

MTEXによるMgのTD-splitシミュレーション

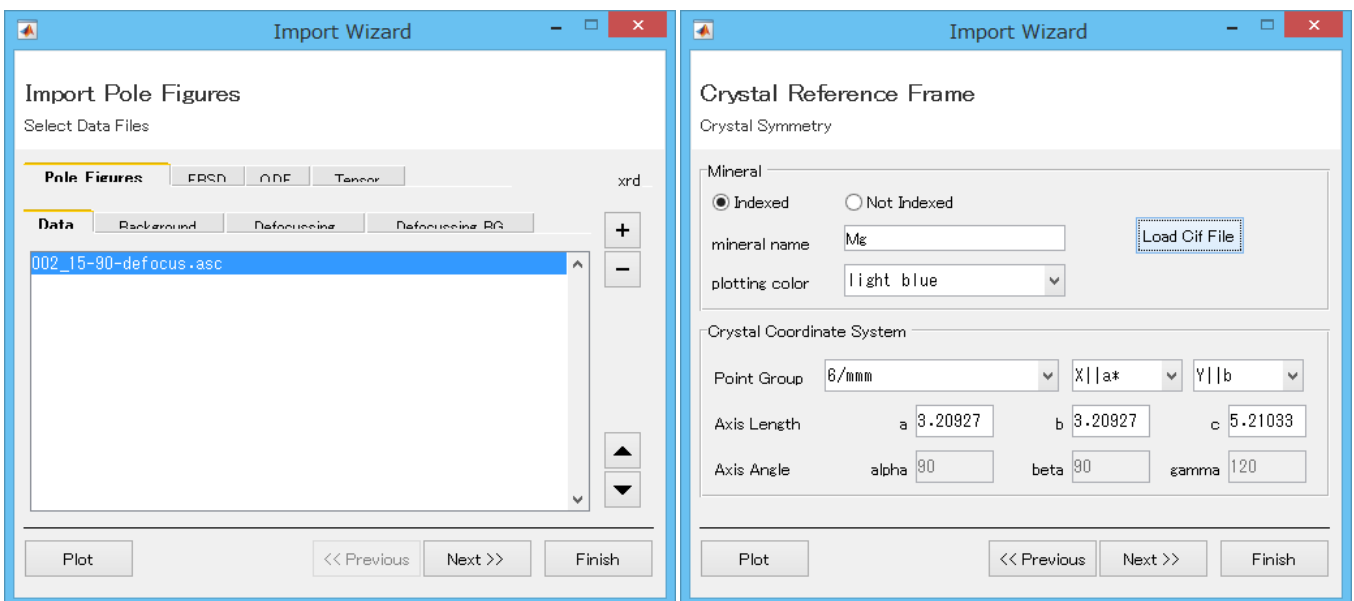
