

Misorientation Analysis

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MTEX Workshop 2015

Coordinate Transforms

Consider a Magnetite grain in cube orientation

```
CS_Mag = loadCIF('Magnetite')
```

```
O_Mag = orientation.id(CS_Mag)
```

```
CS_Mag = crystalSymmetry (show methods, plot)
```

```
mineral : Magnetite
```

```
symmetry: m-3m
```

```
a, b, c : 8.4, 8.4, 8.4
```

```
O_Mag = orientation (show methods, plot)
```

```
size: 1 x 1
```

```
crystal symmetry : Magnetite (m-3m)
```

```
specimen symmetry: 1
```

```
Bunge Euler angles in degree
```

```
phi1  Phi phi2 Inv.
```

```
0     0     0     0
```

Remember, orientations convert crystal into specimen coordinates.

```
r = O_Mag * Miller(1,1,1,CS_Mag)
```

Take a Hematite grain with orientation

```
CS_Hem = loadCIF('Hematite')
```

Coordinate Transforms

Consider a Magnetite grain in cube orientation

```
CS_Mag = loadCIF('Magnetite')
```

```
O_Mag = orientation.id(CS_Mag)
```

Remember, orientations convert crystal into specimen coordinates.

```
r = O_Mag * Miller(1,1,1,CS_Mag)
```

```
r = vector3d (show methods, plot)
```

```
size: 1 x 1
```

```
      x           y           z
0.119107 0.119107 0.119107
```

Take a Hematite grain with orientation

```
CS_Hem = loadCIF('Hematite')
```

```
O_Hem = orientation('Euler', ...
```

```
135*degree, 55*degree, 60*degree, CS_Hem)
```

inverse orientations convert specimen into crystal coordinates

```
inv(O_Hem) * r
```

Coordinate Transforms

Consider a Magnetite grain in cube orientation

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Take a Hematite grain with orientation

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CS_Hem = loadCIF('Hematite')
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```
O_Hem = orientation('Euler', ...
```

```
135*degree, 55*degree, 60*degree, CS_Hem)
```

```
O_Hem = orientation(show methods, plot)
```

```
size: 1 x 1
```

```
crystal symmetry : Hematite (-3m1, X||a*, Y||b, Z||c)
```

```
specimen symmetry: 1
```

```
Bunge Euler angles in degree
```

```
phi1      Phi      phi2      Inv.
```

```
135 54.7356      60      0
```

inverse orientations convert specimen into crystal coordinates

Coordinate Transforms

Consider a Magnetite grain in cube orientation

```
CS_Mag = loadCIF('Magnetite')
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O_Mag = orientation.id(CS_Mag)
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Remember, orientations convert crystal into specimen coordinates.

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r = O_Mag * Miller(1,1,1,CS_Mag)
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Take a Hematite grain with orientation

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CS_Hem = loadCIF('Hematite')
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O_Hem = orientation('Euler',...
```

```
135*degree,55*degree,60*degree,CS_Hem)
```

inverse orientations convert specimen into crystal coordinates

```
inv(O_Hem) * r
```

```
ans = Miller (show methods, plot)
```

```
mineral: Hematite (-3m1, X||a*, Y||b, Z||c)
```

```
h 0
```

```
k 0
```

```
i 0
```

```
l 1
```

Misorientations

Hence, $\text{inv}(\mathbf{O_Hem}) \cdot \mathbf{O_Mag}$ converts crystal into crystal coordinates

$\text{inv}(\mathbf{O_Hem}) * \mathbf{O_Mag} * \text{Miller}(1, 1, 1, 0, \text{CS_Mag})$

```
ans = Miller (show methods, plot)
  size: 1 x 1
  mineral: Hematite (-3m1, X||a*, Y||b, Z||c)
  h 0
  k 0
  i 0
  l 1
```

A **misorientation** transforms coordinates with respect to one crystal into coordinates with respect to another crystal.

$\text{Mag2Hem} = \text{inv}(\mathbf{O_Hem}) * \mathbf{O_Mag}$

As $\mathbf{O_Mag}$ and $\mathbf{O_Hem}$ are suspect to crystal symmetry, there are many symmetrically equivalent misorientations to **Mag2Hem**.

$\text{Mag2Hem}.\text{symmetrise}$

Misorientations

Hence, $\text{inv}(\mathbf{O_Hem}) \cdot \mathbf{O_MAG}$ converts crystal into crystal coordinates

$\text{inv}(\mathbf{O_Hem}) * \mathbf{O_Mag} * \mathbf{Miller}(1, 1, 1, 0, \mathbf{CS_Mag})$

A **misorientation** transforms coordinates with respect to one crystal into coordinates with respect to another crystal.

$\text{Mag2Hem} = \text{inv}(\mathbf{O_Hem}) * \mathbf{O_Mag}$

```
Mag2Hem = misorientation (show methods, plot)
size: 1 x 1
crystal symmetry : Magnetite (m-3m)
crystal symmetry : Hematite (-3m1, X||a*, Y||b, Z||c)

Bunge Euler angles in degree
phi1  Phi phi2 Inv.
120   55   45   0
```

As $\mathbf{O_Mag}$ and $\mathbf{O_Hem}$ are suspect to crystal symmetry, there are many symmetrically equivalent misorientations to Mag2Hem .

$\text{Mag2Hem}.\text{symmetrise}$

Misorientations

Hence, $\text{inv}(\mathbf{O_Hem}) \cdot \mathbf{O_MAG}$ converts crystal into crystal coordinates

```
 $\text{inv}(\mathbf{O\_Hem}) * \mathbf{O\_Mag} * \mathbf{Miller}(1, 1, 1, 0, \mathbf{CS\_Mag})$ 
```

A **misorientation** transforms coordinates with respect to one crystal into coordinates with respect to another crystal.

```
 $\text{Mag2Hem} = \text{inv}(\mathbf{O\_Hem}) * \mathbf{O\_Mag}$ 
```

As $\mathbf{O_Mag}$ and $\mathbf{O_Hem}$ are suspect to crystal symmetry, there are many symmetrically equivalent misorientations to **Mag2Hem**.

```
 $\text{Mag2Hem}.\text{symmetrise}$ 
```

```
Mag2Hem = misorientation (show methods, plot)
size: 576 x 1
crystal symmetry : Magnetite (m-3m)
crystal symmetry : Hematite (-3m1, X||a*, Y||b, Z||c)
```

```
 $\text{Mag2Hem}.\text{symmetrise}('unique')$ 
```


Misorientations

Hence, **inv(O_Hem) · O_MAG** converts crystal into crystal coordinates

```
inv(O_Hem) * O_Mag * Miller(1,1,1,0,CS_Mag)
```

A **misorientation** transforms coordinates with respect to one crystal into coordinates with respect to another crystal.

```
Mag2Hem = inv(O_Hem) * O_Mag
```

As **O_Mag** and **O_Hem** are suspect to crystal symmetry, there are many symmetrically equivalent misorientations to **Mag2Hem**.

