Carnegie Mellon

Texture Analysis with MTEX inside Matlab

For 27-750

Texture, Microstructure and Anisotropy

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MSE

In-Class Questions

- What is “texture”? Texture quantifies any bias in crystal orientations with respect to a reference frame associated with the specimen shape, or equivalent. This is extended to grain boundary (GB) texture or preference for one type of GB over another. GB texture can be present even when the orientation texture is random.
- Why do we have to work with general 3D rotations in order to quantify texture? General 3D rotations are required because crystals have a 3D basis set for their crystal structure and three parameters are required to relate the (three) associated axes with the reference frame (however that is chosen).
- How does a rotation specified by a combination of axis and angle correspond to a set of three Euler angles (flippant answer: not very easily!)? The most straightforward correspondence is via the 3x3 rotation matrix; conversions between Euler angles and matrix can be found e.g. in Bunge’s book, similarly for axis+angle.
- How does texture apply to CdTe? The most relevant aspect is grain boundary texture, although some deposits also have a very strong orientation texture.

In-Class Questions: 2

- How does misorientation apply to CdTe (or any other polycrystalline material)? Misorientation is the term used to describe the *difference* in orientation, generally across a grain boundary (but between any pair of orientations in general).
- How is crystal symmetry taken into account in texture and grain boundary analysis? The symmetry of a crystal defines a point group; that point group must be used to calculate the minimum set of orientations or misorientations that are physically possible.
- What is the procedure that one can follow to use Matlab+MTex to construct an orientation distribution from pole figure data? This procedure is described in these lecture notes.
- What is the procedure that one can follow to use Matlab+MTex to construct an orientation distribution from EBSD data? As with pole figures, this is described in the notes. In general, it is reasonable to use the procedure provided by the MTEX package.
- What else can one obtain from a Matlab+MTex analysis? In principle, one can perform any analysis although some degree of exploration may be required to implement any given type of analysis.

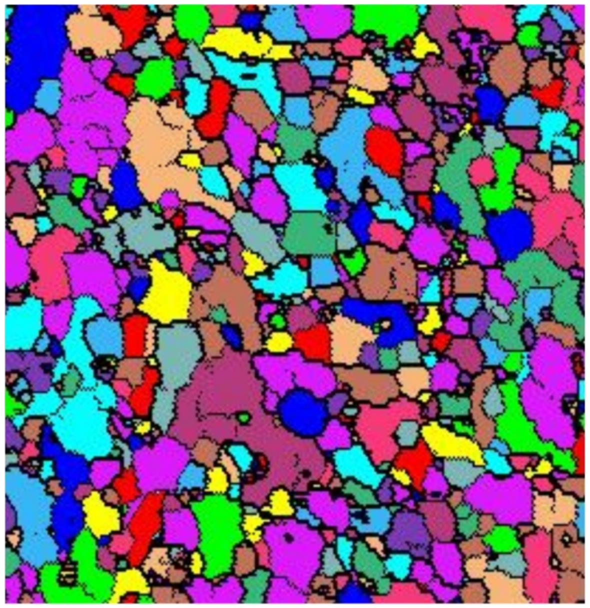
Objectives

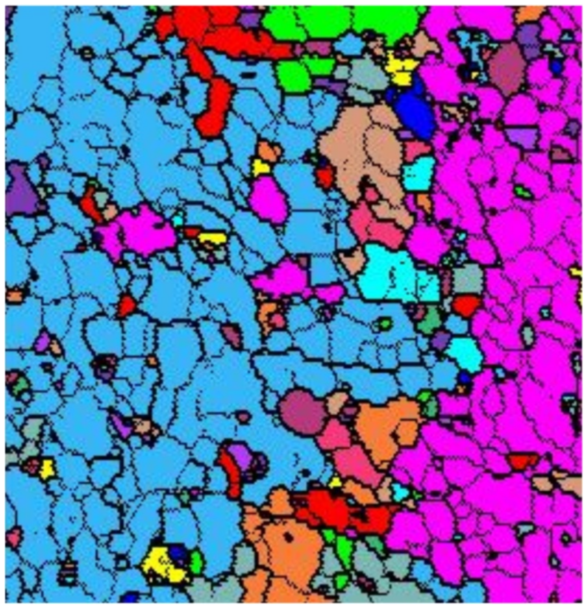
1. Introduce students to *texture* i.e. *crystallographic preferred orientation*, also known as *fabric* in geology.
2. Explain briefly two standard types of data, namely *pole figures* and *orientation maps* from e.g. electron back-scatter diffraction (EBSD).
3. Demonstrate how to use the MTEX package within Matlab to perform analyses on relevant data.

Grain Definitions

- Given an orientation map with continuously varying orientations from one point to the next, one imposes a grain structure by aggregating points with similar orientation. This requires choice of a threshold in misorientation, below which two adjacent points belong to the same grain. From percolation, the procedure is known as the "burn algorithm".

Examples of varying the misorientation threshold:


3 degrees


15 degrees

Note that each color represents 1 grain

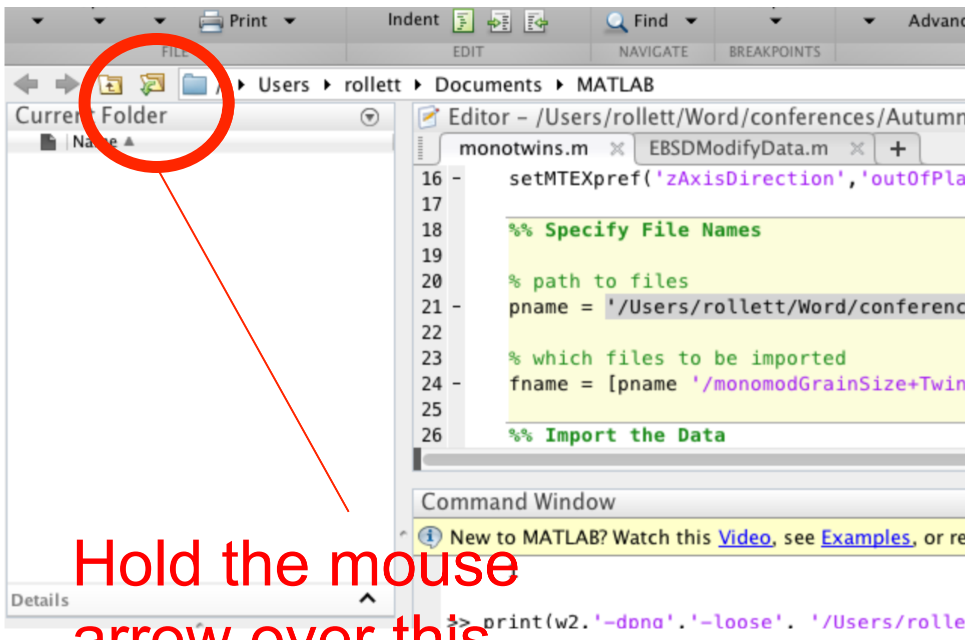
Variation in Boundary Properties

- Rhetorical question: do grain boundaries have variable properties? Answer: yes, even GB energy is highly variable.
- GB energy depends primarily on the two surfaces that are joined at the boundary. Low energy surfaces result in low energy GBs. In fcc metals, for example, {111} is the close packed (highest atomic density) surface and therefore lowest energy. GBs with {111} surface(s) are demonstrably low energy. Thus the coherent twin has the lowest energy of all, and {111} twist GBs are generally lower than most other GB types.
- GB energy correlates (positively) with excess free volume (per atom).
- Other properties also correlate with excess free volume such as diffusion.
- In grain growth, high energy GBs disappear faster than low energy GBs; therefore populations of GBs are anti-correlated with energy.
- GB mobility is poorly understood: some GBs exhibit anti-Arrhenius behavior (mobility decreases with increasing temperature).

Installation of MTex

- Find MTEX by searching on "mtex google code"; the author of MTEX, Ralf Hielscher, now hosts the code on his own website, http://mtex-toolbox.github.io/. As of Jan. 19th 2016, this is still valid.
- MTEX has its own installation procedure. As detailed in the instructions found on-line, the steps include
  a) download the package (from the "downloads" page)
  b) set the Matlab "path" to the folder/directory where the MTex package is located (*see next slide* for screenshots); I put mine in /Users/Shared (on a Mac).
  c) in the Matlab command window, type "*startup_mtex*".
- ~~Then click on "*Install MTEX for future sessions*~~" (no longer required)
- Fortunately, this takes care of replacing any previous, older installations of MTex.
- The Matlab documentation now includes documentation on MTex.
- Caution: if you manually add the MTEX folder to your MATLAB path then there is a significant risk that MTEX will give errors (e.g. when you try to read in EBSD data). What you should do instead to get it to work is to put MTEX in a different folder and run startup_mtex from that directory.

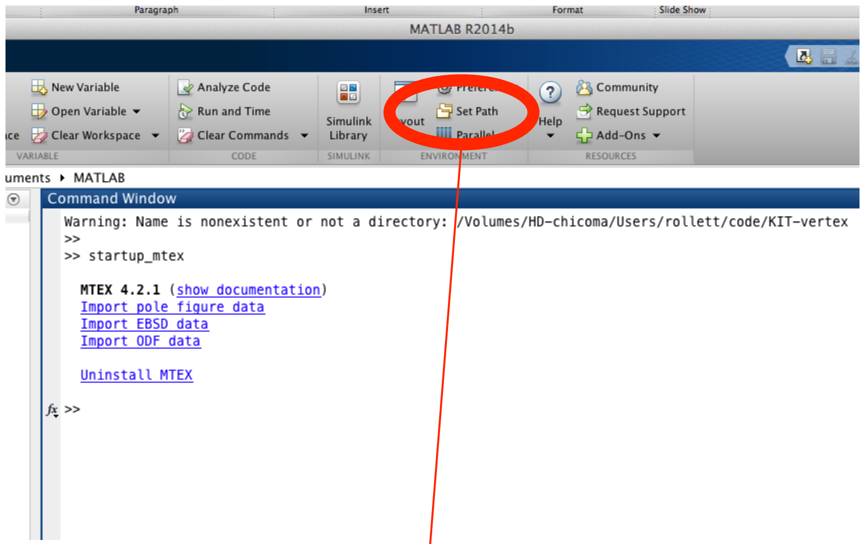
Change Folder



```
setMTEXpref('zAxisDirection','outOfPla

%% Specify File Names

% path to files
pname = '/Users/rollett/Word/conferenc

% which files to be imported
fname = [pname '/monomodGrainSize+Twin

%% Import the Data
```

New to MATLAB? Watch this Video, see Examples, or re

```
>> print(w2,'-dpng','-loose', '/Users/rolle
```



```
Warning: Name is nonexistent or not a directory: /Volumes/HD-chicoma/Users/rollett/code/KIT-vertex
>>
>> startup_mtex

  MTEX 4.2.1 (show documentation)
  Import pole figure data
  Import EBSD data
  Import ODF data

  Uninstall MTEX

>>
```

Hold the mouse arrow over this icon and you will see “Browse for folder”

Or this: “Set Path”

What can MTex do?

- We will explore two things:
  a) analysis of pole figure data;
  b) analysis of EBSD data.
- Useful links:
  This one describes ways to plot individual orientations.
  http://merkel.zoneo.net/RDX/index.php?n=Texture.PlotIndividualOrientationsInMTex
  This one has useful hints (although be careful that many details have changed from v3 to v4):
  http://mtex-toolbox.github.io/files/doc/BoundaryPlots.html

Navigating the file structure

```
>> pwd
```

will tell you which directory you are in,
probably "~/Documents/MATLAB"

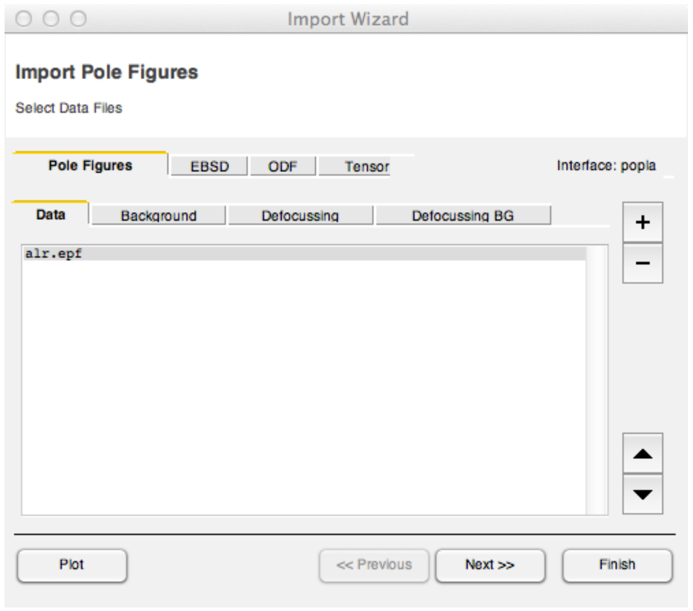
```
>> cd /directory-of-your-choice
```

will place you in whatever folder/directory you like, i.e. where you have your data. Note, on a Mac, you can Copy a highlighted folder, Paste in Terminal, highlight and copy the full path that you see, and then Paste that after the "cd " entry in the Matlab window.

You can then click on "Import pole figure data" or "Import EBSD data", for example, to set up the script to read in your data. Or (next slide) you can type "import_wizard".