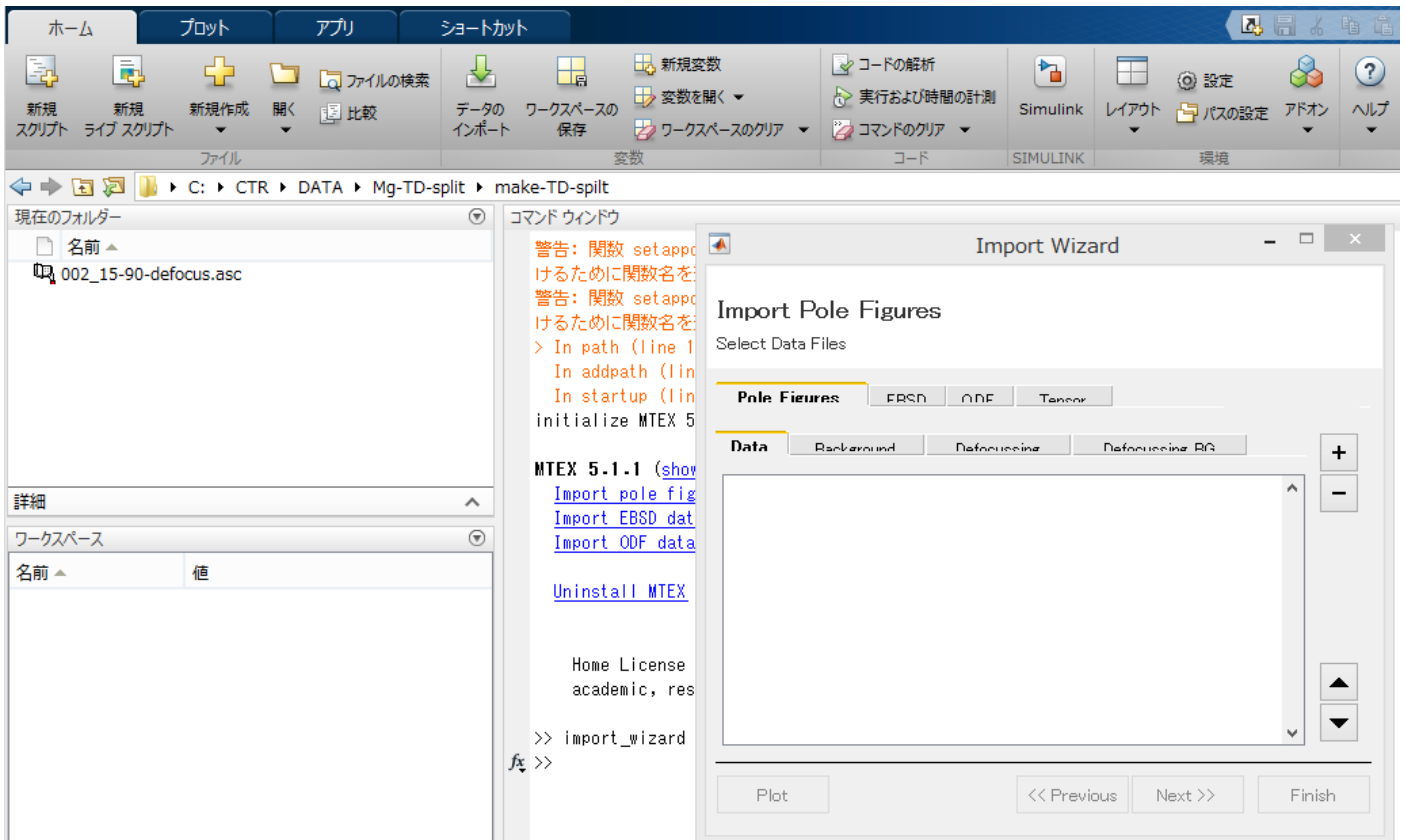
2019年01月27日

