位密度で行っているが、Ｈｅｘａｌｇｏｎａｌは
Ｃｕｂｉｃとは異なる。
方法として、１つの極点図をＭｇとして読み込み、crystalSystem、specimen，plottingconversion を
読み込む方法で行い、Mg の TD-split のＥｕｌｅｒ角度からＯＤＦを決定する。

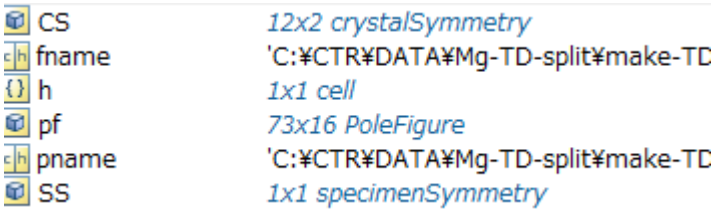
２．ＭＴＥＸ操作





Ｍｇを選択





ＣＳとＳＳを使用する。

２．１ＴＤ－Ｓｐｉｌｔを Ｍｉｌｌｅｒ設定できないのでＥｕｌｅｒ角度を設定

```
>> ori=orientation('Miller',[0,1,-1,3],[2,-1,-1,0],CS,SS)
エラー: Miller2quat (line 44)
Miller indece have to be orthogonal

エラー: orientation (line 97)
        o = orientation(Miller2quat(varargin{2:3},o.CS),o.CS,o.SS);
```

出来る時もある。？？？

```
>> ori=orientation('Euler',0*degree,31.4*degree,30*degree,CS,SS)

ori = orientation (show methods, plot)
  size: 1 x 1
  crystal symmetry : Mg (6/mmm, X||a*, Y||b, Z||c)
  specimen symmetry: 1

  Bunge Euler angles in degree
  phi1  Phi phi2 Inv.
     0 31.4   30    0
```

２．２方位密度の半価幅を設定

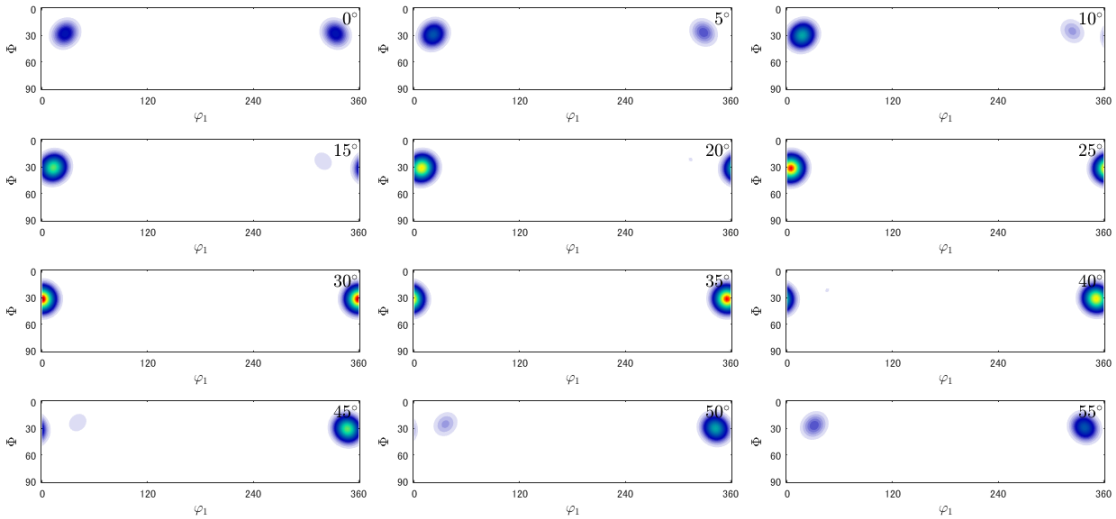
```
>> psi=vonMisesFisherKernel('HALFWIDTH',5*degree)

psi = vonMisesFisherKernel (show methods, plot)
  bandwidth: 59
  halfwidth: 5°
```

２．３ＯＤＦ図を計算

```
>> odf=calcODF(ori,psi)

odf = ODF (show methods, plot)
  crystal symmetry : Mg (6/mmm, X||a*, Y||b, Z||c)
  specimen symmetry: 1

  Radially symmetric portion:
    kernel: de la Vallee Poussin, halfwidth 10°
    center: (0° ,31° ,30° )
    weight: 1
```