Part 1: PF analysis

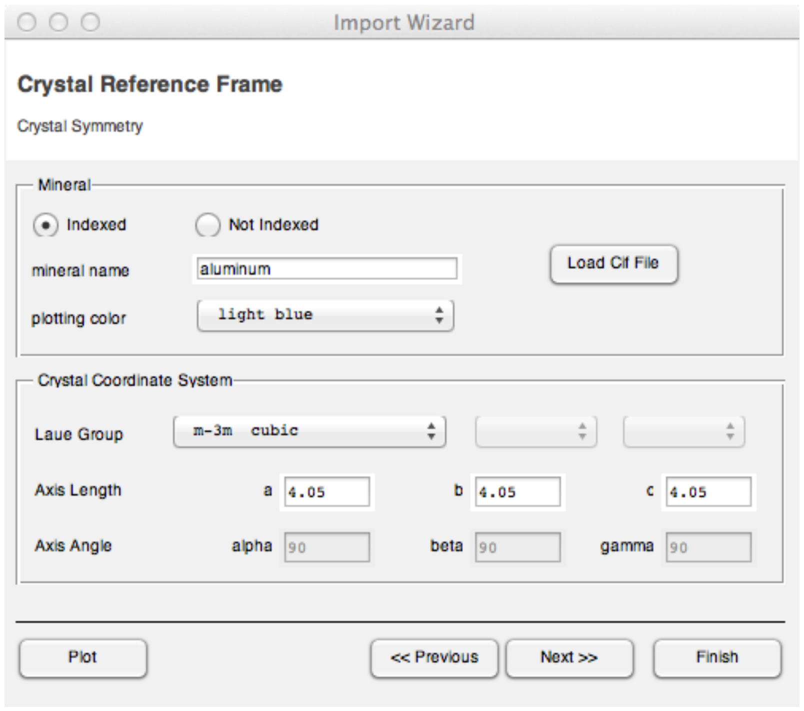
- Look in the "Mtex Toolbox" for "Short Pole Figure Analysis Tutorial". Do not use this!
- Instead, type import_wizard or click on that in the list of links. Note, if you have just started MatLab (after installing MTEX in a previous session), you need to navigate (Change Folder) to the MTEX folder and type "startup_mtex" before doing anything else.
- A new, small window will open. It should be set to the "Pole Figures" tab by default (but if not, click on that tab).
  Click on the "+" and navigate to where you have "alr.epf" stored. You should see the window below.



alr.epf

PF analysis – p2

- Click on “Next >>” in the same window. You can enter the lattice parameter as 4.05 if you wish (although it should not make any difference because this is cubic).
  The wizard is quite clever: if you enter “Fe” or “Iron” as the mineral name, it will recognize this material and make the appropriate entries for you.



Crystal Reference Frame

Crystal Symmetry

Mineral

Indexed [✓] Not Indexed

mineral name: aluminum

plotting color: light blue

Crystal Coordinate System

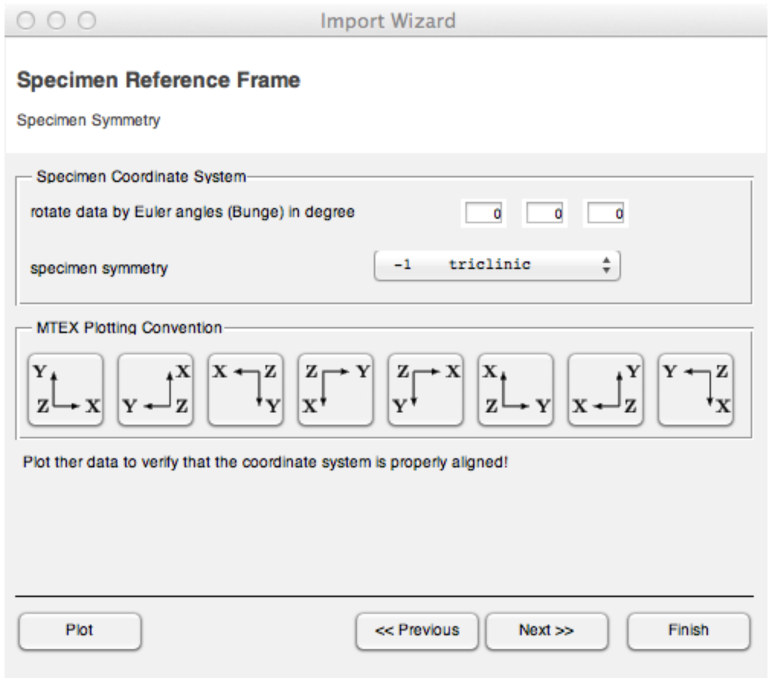
Laue Group: m-3m cubic

Axis Length: a 4.05 b 4.05 c 4.05

Axis Angle: alpha 90 beta 90 gamma 90

PF analysis – p3

- I prefer to set the plotting axes so that "x" points to the right (East), as for normal plots. For now re-set the "specimen symmetry" to "orthorhombic".



Specimen Reference Frame

Specimen Symmetry

Specimen Coordinate System

rotate data by Euler angles (Bunge) in degree 0 0 0

specimen symmetry -1 triclinic

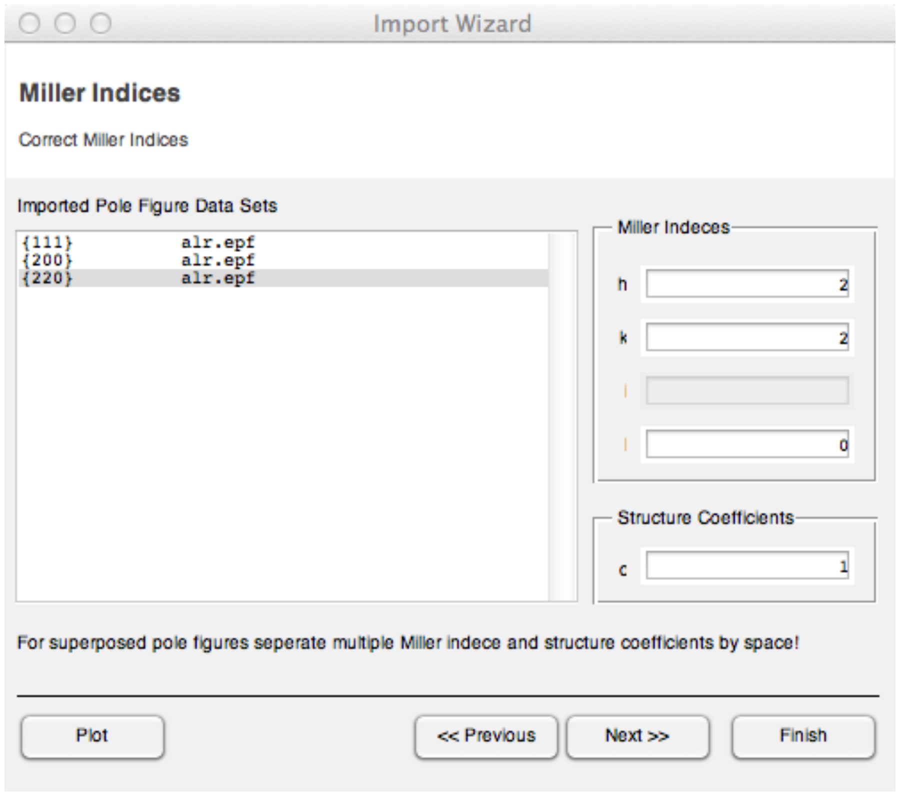
MTEX Plotting Convention

Plot ther data to verify that the coordinate system is properly aligned!