*HelperTex Office*

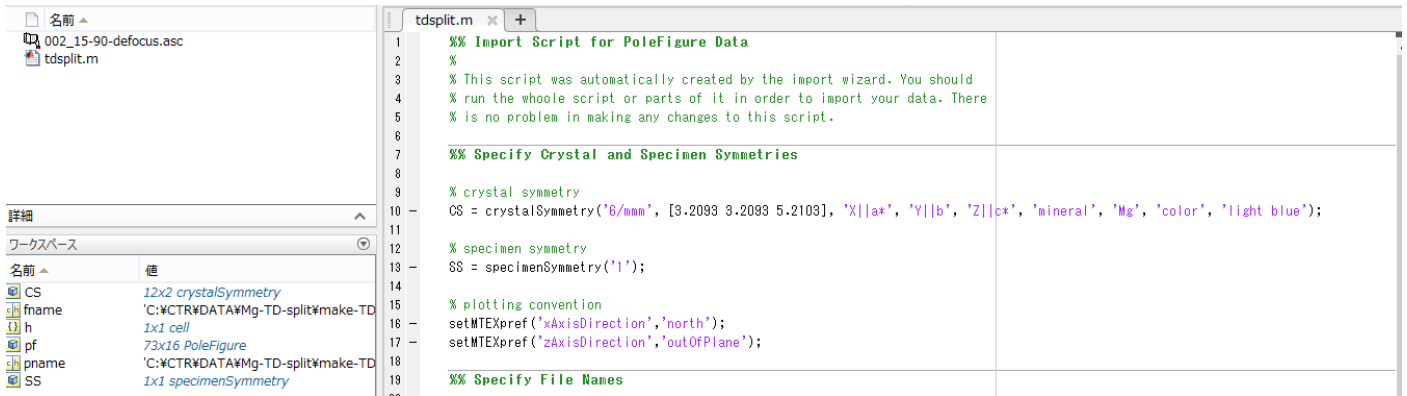
## 1. 概要

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、Hexagonal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	12x2 crystalSymmetry
fname	'C:\CTR\DATA\Mg-TD-split\make-TD'
h	1x1 cell
pf	73x16 PoleFigure
pname	'C:\CTR\DATA\Mg-TD-split\make-TD'
SS	1x1 specimenSymmetry

CSとSSを使用する。

## 2. 1TD-Split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. 3 ODF 図を計算

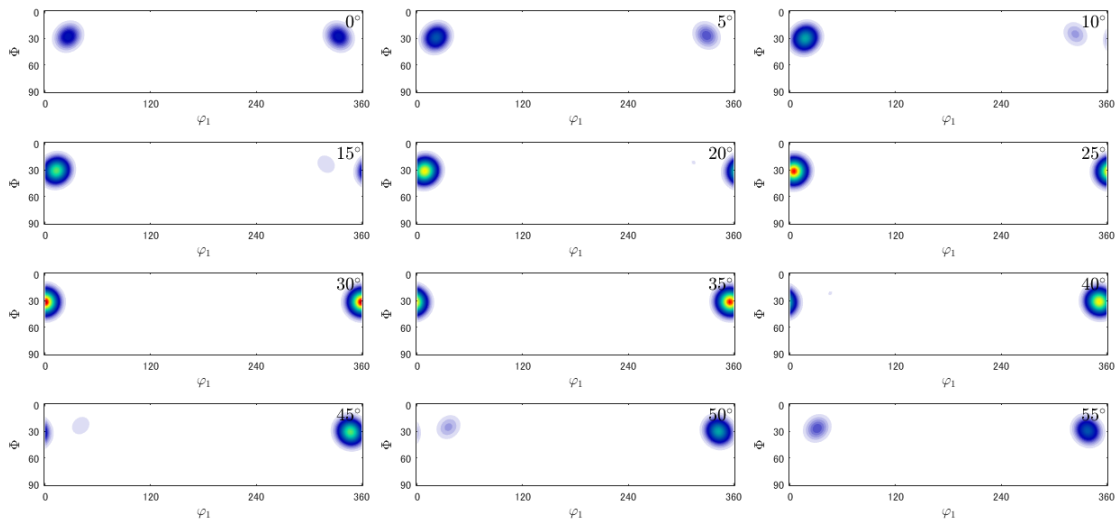
```
>> odf=calcODF(ori,psi)

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

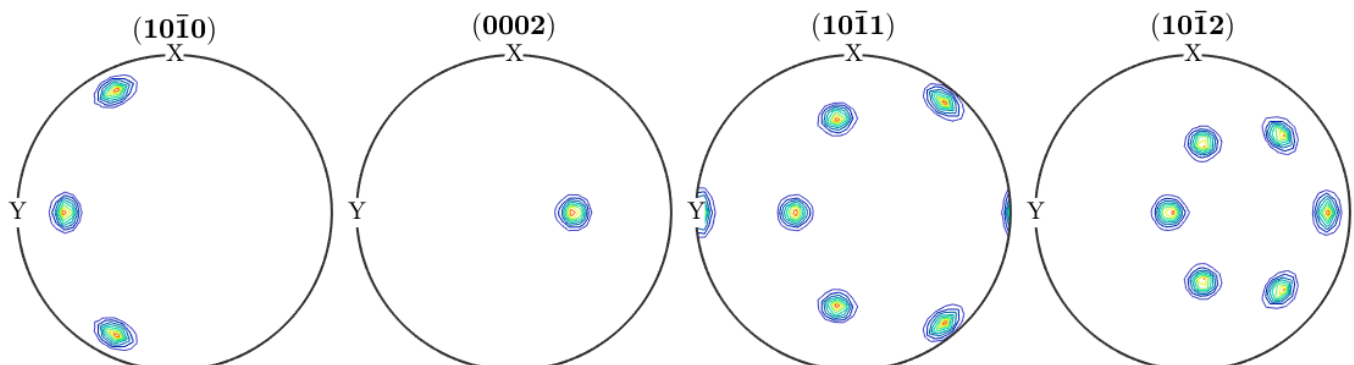
```
>> h=[Miller(1,0,-1,0,CS),Miller(0,0,0,2,CS),Miller(1,0,-1,1,CS),Miller(1,0,-1,2,CS)]
```