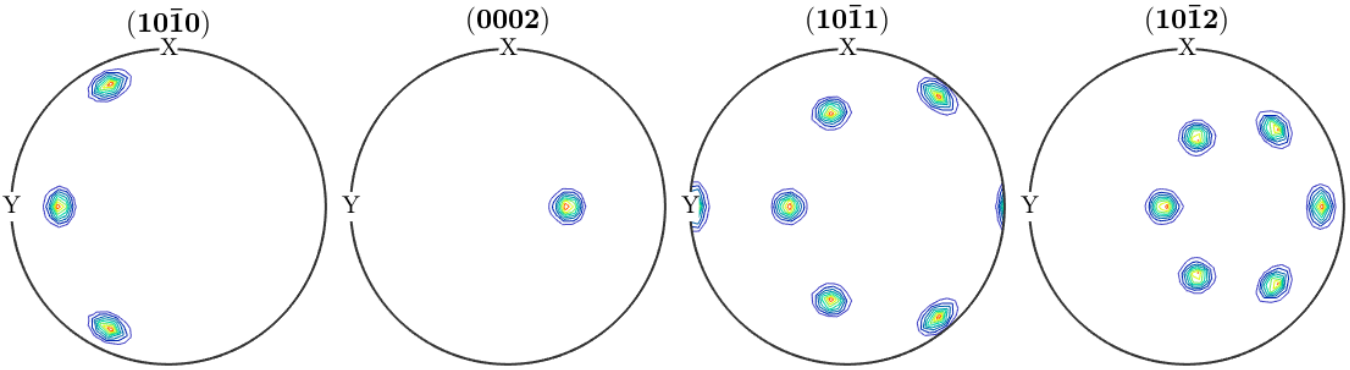
ＯＤＦ図を表示

```
>> plot(odf,'sections',12)
```



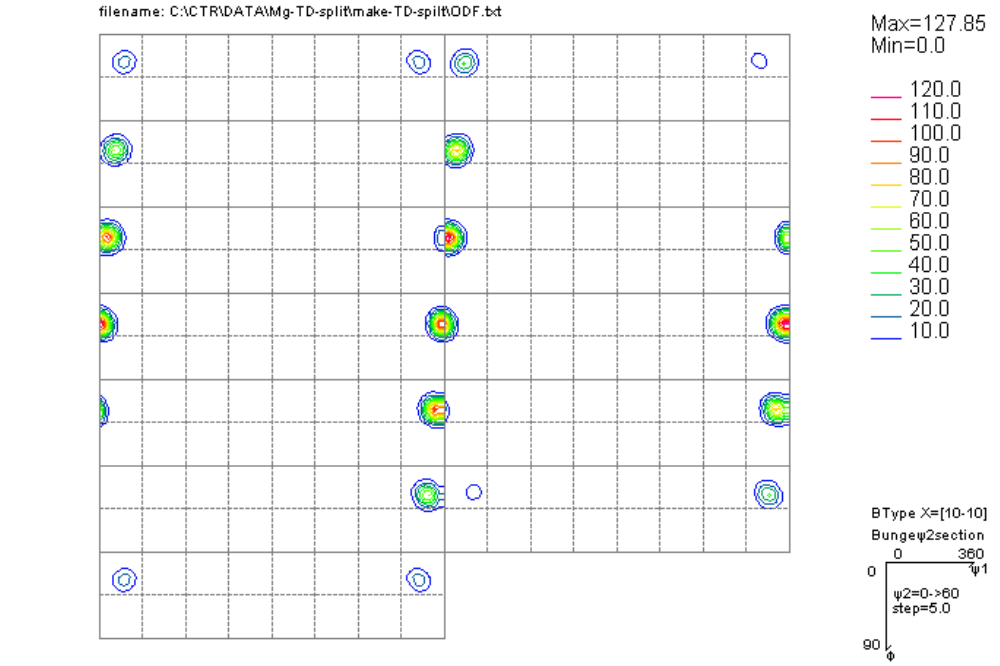
２．４極点図を作成

```
>> h=[Miller(1,0,-1,0,CS),Miller(0,0,0,2,CS),Miller(1,0,-1,1,CS),Miller(1,0,-1,2,CS)]

h = Miller (show methods, plot)
 size: 1 x 4
 mineral: Mg (6/mmm, X||a*, Y||b, Z||c)
  h  1  0  1  1
  k  0  0  0  0
  i -1  0 -1 -1
  l  0  2  1  2

>> rpf=calcPoleFigure(odf,h)

rpf = PoleFigure (show methods, plot)
  crystal symmetry : Mg (6/mmm, X||a*, Y||b, Z||c)
  specimen symmetry: 1

  h = (10-10), r = 72 x 19 points
  h = (0002), r = 72 x 19 points
  h = (10-11), r = 72 x 19 points
  h = (10-12), r = 72 x 19 points
```