```
Mag2Hem.symmetrise
```

```
Mag2Hem.symmetrise('unique')
```

```
Mag2Hem = misorientation (show methods, plot)
size: 96 x 1
crystal symmetry : Magnetite (m-3m)
crystal symmetry : Hematite (-3m1, X||a*, Y||b, Z||c)
```

Phase Transitions

The phase transition from **O_Mag** to **O_Hem** is characterized by $\{111\}_m || \{0001\}_h$ and $\{\bar{1}01\}_m || \{00\bar{1}0\}_h$

```
Mag2Hem = orientation( 'map' , ...
    Miller(1,1,1,CS_Mag), Miller(0,0,0,1,CS_Hem) , ...
    Miller(-1,0,1,CS_Mag), Miller(1,0,-1,0,CS_Hem))
```

```
Mag2Hem = misorientation (show methods, plot)
size: 1 x 1
crystal symmetry : Magnetite (m-3m)
crystal symmetry : Hematite (-3m1, X||a*, Y||b, Z||c)

Bunge Euler angles in degree
phi1 Phi phi2 Inv.
120 54.7356 45 0
```

For measured hematite orientation **O_Hem** we can compute the initial magnetite orientation by

```
O_Mag = O_Hem * Mag2Hem
```

MTEX keeps track about the symmetries throughout all computations and

Phase Transitions

The phase transition from **O_Mag** to **O_Hem** is characterized by $\{111\}_m || \{0001\}_h$ and $\{\bar{1}01\}_m || \{00\bar{1}0\}_h$

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Mag2Hem = orientation( 'map' , ...
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    Miller(-1,0,1,CS_Mag), Miller(1,0,-1,0,CS_Hem))
```

For measured hematite orientation **O_Hem** we can compute the initial magnetite orientation by

```
O_Mag = O_Hem * Mag2Hem
```

```
O_Mag = orientation (show methods, plot)
size: 1 x 1
crystal symmetry : Magnetite (m-3m)
specimen symmetry: 1

Bunge Euler angles in degree
  phi1      Phi      phi2      Inv.
134.739  54.7356      45         0
```

MTEX keeps track about the symmetries throughout all computations and

Phase Transitions

The phase transition from **O_Mag** to **O_Hem** is characterized by $\{111\}_m || \{0001\}_h$ and $\{\bar{1}01\}_m || \{00\bar{1}0\}_h$

```
Mag2Hem = orientation( 'map' , ...
    Miller( 1 , 1 , 1 , CS_Mag ) , Miller( 0 , 0 , 0 , 1 , CS_Hem ) , ...
    Miller( -1 , 0 , 1 , CS_Mag ) , Miller( 1 , 0 , -1 , 0 , CS_Hem ) )
```

For measured hematite orientation **O_Hem** we can compute the initial magnetite orientation by

```
O_Mag = O_Hem * Mag2Hem
```

MTEX keeps track about the symmetries throughout all computations and warns in case of mismatch.

Phase Transition

We should care about symmetric equivalence

```
O_Mag = O_Hem * symmetrise(Mag2Hem, 'unique')
```

```
ori_Mag = orientation (show methods, plot)
size: 1 x 96
crystal symmetry : Magnetite (m-3m)
specimen symmetry: 1
```

How many are crystallographically not equivalent?

```
unique(O_Mag)
```

Pole figures of misorientations

```
plotPDF(Mag2Hem, Miller({0 0 0 1},{1 1 -2 1},CS_Hem))
plotIPDF(Mag2Hem, Miller({0 0 1},{1 1 1},CS_Mag))
```

Phase Transition

We should care about symmetric equivalence

```
O_Mag = O_Hem * symmetrise(Mag2Hem, 'unique')
```

How many are crystallographically not equivalent?

```
unique(O_Mag)
```

```
ans = orientation (show methods, plot)
size: 1 x 2
crystal symmetry : Magnetite (m-3m)
specimen symmetry: 1

Bunge Euler angles in degree
  phi1      Phi      phi2      Inv.
314.739 125.264      225         0
254.739 125.264      315         0
```

Pole figures of misorientations

```
plotPDF(Mag2Hem, Miller({0 0 0 1},{1 1 -2 1},CS_Hem))
plotIPDF(Mag2Hem, Miller({0 0 1},{1 1 1},CS_Mag))
```

Phase Transition

We should care about symmetric equivalence

```
O_Mag = O_Hem * symmetrise(Mag2Hem, 'unique')
```

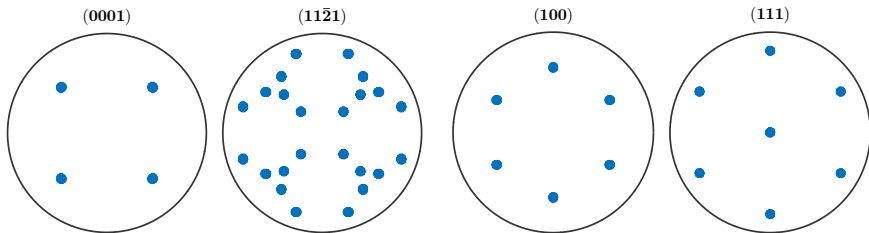
How many are crystallographically not equivalent?

```
unique(O_Mag)
```

Pole figures of misorientations

```
plotPDF(Mag2Hem, Miller({0 0 0 1}, {1 1 -2 1}, CS_Hem))
```

```
plotIPDF(Mag2Hem, Miller({0 0 1}, {1 1 1}, CS_Mag))
```



Relationship Between Lattice Planes

Problem: compute the minimal angle between two lattice planes of two different grains having different orientation and different phase.

```
m_Mag = Miller(1,0,0,cs_Magnetite);
m_Hem = Miller(1,1,-2,0,cs_Hematite);
```

```
m_Mag = Miller (show methods, plot)
size: 1 x 1
mineral: Magnetite (432)
  h 1
  k 0
  l 0

m_Hem = Miller (show methods, plot)
size: 1 x 1
mineral: Hematite (321, X||a*, Y||b, Z||c)
  h 1
  k 1
  i -2
  l 0
```

The orientation relation should be given by

Relationship Between Lattice Planes

Problem: compute the minimal angle between two lattice planes of two different grains having different orientation and different phase.

```
m_Mag = Miller(1,0,0,cs_Magnetite);
m_Hem = Miller(1,1,-2,0,cs_Hematite);
```

The orientation relation should be given by

```
Mag2Hem = orientation( 'map' , ...
    Miller(1,1,1,CS_Mag), Miller(0,0,0,1,CS_Hem) , ...
    Miller(-1,0,1,CS_Mag), Miller(1,0,-1,0,CS_Hem))
```

```
Mag2Hem = misorientation (show methods, plot)
size: 1 x 1
crystal symmetry : Magnetite (m-3m)
crystal symmetry : Hematite (-3m1, X||a*, Y||b, Z||c)

Bunge Euler angles in degree
phi1 Phi phi2 Inv.
120 54.7356 45 0
```

Relationship Between Lattice Planes

Problem: compute the minimal angle between two lattice planes of two different grains having different orientation and different phase.

```
m_Mag = Miller ( 1 , 0 , 0 , cs_Magnetite );
m_Hem = Miller ( 1 , 1 , -2 , 0 , cs_Hematite );
```

The orientation relation should be given by

```
Mag2Hem = orientation ( 'map' , ...
    Miller ( 1 , 1 , 1 , CS_Mag ) , Miller ( 0 , 0 , 0 , 1 , CS_Hem ) , ...
    Miller ( -1 , 0 , 1 , CS_Mag ) , Miller ( 1 , 0 , -1 , 0 , CS_Hem ) )
```