```
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)
```

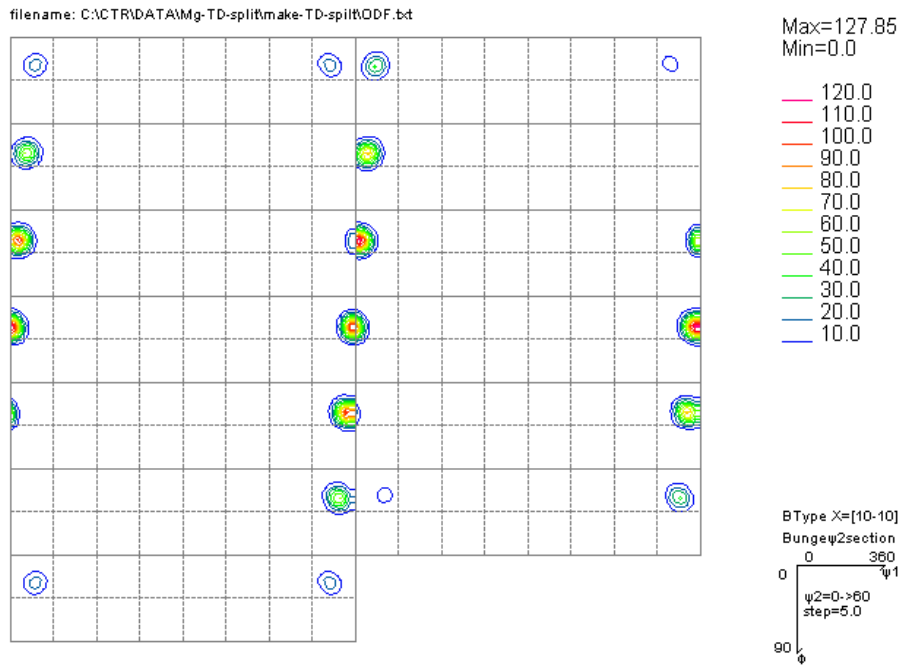
```
rpf = PoleFigure (show methods, plot)
crystal symmetry : Mg (6/mmm, X||a*, Y||b, Z||c)
specimen symmetry: 1
```