There is now a control to enforce plotting with X to the right (east): plotx2east

PF analysis – p4

- After clicking “Next >>”, you should see this window.



Import Wizard

Miller Indices

Correct Miller Indices

Imported Pole Figure Data Sets

```
{111}         alr.epf
{200}         alr.epf
{220}         alr.epf
```

Miller Indeces

h 2

k 2

i

l 0

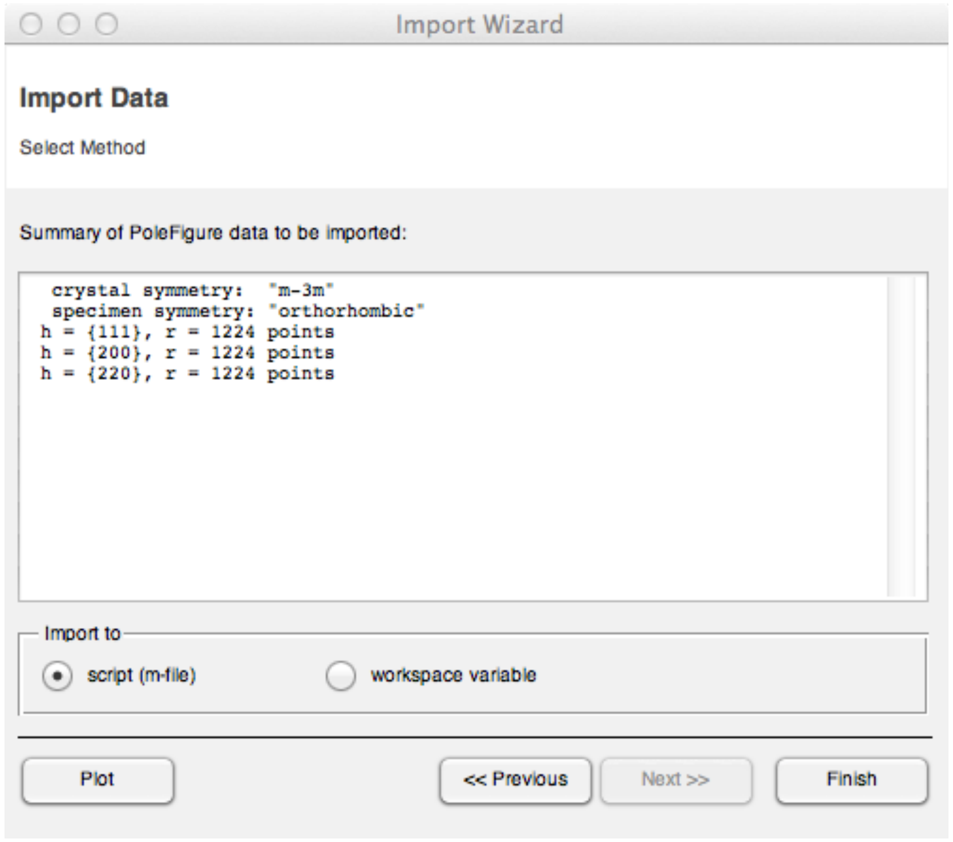
Structure Coefficients

c 1

For superposed pole figures seperate multiple Miller indece and structure coefficients by space!

PF analysis – p5

- After clicking “Next >>”, you should see this window (but with “orthorhombic” for the sample symmetry). Now click “Finish” to be done.



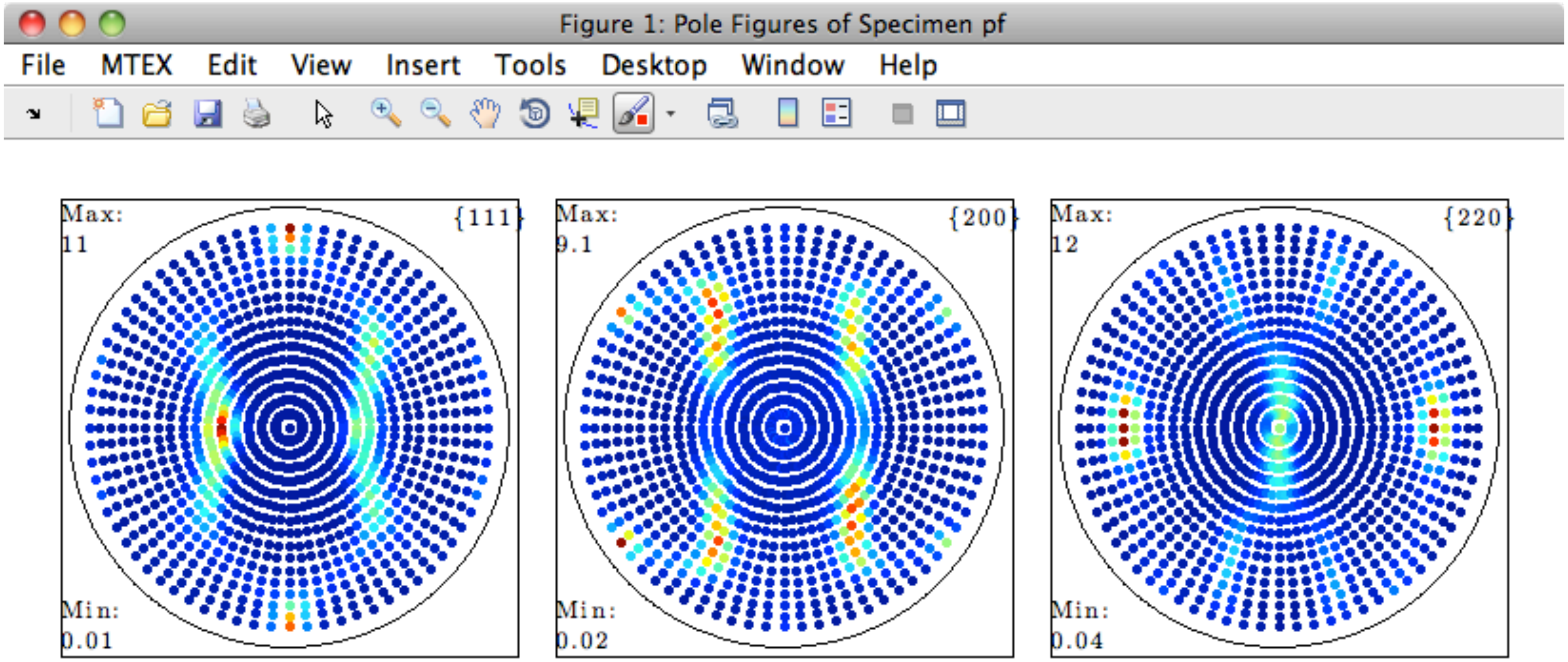
Summary of PoleFigure data to be imported:

```
  crystal symmetry:  "m-3m"
  specimen symmetry: "orthorhombic"
 h = {111}, r = 1224 points
 h = {200}, r = 1224 points
 h = {220}, r = 1224 points
```