The minimum angle

```
min ( angle ( Mag2Hem * m_Mag . symmetrise , m_Hem ) ) / degree
```

```
35.2644
```

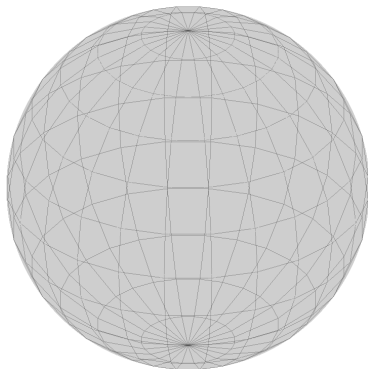
The Misorientation Space - Disjoint Symmetries

plot(orientationRegion)

```
cs3 = crystalSymmetry('3')  
oR = orientationRegion(cs3)  
plot(oR, 'color', 'r')
```

```
cs4 = crystalSymmetry('4')  
oR = orientationRegion(cs4)  
plot(oR, 'color', 'g')
```

```
oR = orientationRegion(cs3, cs4)  
plot(oR, 'color', 'r')
```



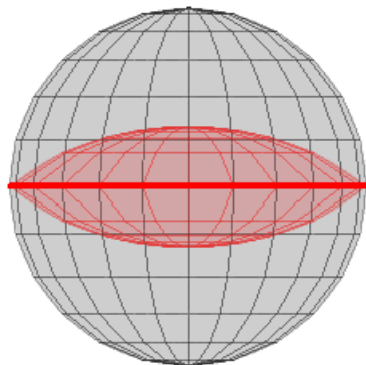
The Misorientation Space - Disjoint Symmetries

```
plot(orientationRegion)
```

```
cs3 = crystalSymmetry('3')  
oR = orientationRegion(cs3)  
plot(oR, 'color', 'r')
```

```
cs4 = crystalSymmetry('4')  
oR = orientationRegion(cs4)  
plot(oR, 'color', 'g')
```

```
oR = orientationRegion(cs3, cs4)  
plot(oR, 'color', 'r')
```



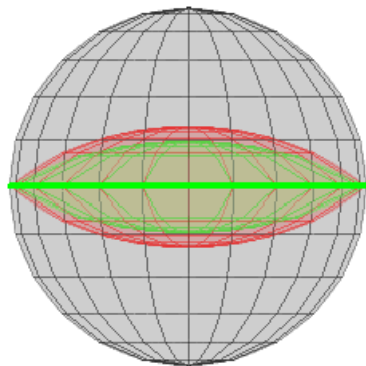
The Misorientation Space - Disjoint Symmetries

```
plot(orientationRegion)
```

```
cs3 = crystalSymmetry('3')
oR = orientationRegion(cs3)
plot(oR, 'color', 'r')
```

```
cs4 = crystalSymmetry('4')
oR = orientationRegion(cs4)
plot(oR, 'color', 'g')
```

```
oR = orientationRegion(cs3, cs4)
plot(oR, 'color', 'r')
```



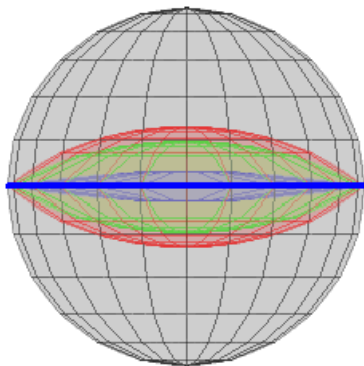
The Misorientation Space - Disjoint Symmetries

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plot(orientationRegion)
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cs3 = crystalSymmetry('3')
oR = orientationRegion(cs3)
plot(oR, 'color', 'r')
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```
cs4 = crystalSymmetry('4')
oR = orientationRegion(cs4)
plot(oR, 'color', 'g')
```

```
oR = orientationRegion(cs3, cs4)
plot(oR, 'color', 'r')
```



The Misorientation Space - Disjoint Symmetries

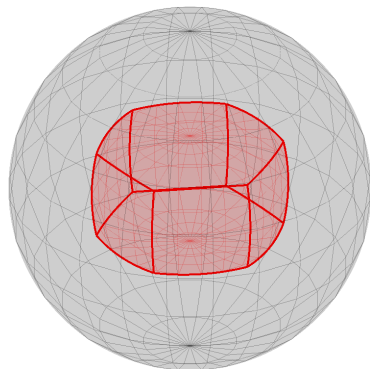
```
plot(orientationRegion)
```

```
cs3 = crystalSymmetry('3')
oR = orientationRegion(cs3)
plot(oR, 'color', 'r')
```

```
cs4 = crystalSymmetry('4')
oR = orientationRegion(cs4)
plot(oR, 'color', 'g')
```

```
oR = orientationRegion(cs3, cs4)
plot(oR, 'color', 'r')
```

```
cs2 = crystalSymmetry('211')
oR = orientationRegion(cs3, cs2)
plot(oR, 'color', 'r')
```



The Misorientation Space - Disjoint Symmetries

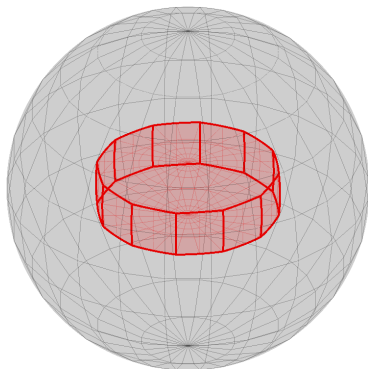
```
plot(orientationRegion)
```

```
cs3 = crystalSymmetry('3')  
oR = orientationRegion(cs3)  
plot(oR, 'color', 'r')
```

```
cs4 = crystalSymmetry('4')  
oR = orientationRegion(cs4)  
plot(oR, 'color', 'g')
```

```
oR = orientationRegion(cs3, cs4)  
plot(oR, 'color', 'r')
```

```
cs2 = crystalSymmetry('222')  
oR = orientationRegion(cs3, cs2)  
plot(oR, 'color', 'r')
```



The Misorientation Space - Common Symmetries

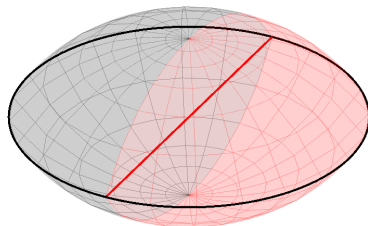
```
cs = crystalSymmetry( '211' )
oR = orientationRegion( cs , cs )
plot( oR , 'color' , 'r' )
```

```
cs = crystalSymmetry( '3' )
oR = orientationRegion( cs , cs )
```

```
cs = crystalSymmetry( '222' )
oR = orientationRegion( cs , cs )
```

```
cs = crystalSymmetry( '222' )
oR = orientationRegion( cs , cs , ...
    'antipodal' )
```

```
cs = crystalSymmetry( '432' )
oR = orientationRegion( cs )
```



The Misorientation Space - Common Symmetries

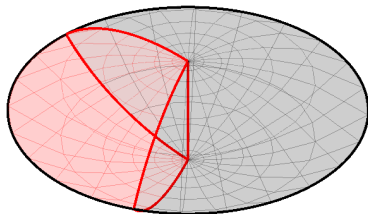
```
cs = crystalSymmetry( '211 ' )
oR = orientationRegion( cs , cs )
plot( oR , 'color' , 'r' )
```