```
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
```

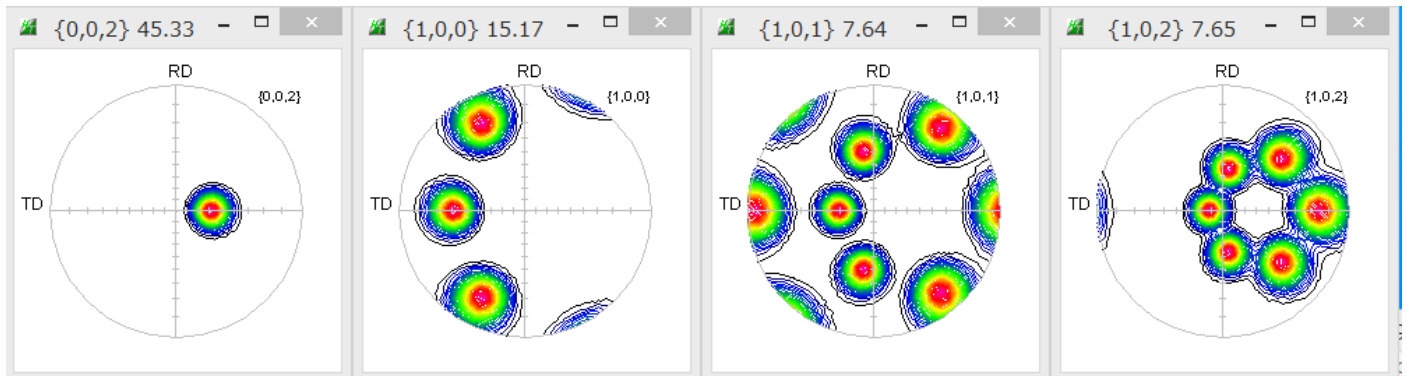


### 3. ODF図、極点図をExport

```
>> 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

PFtoODF3 8.41SKT[19/03/31] by CTR

File Option Symmetric Software Data Help

Lattice constant

Material A-Iron-Measure-IntegralData.txt

Structure Code(Symmetries after Schoenfiles) 7 - O (cubic)

a 1.0 <=b 1.0 <=c 1.0 alpha 90.0 beta 90.0 gamm 90.0

Initialize Start

getHKL<-Filename

AllFileSelect

PF Data

SelectFile(TXT(b,intens),TXT2(a,b,intens))	h,k,l	2Theta	Alpha scope	AlphaS	AlphaE	Select
002_txt-rp_2.TXT	0,0,2	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>
100_txt-rp_2.TXT	1,0,0	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>
101_txt-rp_2.TXT	1,0,1	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>
102_txt-rp_2.TXT	1,0,2	0.0	0.0->90.0	0.0	90.0	<input checked="" type="checkbox"/>
	2,1,1	0.0		0.0	0.0	<input type="checkbox"/>
	3,1,1	0.0		0.0	0.0	<input type="checkbox"/>
	4,0,0	0.0		0.0	0.0	<input type="checkbox"/>
	3,3,1	0.0		0.0	0.0	<input type="checkbox"/>
	4,2,2	0.0		0.0	0.0	<input type="checkbox"/>
	5,1,1	0.0		0.0	0.0	<input type="checkbox"/>
	5,2,1	0.0		0.0	0.0	<input type="checkbox"/>
	5,3,1	0.0		0.0	0.0	<input type="checkbox"/>

Comment 002\_txt-rp\_2.TXT 100\_txt-rp\_2.TXT 101\_txt-rp\_2.TXT 102\_txt-rp\_2.TXT

Symmetric type Half

CenterData Average

Asc file save

Labotex(EPF),popLA(RAW) filename ASC

C: > CTR > DATA > Mg-TD-split > make-TD-spilt > MTEX

現在のフォルダー

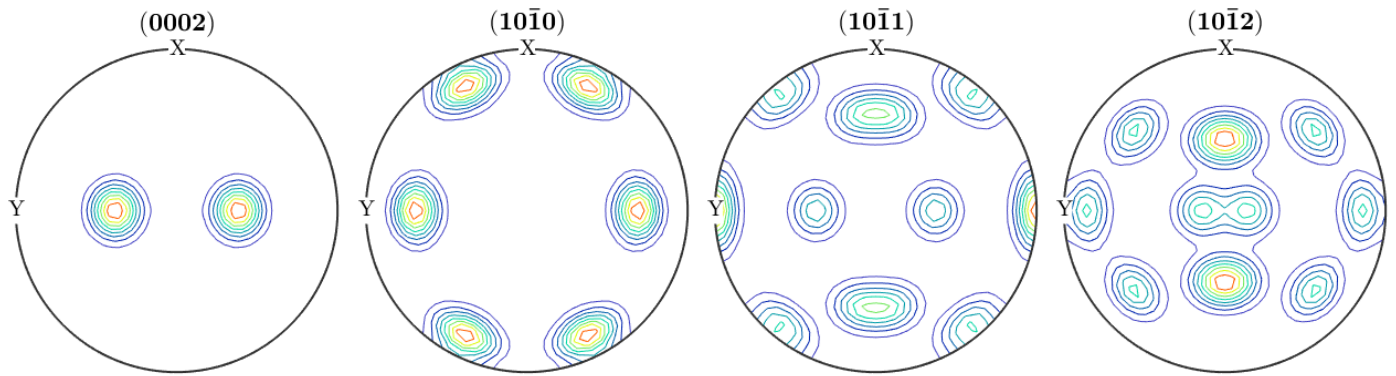
- 名前 ▲
- 002TR.ASC
- 100TR.ASC
- 101TR.ASC
- 102TR.ASC