Import to: [✓ script (m-file)] workspace variable

Plot experimental PFs

- Plot(pf) should show you discrete pole figures in which the color is red for high intensity and blue for low; “pf” was the default name of the PF data that you read in.



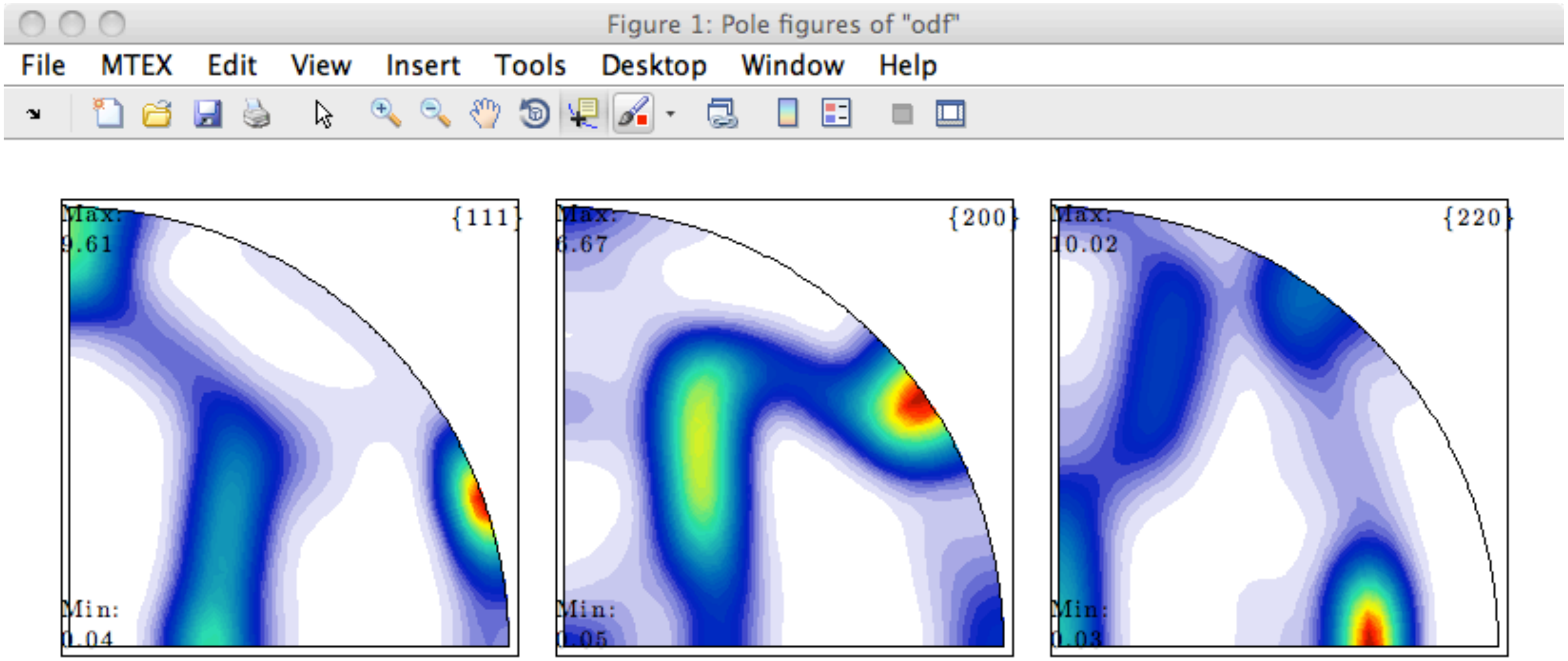
ODF analysis

- At this point you can run the ODF analysis:

```
odf = calcODF(pf)
------ MTEX -- PDF to ODF inversion ------------------
Call c-routine
initialize solver
start iteration
error: 7.1530E-01 4.2632E-01 2.1810E-01 1.3615E-01 9.8065E-02 7.7246E-02 7.1090E-02 6.7171E-02 6.4644E-02
6.2644E-02 6.0870E-02
Finished PDF-ODF inversion.
error: 6.0870E-02
alpha: 1.0518E+00 1.0678E+00 1.1113E+00
required time: 6s

odf = ODF (show methods, plot)
  comment: ODF recalculated from /Users/rollett/Word/teaching/Micro14/MatLab_Casper/Al-PFs/alr.epf
  crystal symmetry: aluminum (m-3m)
  sample symmetry : orthorhombic

  Radially symmetric portion:
    kernel: de la Vallee Poussin, hw = 5°
    center: 1232 orientations, resolution: 5°
    weight: 1
```