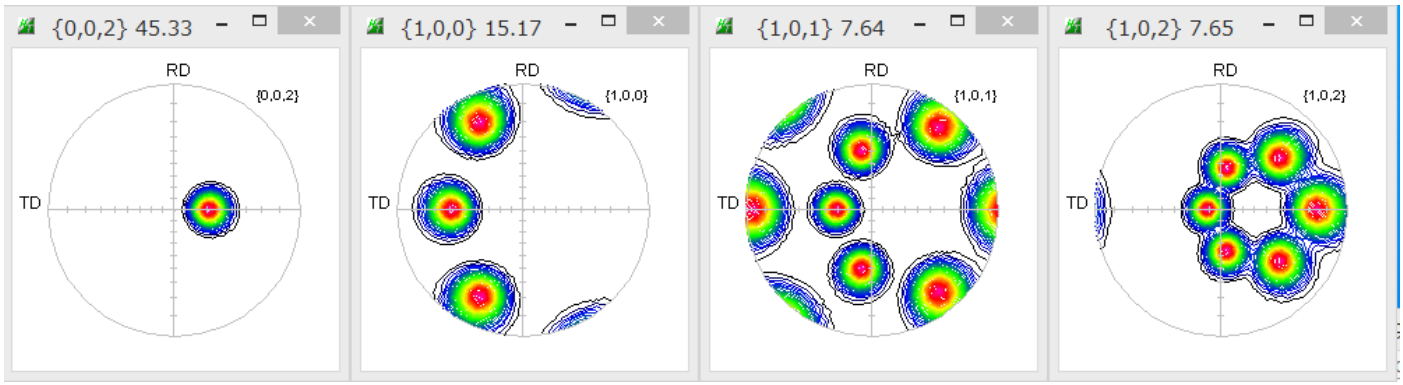


３．ＯＤＦ図、極点図をＥｘｐｏｒｔ

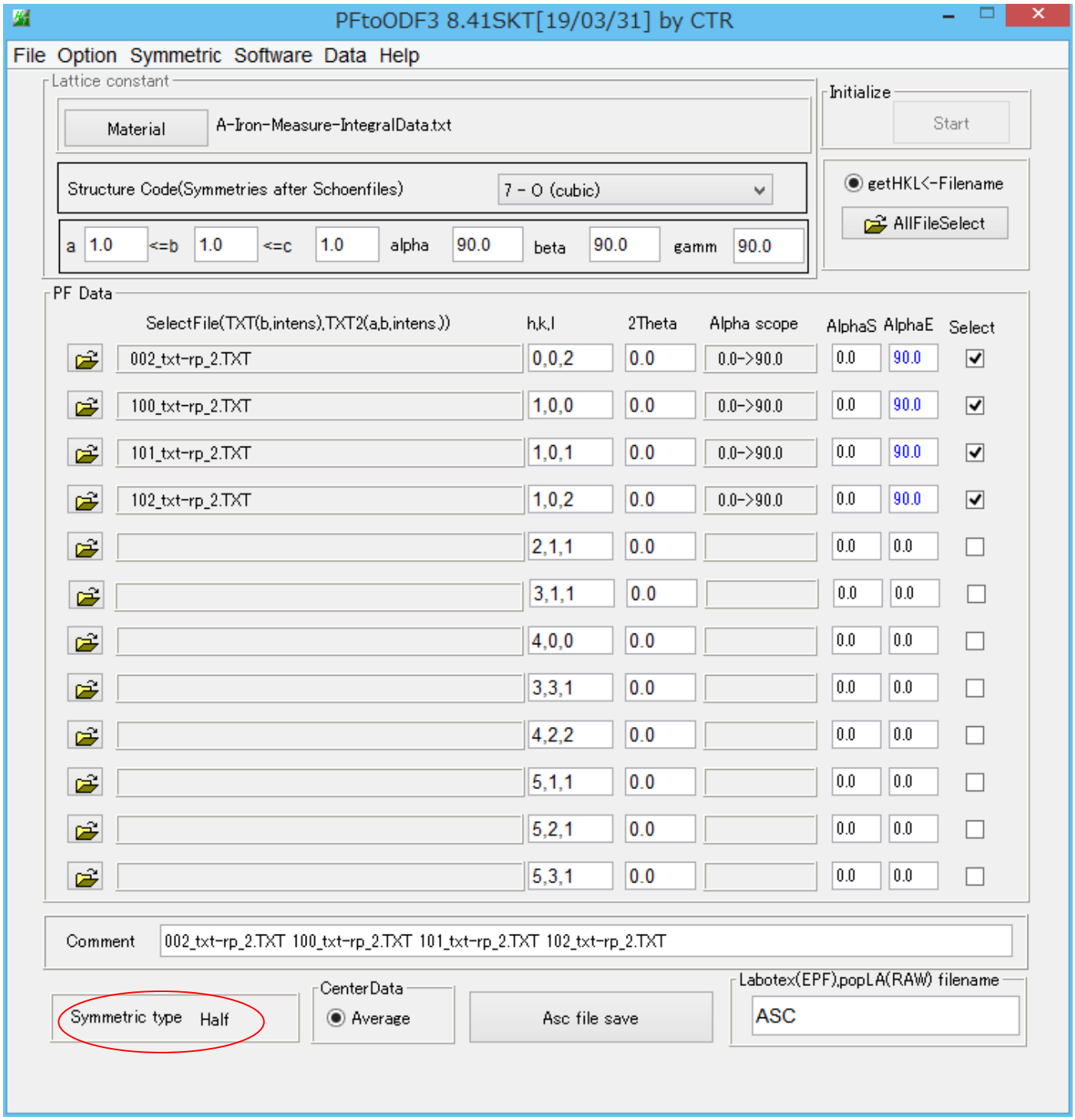
```
>> plot(rpf,'contour')
>> export(odf,'ODF.txt')
>> export(rpf,'rpf.txt')
```