コマンド ウィンドウ

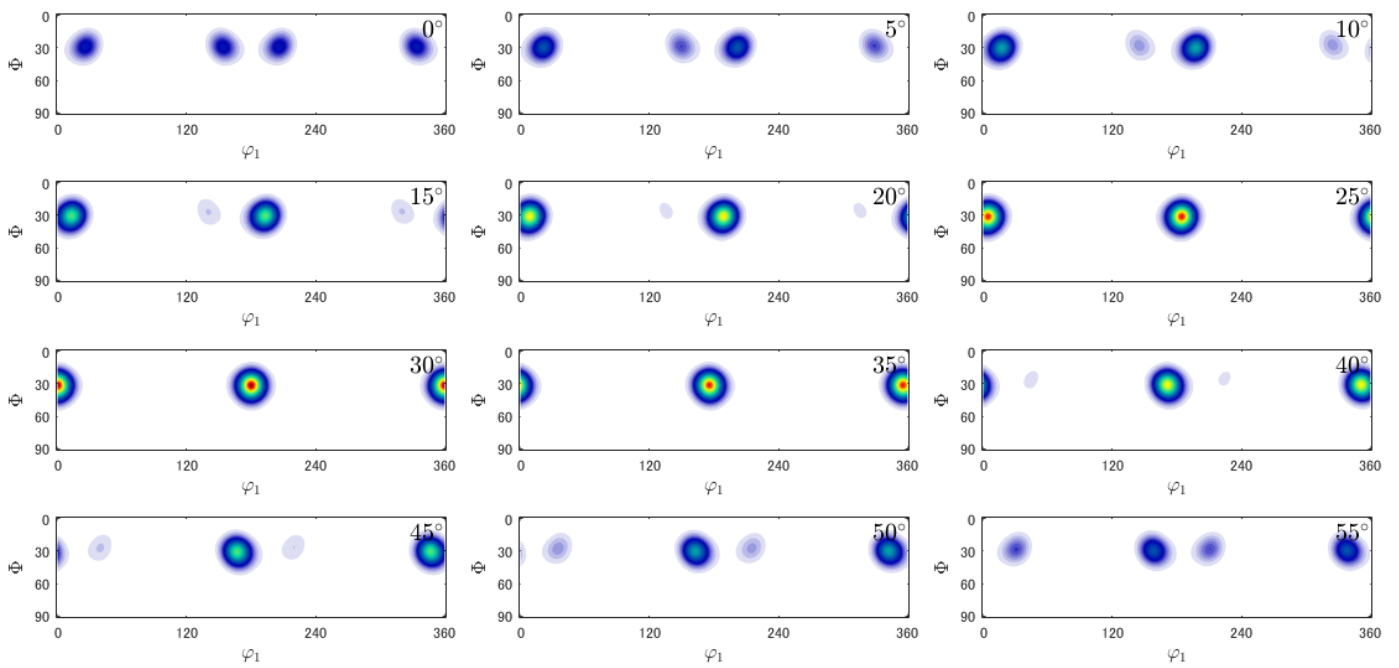
```
odf = ODF (show methods
crystal symmetry : Mg
specimen symmetry: 1

Radially symmetric poi
```