```
cs = crystalSymmetry( '3 ' )
oR = orientationRegion( cs , cs )
```

```
cs = crystalSymmetry( '222 ' )
oR = orientationRegion( cs , cs )
```

```
cs = crystalSymmetry( '222 ' )
oR = orientationRegion( cs , cs , ...
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cs = crystalSymmetry( '432 ' )
oR = orientationRegion( cs )
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The Misorientation Space - Common Symmetries

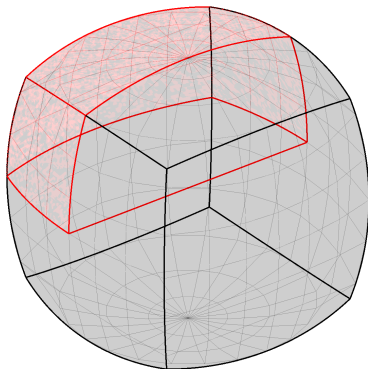
```
cs = crystalSymmetry( '211' )
oR = orientationRegion( cs , cs )
plot( oR , 'color' , 'r' )
```

```
cs = crystalSymmetry( '3' )
oR = orientationRegion( cs , cs )
```

```
cs = crystalSymmetry( '222' )
oR = orientationRegion( cs , cs )
```

```
cs = crystalSymmetry( '222' )
oR = orientationRegion( cs , cs , ...
    'antipodal' )
```

```
cs = crystalSymmetry( '432' )
oR = orientationRegion( cs )
```



The Misorientation Space - Common Symmetries

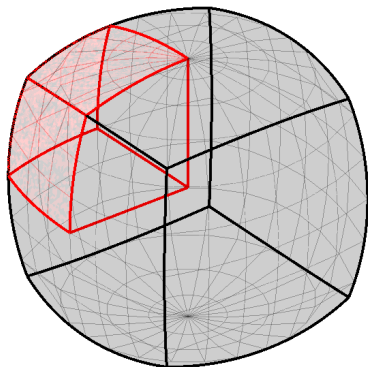
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cs = crystalSymmetry( '222' )
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The Misorientation Space - Common Symmetries

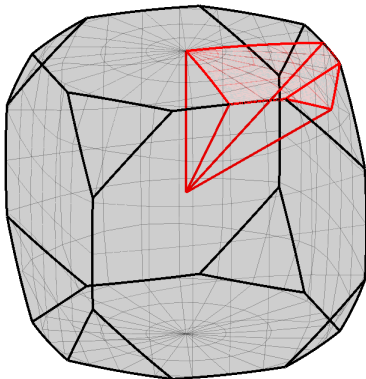
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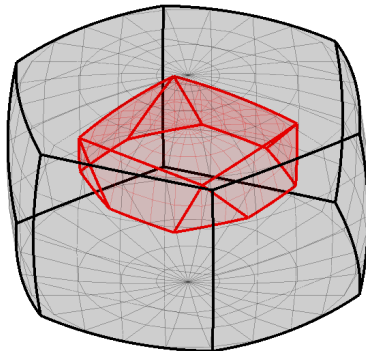
The Misorientation Space - Phase Transitions

```
cs1 = crystalSymmetry( '23' )  
cs2 = crystalSymmetry( '32' )  
oR = orientationRegion( cs1 , cs2 )
```

```
cs1 = crystalSymmetry( '432' )  
cs2 = crystalSymmetry( '321' )  
oR = orientationRegion( cs1 , cs2 )
```

```
Mag2Hem = orientation( 'map' , ...  
    Miller( 1, 1, 1, cs1 ), ...  
    Miller( 0, 0, 0, 1, cs2 ), ...  
    Miller( -1, 0, 1, cs1 ), ...  
    Miller( 1, 0, -1, 0, cs2 ) )  
plot( Mag2Hem )
```

```
plotSection( Mag2Hem )
```



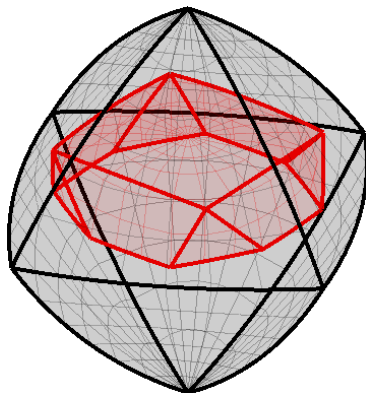
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cs1 = crystalSymmetry( '432' )  
cs2 = crystalSymmetry( '321' )  
oR = orientationRegion( cs1, cs2 )
```

```
Mag2Hem = orientation( 'map', ...  
    Miller(1,1,1, cs1), ...  
    Miller(0,0,0,1, cs2), ...  
    Miller(-1,0,1, cs1), ...  
    Miller(1,0,-1,0, cs2) )  
plot( Mag2Hem )
```

```
plotSection( Mag2Hem )
```



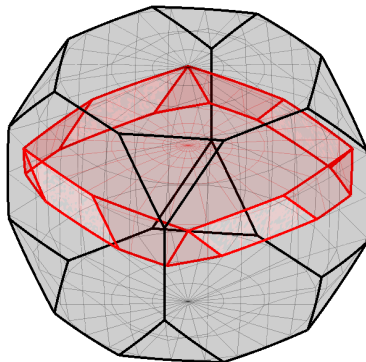
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oR = orientationRegion( cs1 , cs2 )
```

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Mag2Hem = orientation( 'map' , ...  
    Miller( 1, 1, 1, cs1 ), ...  
    Miller( 0, 0, 0, 1, cs2 ), ...  
    Miller( -1, 0, 1, cs1 ), ...  
    Miller( 1, 0, -1, 0, cs2 ) )  
plot( Mag2Hem )
```

```
plotSection( Mag2Hem )
```



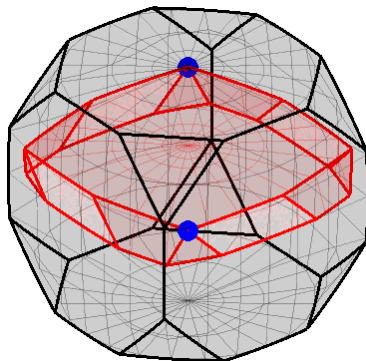
The Misorientation Space - Phase Transitions

```
cs1 = crystalSymmetry( '23' )  
cs2 = crystalSymmetry( '32' )  
oR = orientationRegion( cs1 , cs2 )
```

```
cs1 = crystalSymmetry( '432' )  
cs2 = crystalSymmetry( '321' )  
oR = orientationRegion( cs1 , cs2 )
```

```
Mag2Hem = orientation( 'map' , ...  
    Miller( 1, 1, 1, cs1 ), ...  
    Miller( 0, 0, 0, 1, cs2 ), ...  
    Miller( -1, 0, 1, cs1 ), ...  
    Miller( 1, 0, -1, 0, cs2 ) )  
plot( Mag2Hem )
```