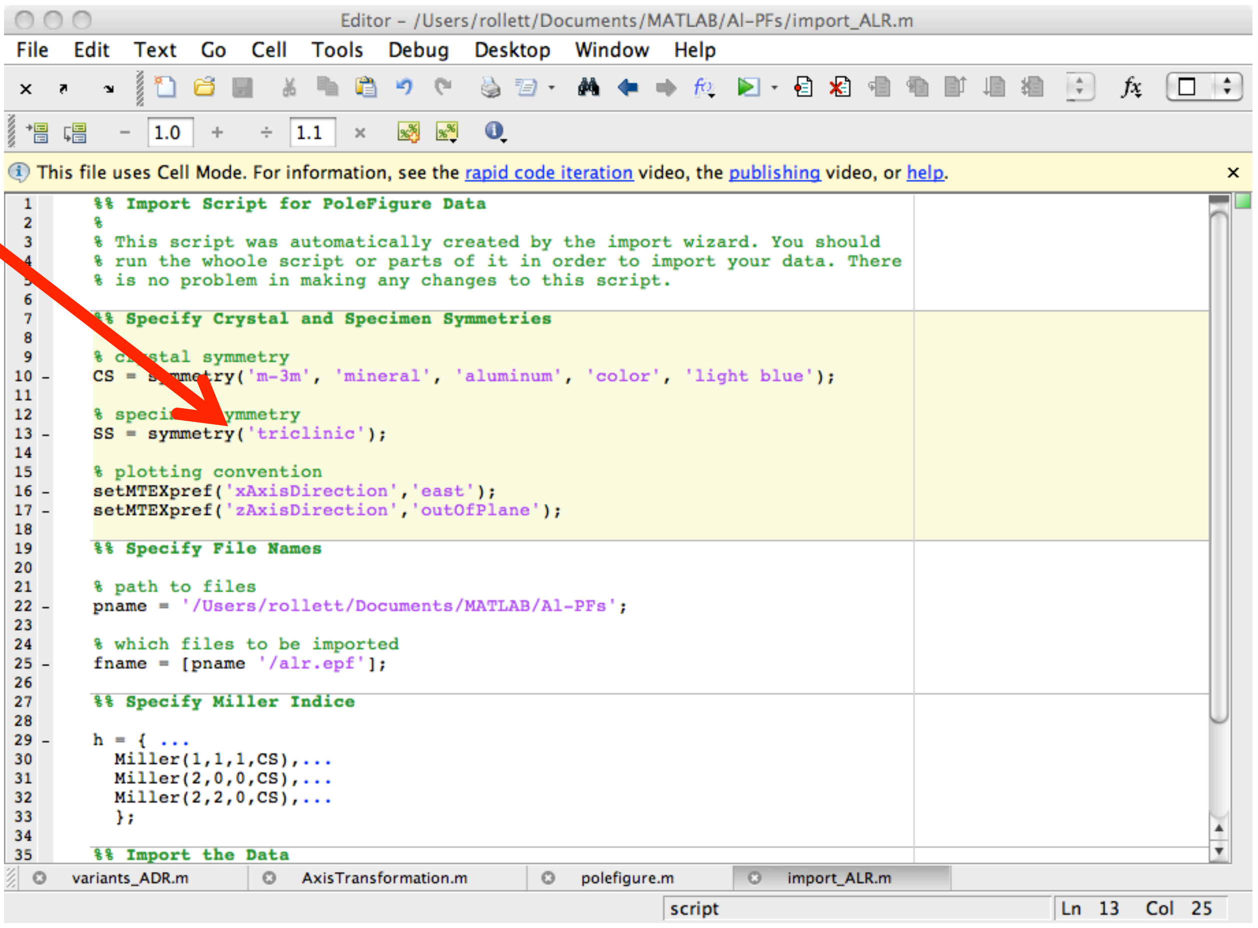
Recalculated PFs

- Type "plotPDF(odf,h,'antipodal')" to plot the same set of pole figures but based on the ODF. Note that these are quadrant PFs because of the assumed orthorhombic sample symmetry.



Adjust sample symmetry

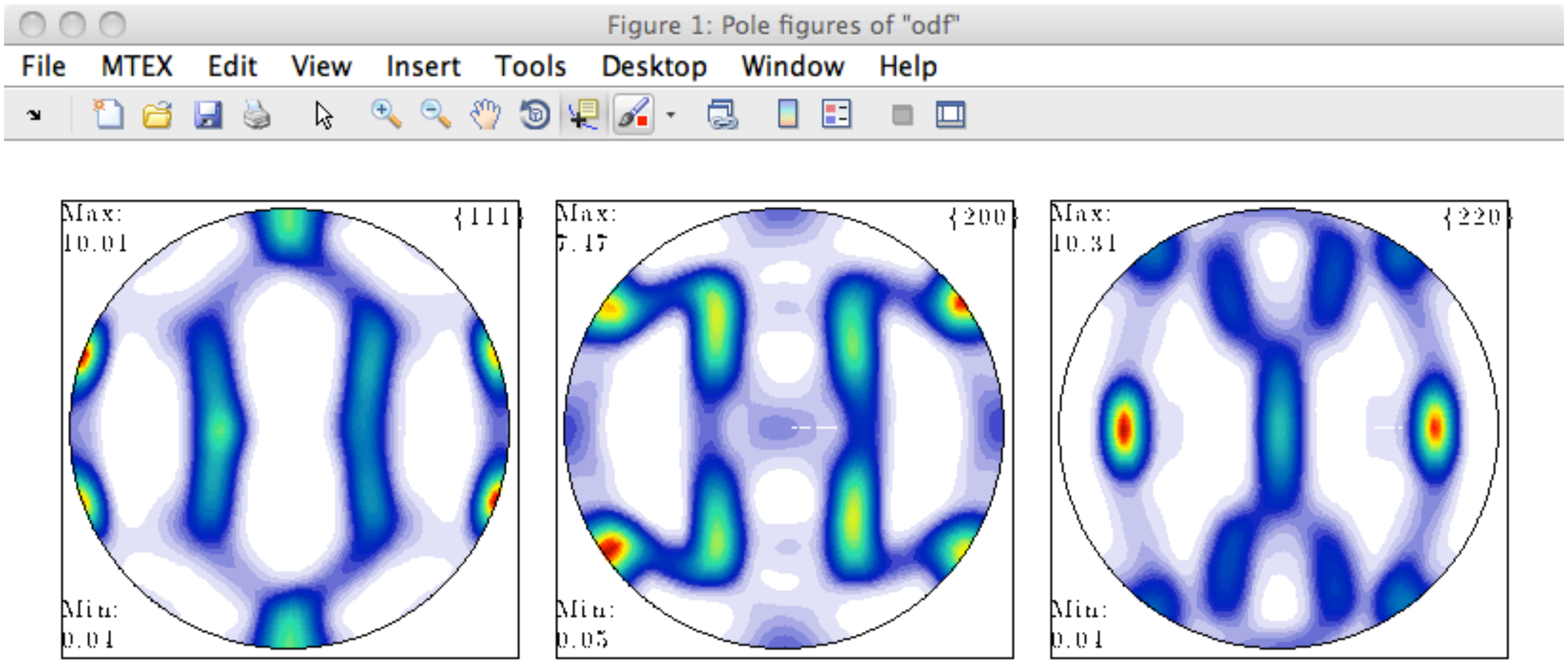
- Now go into the script that you had generated for the PF import, and change (by editing it) the sample symmetry from orthorhombic to triclinic.