### 3. 3 読み込み極点図を描画



### 3. 4 ODF計算



4. 2. 3 ODF図を *triclinic* から *orthorhombic* 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)
```

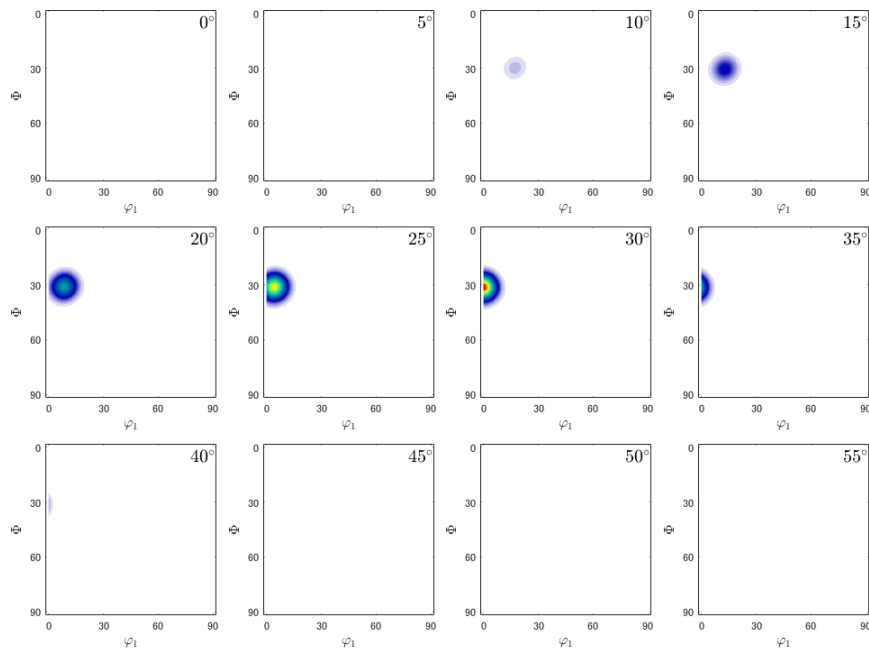
```
specimen symmetry: mmm
```

```
Bunge Euler angles in degree
```

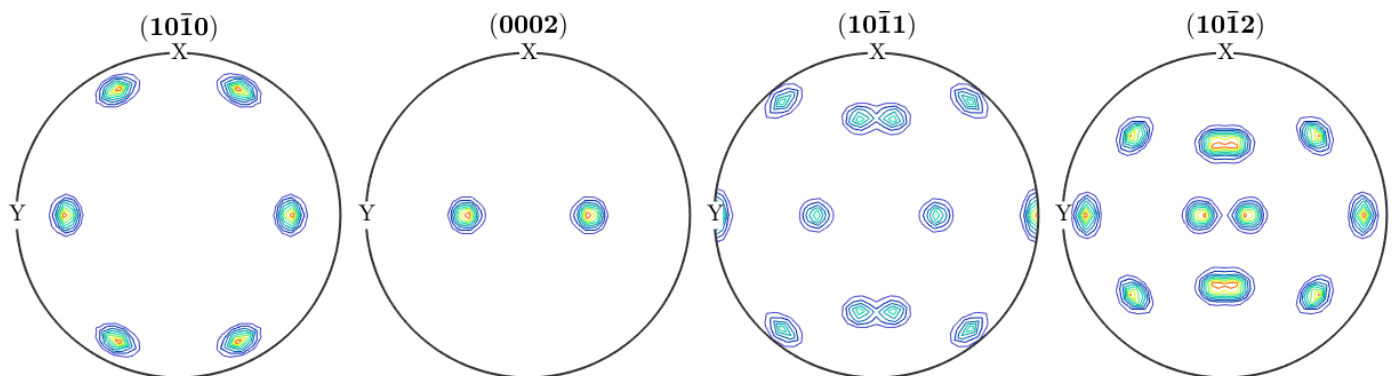
```
phi1 Phi phi2 Inv.
```

```
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')
```