```
plotSection( Mag2Hem )
```



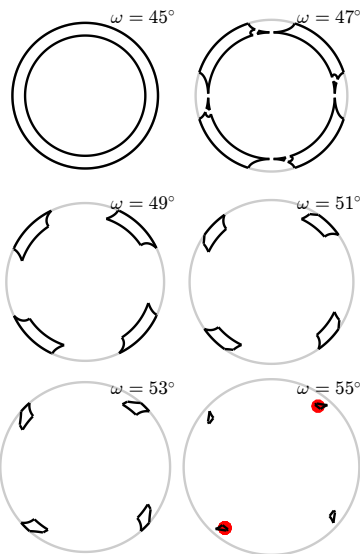
The Misorientation Space - Phase Transitions

```
cs1 = crystalSymmetry( '23' )
cs2 = crystalSymmetry( '32' )
oR = orientationRegion( cs1 , cs2 )
```

```
cs1 = crystalSymmetry( '432' )
cs2 = crystalSymmetry( '321' )
oR = orientationRegion( cs1 , cs2 )
```

```
Mag2Hem = orientation( 'map' , ...
  Miller( 1, 1, 1, cs1 ), ...
  Miller( 0, 0, 0, 1, cs2 ), ...
  Miller( -1, 0, 1, cs1 ), ...
  Miller( 1, 0, -1, 0, cs2 ) )
plot( Mag2Hem )
```

```
plotSection( Mag2Hem )
```



Austenite to Martensite transition

```
ebsd=loadEBSD('martensite.ctf')
```

```
ebsd = EBSD (show methods, plot)
```

Phase	Orientations	Mineral	Symmetry
1	25389 (69)	fcc	m-3m
2	1884 (5.1)	bcc	m-3m
3	9693 (26)	hcp	6/mmm

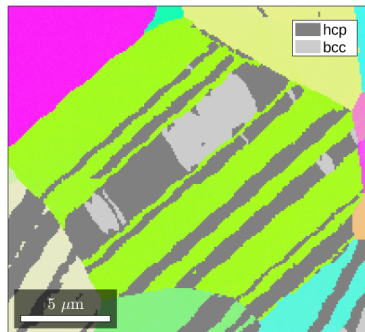
Properties: bands, bc, bs, error, mad
Scan unit : um

```
grains=calcGrains(ebsd);  
plot(grains.boundary)  
gB=grains.boundary('fcc','hcp')
```

```
plotSection(gB.misorientation)
```

```
mdf=calcMDF(gB.misorientation)  
plotSection(mdf)
```

```
plot(gB.misorientation, ...  
      mdf.eval(gB.misorientation))
```



Austenite to Martensite transition

```
ebsd=loadEBSD('martensite.ctf')
```

```
grains=calcGrains(ebsd);
```

```
plot(grains.boundary)
```

```
gB=grains.boundary('fcc','hcp')
```

```
gB = grainBoundary (show methods, plot)
```

Segments	mineral 1	mineral 2
3829	fcc	hcp

```
plotSection(gB.misorientation)
```

```
mdf=calcMDF(gB.misorientation)
```

```
plotSection(mdf)
```

```
plot(gB.misorientation, ...  
      mdf.eval(gB.misorientation))
```



Austenite to Martensite transition

```
ebsd=loadEBSD('martensite.ctf')
```

```
grains=calcGrains(ebsd);
```

```
plot(grains.boundary)
```

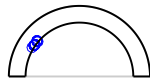
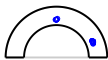
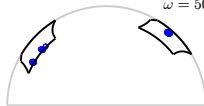
```
gB=grains.boundary('fcc','hcp')
```

```
plotSection(gB.misorientation)
```

```
mdf=calcMDF(gB.misorientation)
```

```
plotSection(mdf)
```

```
plot(gB.misorientation, ...  
      mdf.eval(gB.misorientation))
```

 $\omega = 20^\circ$ $\omega = 25^\circ$ $\omega = 30^\circ$ $\omega = 35^\circ$  $\omega = 40^\circ$ $\omega = 45^\circ$ $\omega = 50^\circ$ $\omega = 55^\circ$ 

Austenite to Martensite transition

```
ebsd=loadEBSD('martensite.ctf')
```

```
grains=calcGrains(ebsd);
```

```
plot(grains.boundary)
```

```
gB=grains.boundary('fcc','hcp')
```

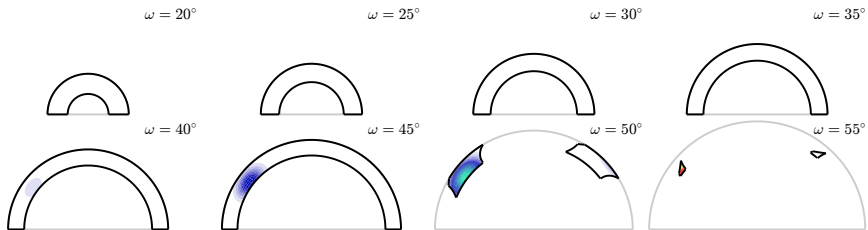
```
plotSection(gB.misorientation)
```

```
mdf=calcMDF(gB.misorientation)
```

```
plotSection(mdf)
```

```
plot(gB.misorientation, ...  
     mdf.eval(gB.misorientation))
```

```
mdf = MDF  
crystal sym: fcc (m-3m)  
crystal sym: hcp (6/mmm)  
  
Harmonic portion:  
degree: 38  
weight: 1
```



Austenite to Martensite transition

```
ebsd=loadEBSD('martensite.ctf')
```

```
grains=calcGrains(ebsd);
```

```
plot(grains.boundary)
```

```
gB=grains.boundary('fcc','hcp')
```

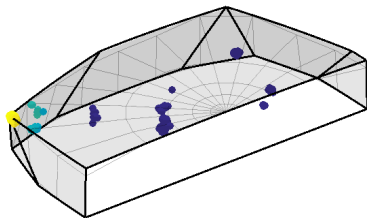
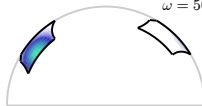
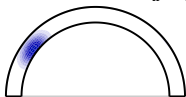
```
plotSection(gB.misorientation)
```

```
mdf=calcMDF(gB.misorientation)
```

```
plotSection(mdf)
```

```
plot(gB.misorientation, ...
```

```
mdf.eval(gB.misorientation))
```

 $\omega = 20^\circ$ $\omega = 25^\circ$ $\omega = 30^\circ$ $\omega = 35^\circ$  $\omega = 40^\circ$ $\omega = 45^\circ$ $\omega = 50^\circ$ $\omega = 55^\circ$ 

Austenite to Martensite transition

```
plot (gB, gB.misorientation . angle)
```

```
oR = fundamentalRegion (csFCC , csHCP)
```

```
mO = orientation (oR.V, csFCC , csHCP)
```

```
tB = gB (gB.isTwinning (mO, 1*degree))
```

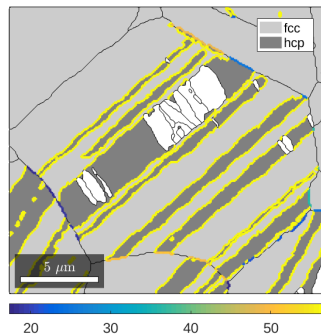
```
plot (tB, 'linccolor', 'r')
```