Editor – /Users/rollett/Documents/MATLAB/Al-PFs/import_ALR.m
File Edit Text Go Cell Tools Debug Desktop Window Help
1.0
1.1
This file uses Cell Mode. For information, see the rapid code iteration video, the publishing video, or help.
variants_ADR.m
AxisTransformation.m
polefigure.m
import_ALR.m
script
Ln 13 Col 25

```
%% Import Script for PoleFigure Data
%
% This script was automatically created by the import wizard. You should
% run the whoole script or parts of it in order to import your data. There
% is no problem in making any changes to this script.

%% Specify Crystal and Specimen Symmetries

% crystal symmetry
CS = symmetry('m-3m', 'mineral', 'aluminum', 'color', 'light blue');

% specimen symmetry
SS = symmetry('triclinic');

% plotting convention
setMTEXpref('xAxisDirection','east');
setMTEXpref('zAxisDirection','outOfPlane');

%% Specify File Names

% path to files
pname = '/Users/rollett/Documents/MATLAB/Al-PFs';

% which files to be imported
fname = [pname '/alr.epf'];

%% Specify Miller Indice

h = { ...
  Miller(1,1,1,CS),...
  Miller(2,0,0,CS),...
  Miller(2,2,0,CS),...
  };

%% Import the Data
```

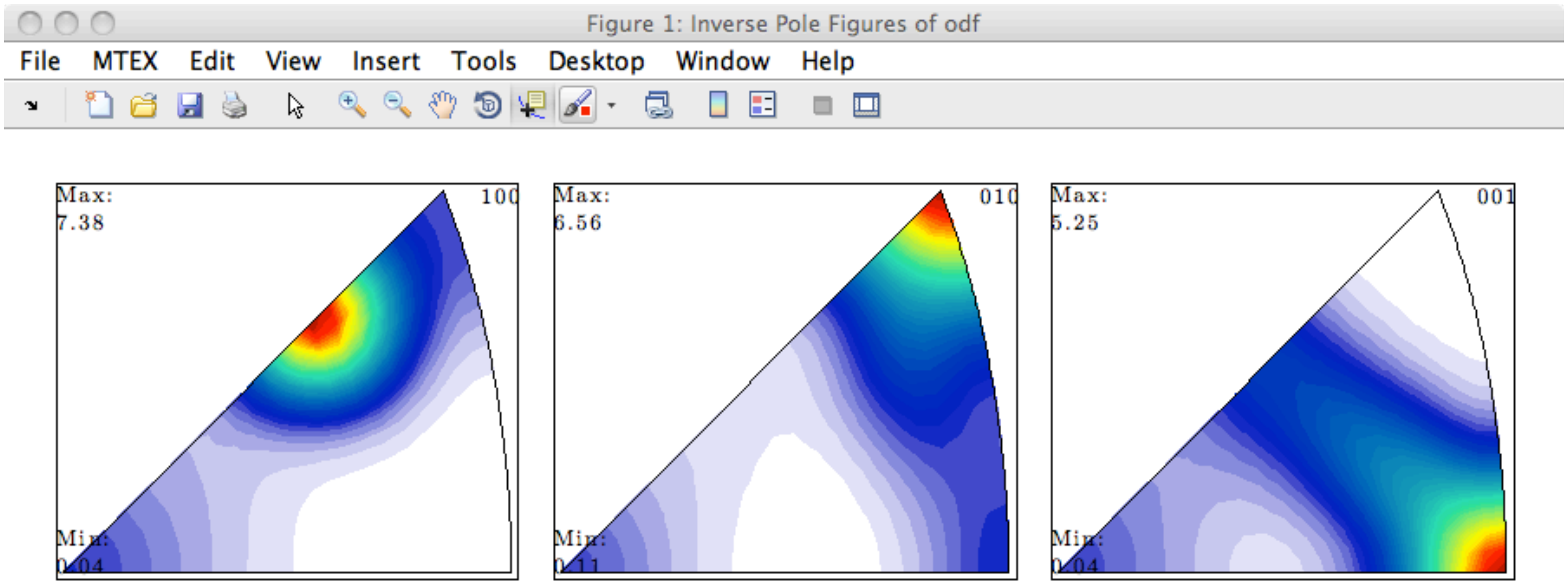
Re-analyze

- Re-run the calcODF and plotpdf commands.



Inverse PFs

- To get a complete set of 3 inverse pole figures, type "plotIPDF(odf,[xvector,yvector,zvector],'antipodal')". The 3 sample directions (X, Y & Z) are specified by the built-in "xvector", "yvector" and "zvector". You may need to use Annotate to label the corners.



Sections through ODF

- plot(odf,’PHI2’,'sections') will give you plots of sections through the ODF. These go to 360° in phi1, because of the triclinic sample symmetry.