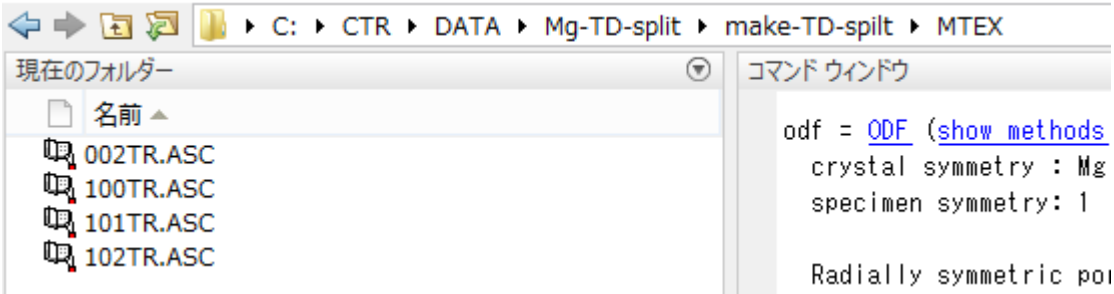


(0,1,3)[1,0,0]f1=0.0,F=31.9,f2=30.0 ODF=127.85

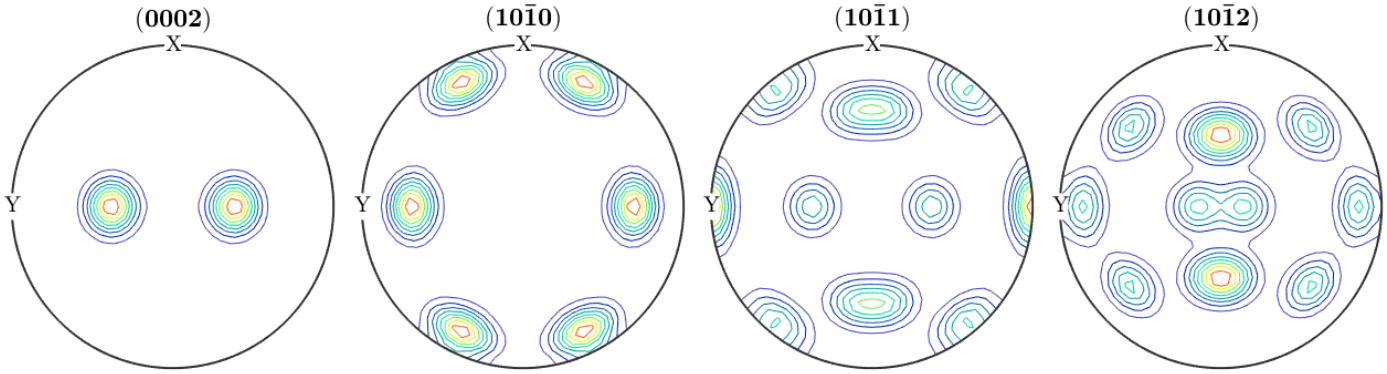


３．１　１／２対称操作でＭＴＥＸに読み込む

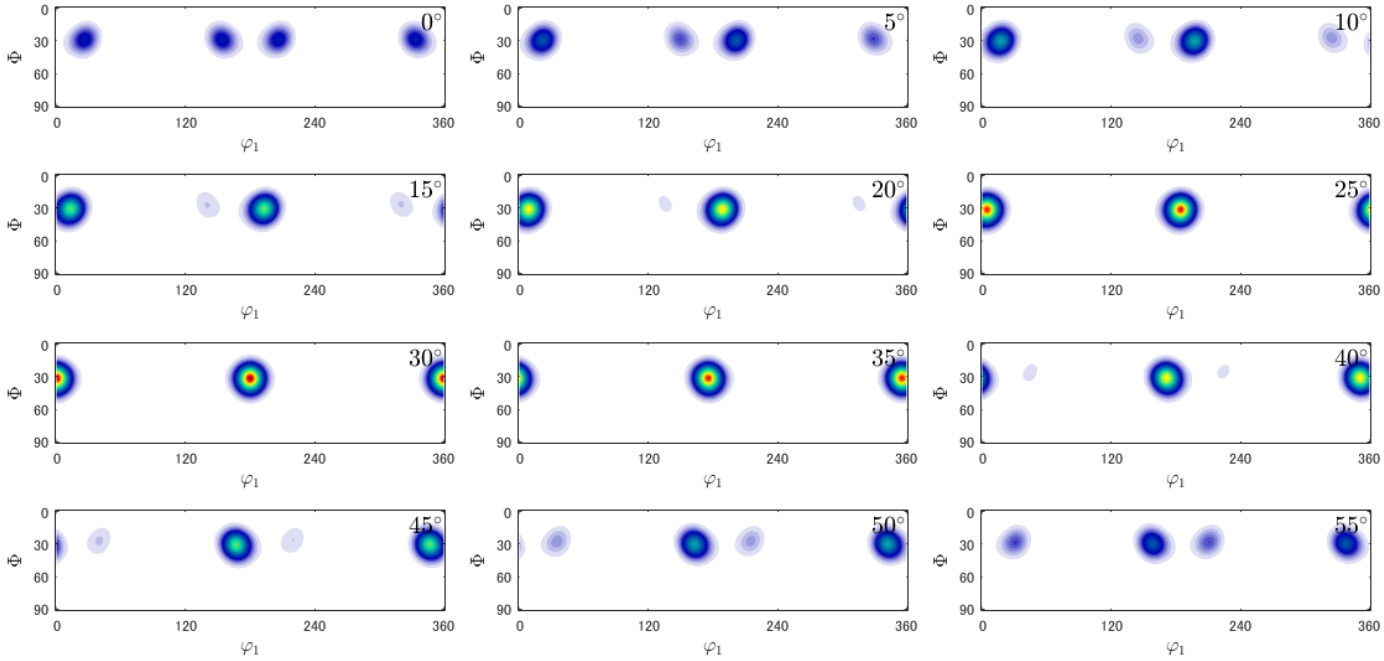




３．３読み込み極点図を描画

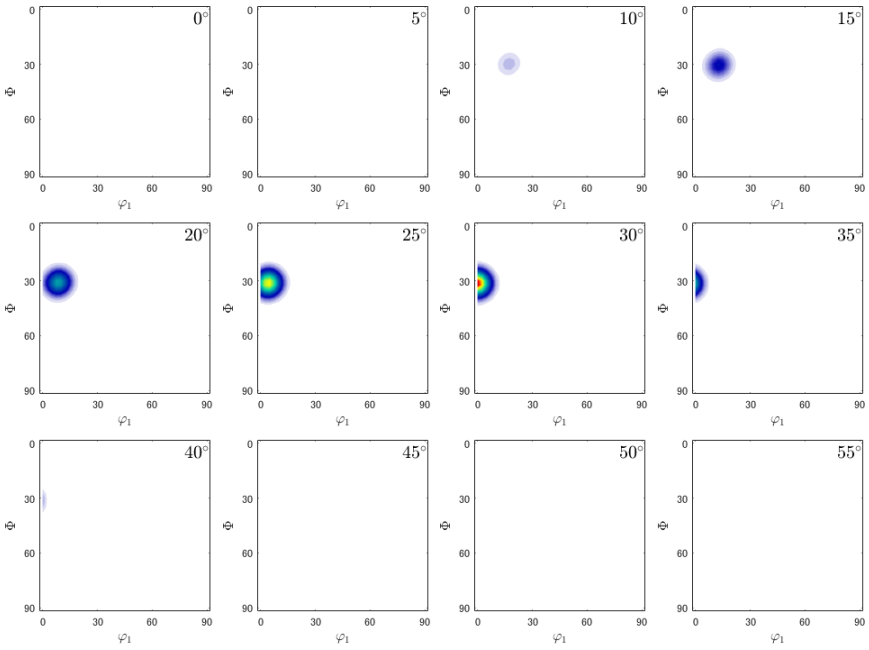


３．４　ＯＤＦ計算

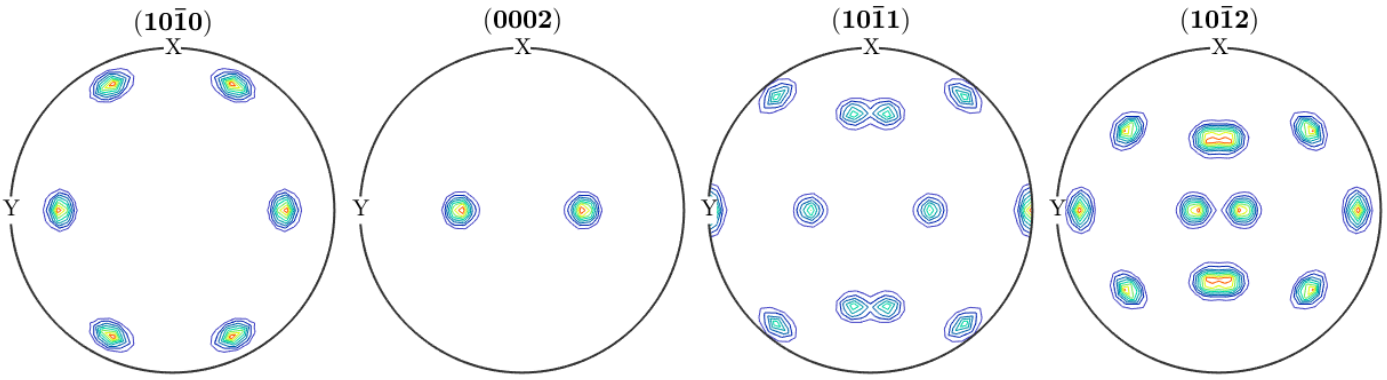


４．　２．３ＯＤＦ図をｔｒｉｃｌｉｎｉｃからｏｒｔｈｏｒｏｍｂｉｃに変える

```
>> SS=specimenSymmetry('mmm')

SS = orthorhombic specimenSymmetry (show methods, plot)

>> ori=orientation('Euler',0*degree,31.4*degree,30*degree,CS,SS)

ori = orientation (show methods, plot)
  size: 1 x 1
  crystal symmetry : Mg (6/mmm, X||a*, Y||b, Z||c)
  specimen symmetry: mmm

  Bunge Euler angles in degree
  phi1  Phi phi2 Inv.
     0 31.4   30    0

>>  odf=unimodalODF(ori,psi)
```



上記ＯＤＦから計算した極点図



コマンド

```
>> ori=orientation('Euler',0*degree,31.4*degree,30*degree,CS,SS)
>> ps=vonMisesFisherKernel('HALFWIDTH',5*degree)
>> odf=calcODF(ori,ps)
>>    h=[Miller(1,0,-1,0,CS),Miller(0,0,0,2,CS),Miller(1,0,1,1,CS),Miller(1,0,-1,2,CS)]
>> odf=calcODF(ori,ps)
>> rpf=calcPoleFigure(odf,h)
>> plot(odf,'sections',12)
>> plot(rpf,'contour')
```