```
[mGrains, parent] = merge (grains, tB)
```

```
plot (mGrains.boundary)
```

```
wasFCC = parent (grains.phase==1);
```

```
mGrains.phase (wasFCC) = 1
```



Austenite to Martensite transition

```
plot (gB, gB.misorientation . angle)
```

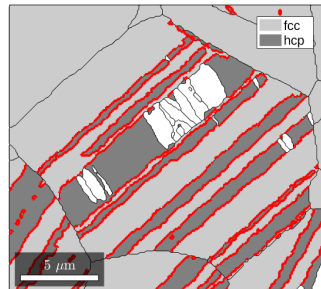
```
oR = fundamentalRegion (csFCC, csHCP)  
mO = orientation (oR.V, csFCC, csHCP)  
tB = gB (gB.isTwinning (mO, 1 * degree))  
plot (tB, 'linccolor', 'r')
```

```
tB = grainBoundary (show methods, plot)
```

Segments	mineral 1	mineral 2
3283	fcc	hcp

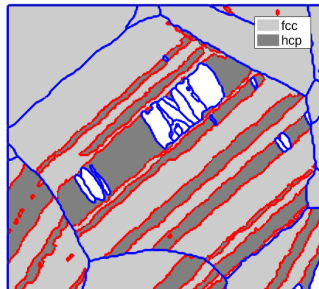
```
[mGrains, parent] = merge (grains, tB)  
plot (mGrains.boundary)
```

```
wasFCC = parent (grains.phase == 1);  
mGrains.phase (wasFCC) = 1
```



Austenite to Martensite transition

```
plot (gB, gB.misorientation.angle)
```



```
oR = fundamentalRegion (csFCC, csHCP)
```

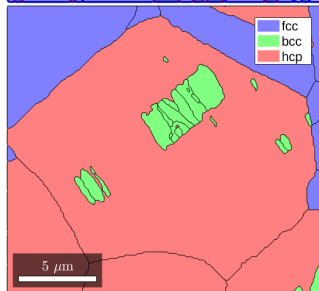
```
mO = orientation (oR.V, csFCC, csHCP)
```

```
tB = gB(gB.isTwinning (mO, 1*degree))
```

```
plot (tB, 'linccolor', 'r')
```

```
[mGrains, parent] = merge (grains, tB)
```

```
plot (mGrains.boundary)
```



```
mGrains = grain2d (show methods, plot)
```

Phase	Grains	Pixels	Mineral	Symmetry
1	8	7156	fcc	m-3m
2	26	1884	bcc	m-3m
3	6	27926	hcp	6/mmm

```
wasFCC = parent (grains.phase==1);
```

```
mGrains.phase (wasFCC) = 1
```

Austenite to Martensite transition

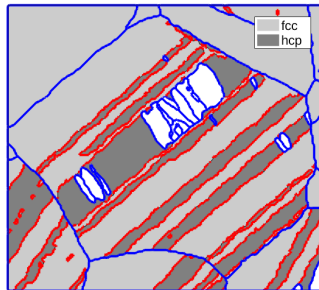
```
plot (gB , gB . misorientation . angle )
```

```
oR = fundamentalRegion (csFCC , csHCP)
```

```
mO = orientation (oR.V , csFCC , csHCP)
```

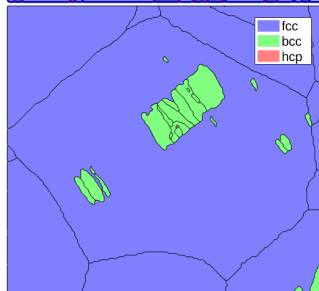
```
tB = gB (gB . isTwinning (mO , 1 * degree ))
```

```
plot (tB , 'linccolor' , 'r')
```



```
[mGrains , parent] = merge (grains , tB)
```

```
plot (mGrains . boundary)
```



```
wasFCC = parent (grains . phase == 1);
```

```
mGrains . phase (wasFCC) = 1
```

```
mGrains = grain2d (show methods , plot)
```

Phase	Grains	Pixels	Mineral	Symmetry
1	13	35079	fcc	m-3m
2	26	1884	bcc	m-3m
3	1	3	hcp	6/mmm

Misorientation angle and axis

the smallest rotational angle of all symmetrically equivalent misorientations to **MO** is called **misorientation angle**

angle(O1, O2), angle(MO), angle(inv(MO))

for boundary misorientations we can do a simple statistics by

```
gB = grain.boundary
```

```
hist(gB('fcc', 'fcc').misorientation.angle ./ degree)
```

nicer plots

```
plotAngleDistribution(gB('fcc', 'fcc').misorientation)
```

Misorientation angle and axis

the smallest rotational angle of all symmetrically equivalent misorientations to **MO** is called **misorientation angle**

```
angle(O1, O2), angle(MO), angle(inv(MO))
```

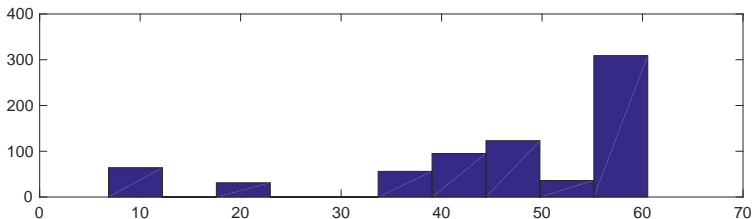
for boundary misorientations we can do a simple statistics by

```
gB = grain.boundary
```

```
hist(gB('fcc', 'fcc').misorientation.angle ./ degree)
```

nicer plots

```
plotAngleDistribution(gB('fcc', 'fcc').misorientation)
```



Misorientation angle and axis

the smallest rotational angle of all symmetrically equivalent misorientations to **MO** is called **misorientation angle**

```
angle(O1, O2), angle(MO), angle(inv(MO))
```

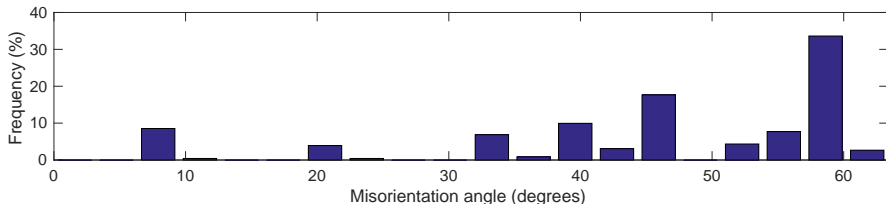
for boundary misorientations we can do a simple statistics by

```
gB = grain.boundary
```

```
hist(gB('fcc', 'fcc').misorientation.angle ./ degree)
```

nicer plots

```
plotAngleDistribution(gB('fcc', 'fcc').misorientation)
```



Angle Distributions

The untextured, uncorrelated angle distribution

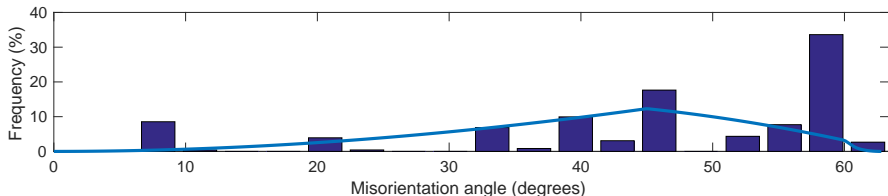
```
plotAngleDistribution (csFCC , csFCC)
```

The textured, uncorrelated angle distribution

```
odf = calcODF (ebsd ( 'fcc ' ). orientations );  
mdf = calcMDF (odf , odf)  
plotAngleDistribution (mdf)
```

The textured, correlated angle distribution

```
mdf = calcMDF (gB ( 'fcc ' , 'fcc ' ). misorientation )  
plotAngleDistribution (mdf)
```



Angle Distributions

The untextured, uncorrelated angle distribution

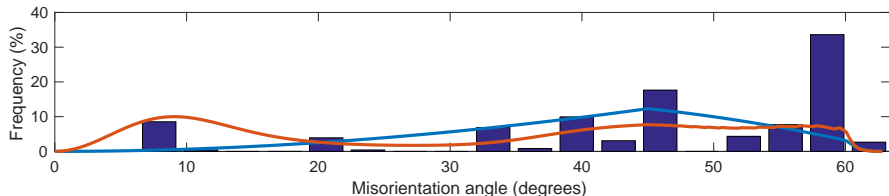
```
plotAngleDistribution (csFCC , csFCC)
```

The textured, uncorrelated angle distribution

```
odf = calcODF(ebsd('fcc').orientations);  
mdf = calcMDF(odf, odf)  
plotAngleDistribution(mdf)
```

The textured, correlated angle distribution

```
mdf = calcMDF(gB('fcc', 'fcc').misorientation)  
plotAngleDistribution(mdf)
```



Angle Distributions

The untextured, uncorrelated angle distribution

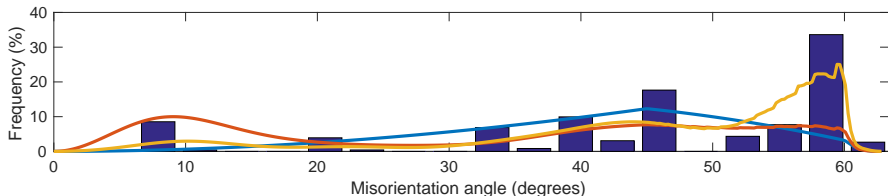
```
plotAngleDistribution (csFCC , csFCC)
```

The textured, uncorrelated angle distribution

```
odf = calcODF(ebsd('fcc').orientations);  
mdf = calcMDF(odf , odf)  
plotAngleDistribution(mdf)
```

The textured, correlated angle distribution

```
mdf = calcMDF(gB('fcc', 'fcc').misorientation)  
plotAngleDistribution(mdf)
```



Misorientation axis in crystal coordinates

the misorientation realizing the minimum angle is

MO. `project2FundamentalRegion`

```
MO = misorientation (show methods, plot)
size: 1 x 1
crystal symmetry : Magnetite (m-3m)
crystal symmetry : Hematite (-3m1)

Bunge Euler angles in degree
  phi1      Phi      phi2      Inv.
60.1624  54.6037  314.719      0
```

its rotational axis is the `misorientation axis`

```
axis(MO)
```

```
axis(inv(MO))
```

```
plotAxisDistribution (...
  gB.misorientation)
```

```
plotAxisDistribution (...
  inv(gB.misorientation))
```

Misorientation axis in crystal coordinates

the misorientation realizing the minimum angle is

MO. project2FundamentalRegion

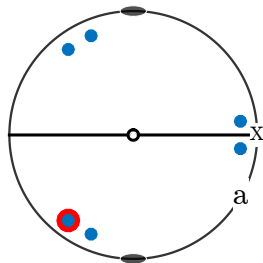
its rotational axis is the **misorientation axis**

axis (MO)

```
ans = Miller (show methods, plot)
  size: 1 x 1
  mineral: Hematite (-3m1)
  h  0.6191
  k  3.8882
  i -4.5073
  l  3.3513
```

axis (inv (MO))

```
plotAxisDistribution (...
  gB.misorientation)
plotAxisDistribution (...
  inv(gB.misorientation))
```



Misorientation axis in crystal coordinates

the misorientation realizing the minimum angle is

MO. project2FundamentalRegion

its rotational axis is the **misorientation axis**

axis (MO)

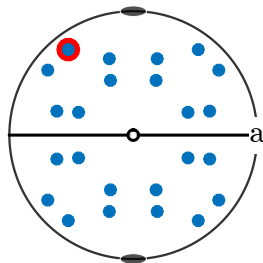
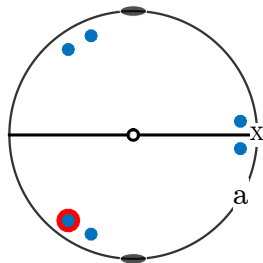
axis (inv (MO))

```
ans = Miller (show methods, plot)
size: 1 x 1
mineral: Magnetite (m-3m)
h 4.9324
k -6.4797
l 2.0431
```

```
plotAxisDistribution (...
    gB.misorientation)
```

```
plotAxisDistribution (...
    inv(gB.misorientation))
```

```
plotAxisDistribution (...
```



Misorientation axis in crystal coordinates

the misorientation realizing the minimum angle is

MO. project2FundamentalRegion

its rotational axis is the **misorientation axis**

axis (MO)

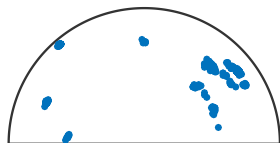
axis (inv (MO))

**plotAxisDistribution (...
gB. misorientation)**

**plotAxisDistribution (...
inv (gB. misorientation))**

**plotAxisDistribution (...
gB. misorientation, 'contourf')**

**plotAxisDistribution (...
inv (gB. misorientation), 'contourf')**



Misorientation axis in crystal coordinates

the misorientation realizing the minimum angle is

MO. project2FundamentalRegion

its rotational axis is the **misorientation axis**

axis (MO)

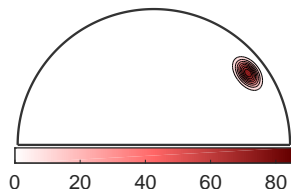
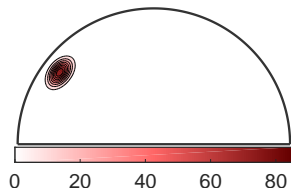
axis (inv (MO))

**plotAxisDistribution (...
gB. misorientation)**

**plotAxisDistribution (...
inv (gB. misorientation))**

**plotAxisDistribution (...
gB. misorientation, 'contourf')**

**plotAxisDistribution (...
inv (gB. misorientation), 'contourf')**



Misorientation axis distributions

The untextured, uncorrelated axis distribution

```
plotAxisDistribution (csHCP , csFCC)
```

The textured, correlated axis distribution

```
mdf = calcMDF(gB.misorientations)
```

```
plotAxisDistribution (mdf)
```

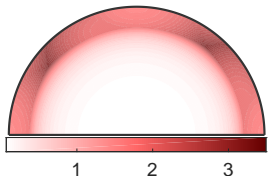
```
[value , mori] = max(mdf)
```

```
plot (mori . axis)
```

The textured, uncorrelated axis distribution

```
mdf = calcMDF(odfFCC , odfHCP)
```

```
plotAxisDistribution (mdf)
```



Misorientation axis distributions

The untextured, uncorrelated axis distribution

```
plotAxisDistribution (csHCP , csFCC)
```

The textured, correlated axis distribution

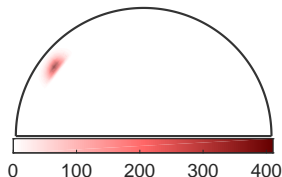
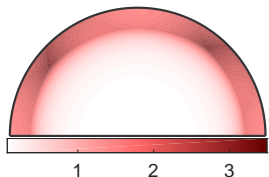
```
mdf = calcMDF(gB.misorientations)  
plotAxisDistribution (mdf)
```

```
mdf = MDF (show methods , plot)  
crystal symmetry : fcc (m-3m)  
crystal symmetry : hcp (6/mmm)  
  
Harmonic portion:  
degree: 58  
weight: 1
```

```
[value , mori] = max(mdf)  
plot (mori.axis)
```

The textured, uncorrelated axis distribution

```
mdf = calcMDF(odfFCC , odfHCP)  
plotAxisDistribution (mdf)
```



Misorientation axis distributions

The untextured, uncorrelated axis distribution

plotAxisDistribution (csHCP , csFCC)

The textured, correlated axis distribution

`mdf = calcMDF(gB.misorientations)`

plotAxisDistribution (mdf)

`[value , mori] = max(mdf)`

plot (mori . axis)

```
value =  
232.1792
```

```
mori = misorientation (show methods, plot)
```

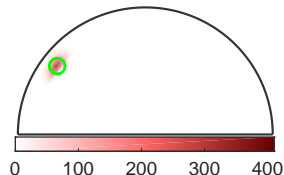
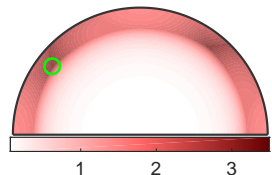
```
size: 1 x 1
```

```
crystal symmetry : fcc (m-3m)
```

```
crystal symmetry : hcp (6/mmm)
```

```
Bunge Euler angles in degree
```

```
phi1      Phi      phi2      Inv.  
210.936  54.7028  134.957      0
```



Misorientation axis distributions

The untextured, uncorrelated axis distribution

```
plotAxisDistribution (csHCP , csFCC)
```

The textured, correlated axis distribution

```
mdf = calcMDF(gB.misorientations)
```

```
plotAxisDistribution (mdf)
```

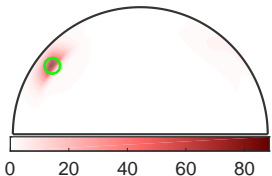
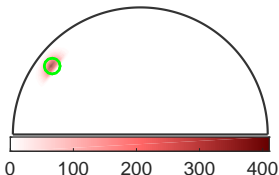
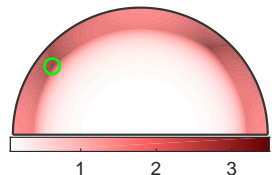
```
[value , mori] = max(mdf)
```

```
plot (mori . axis)
```

The textured, uncorrelated axis distribution

```
mdf = calcMDF(odfFCC , odfHCP)
```

```
plotAxisDistribution (mdf)
```



Misorientation axis in specimen coordinates

Surprisingly the misorientation axis in specimen coordinates is unique

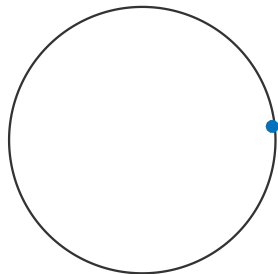
```
axis(O1,O2)
```

```
ans = vector3d (show methods, plot)
size: 1 x 1
      x           y           z
0.0495585  0.992437 -0.112305
```

```
[grains, ebsd.grainId] = ...
calcGrains(ebsd)
```

```
gB = grains.boundary('fcc','hcp')
ids = gB.ebsdId;
oFCC = ebsd(ids(:,1)).orientations
oHCP = ebsd(ids(:,2)).orientations
```

```
plotAxisDistribution(oFCC,oHCP)
```



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```
axis (O1, O2)
```

```
[grains , ebsd.grainId] = ...  
calcGrains (ebsd)
```

```
gB = grains.boundary ('fcc', 'hcp')  
ids = gB.ebsdId;  
oFCC = ebsd(ids(:,1)).orientations  
oHCP = ebsd(ids(:,2)).orientations
```

```
plotAxisDistribution (oFCC, oHCP)
```

```
plotAxisDistribution (oFCC, oHCP, ...  
    'contourf')
```

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```
axis (O1, O2)
```

```
[ grains , ebsd.grainId ] = ...  
calcGrains (ebsd)
```

```
gB = grains.boundary ( 'fcc' , 'hcp' )  
ids = gB.ebsdId ;  
oFCC = ebsd ( ids ( : , 1 ) ). orientations  
oHCP = ebsd ( ids ( : , 2 ) ). orientations
```

```
plotAxisDistribution (oFCC, oHCP)
```

```
plotAxisDistribution (oFCC, oHCP , ...  
    'contourf')
```

Misorientation axis in specimen coordinates

Surprisingly the misorientation axis in specimen coordinates is unique

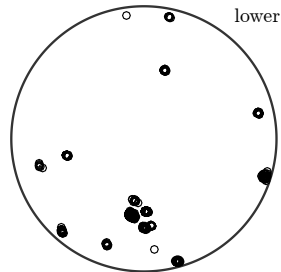
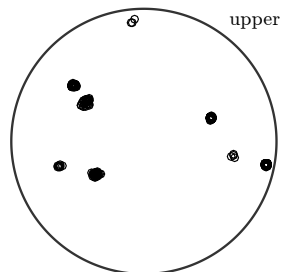
```
axis (O1, O2)
```

```
[grains, ebsd.grainId] = ...  
calcGrains(ebsd)
```

```
gB = grains.boundary('fcc', 'hcp')  
ids = gB.ebsdId;  
oFCC = ebsd(ids(:,1)).orientations  
oHCP = ebsd(ids(:,2)).orientations
```

```
plotAxisDistribution(oFCC, oHCP)
```

```
plotAxisDistribution(oFCC, oHCP, ...  
    'contourf')
```



Misorientation axis in specimen coordinates

Surprisingly the misorientation axis in specimen coordinates is unique

```
axis (O1, O2)
```

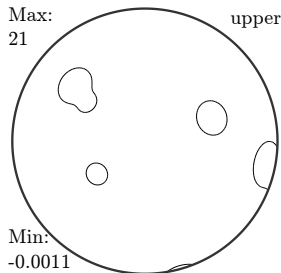
```
[grains, ebsd.grainId] = ...  
calcGrains(ebsd)
```

```
gB = grains.boundary('fcc', 'hcp')  
ids = gB.ebsdId;  
oFCC = ebsd(ids(:,1)).orientations  
oHCP = ebsd(ids(:,2)).orientations
```

```
plotAxisDistribution(oFCC, oHCP)
```

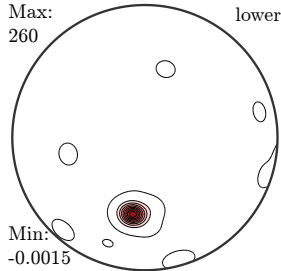
```
plotAxisDistribution(oFCC, oHCP, ...  
    'contourf')
```

Max:
21



Min:
-0.0011

Max:
260



Min:
-0.0015