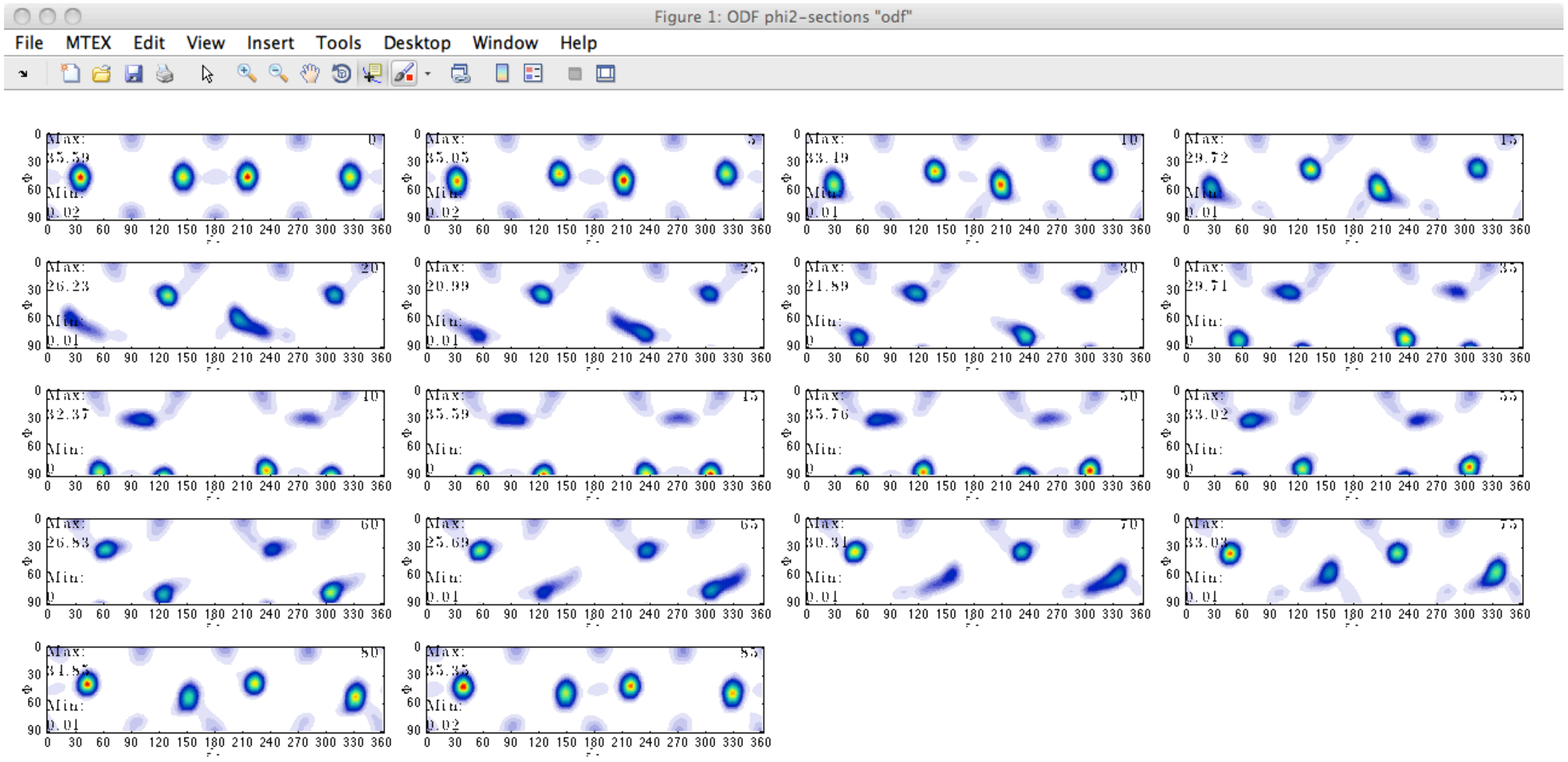


Figure 1: ODF phi2-sections "odf"
File MTEX Edit View Insert Tools Desktop Window Help
Max:
Min:
0 30 60 90 120 150 180 210 240 270 300 330 360

3D view

- “plot(odf,'PHI2','surf3')” – gives rotatable view.

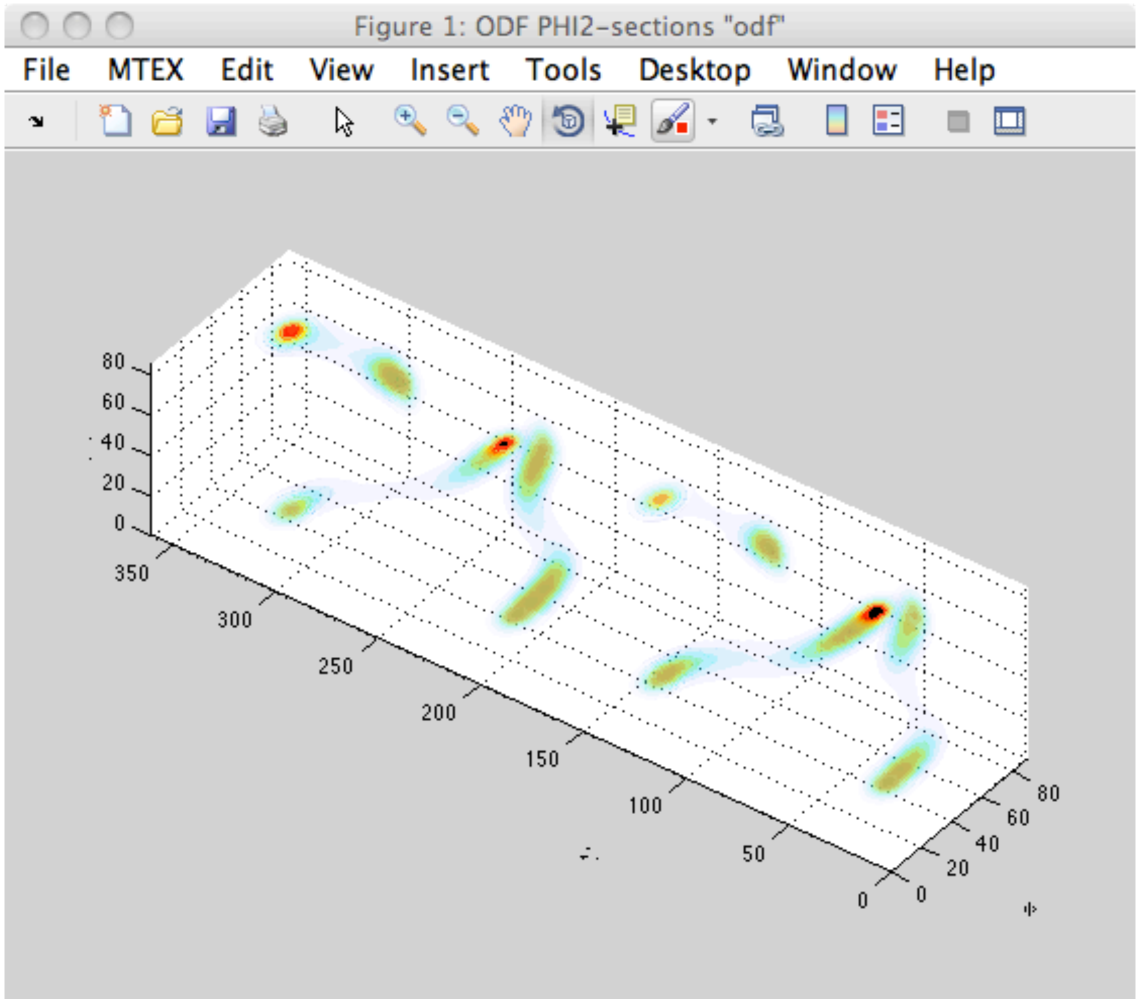


Figure 1: ODF PHI2-sections "odf"
File MTEX Edit View Insert Tools Desktop Window Help
80
60
40
20
0
350
300
250
200
150
100
50
0
0
20
40
60
80

Misc.

```
>> textureindex(odf)
ans =
   10.6263
>> entropy(odf)
ans =
   -1.6371
```

- These values suggest a moderately strong texture.
- The section on “Characterizing ODFs” provides a few other techniques.

Misc., tricks

- Inside a script (*.m file), you can run a portion of it by positioning the cursor at the end of the line where you want to go to, and hit “Control-Enter” to run the script to that position.

Errors

%Error analysis:

%For a more quantitative description of the reconstruction quality one can use the function calcError to compute the fit between the reconstructed ODF and the measured pole figure intensities. The following measured are available:

RP - error ; L1 – error; L2 – error

```
calcError(pf,odf,'RP',1)
ans =
   0.1540    0.1631    0.1319    0.1033    0.1163    0.1763    0.1734
```

%In order to recognize bad pole figure intensities it is often useful to plot difference pole figures between the normalized measured intensities and the recalculated ODF. This can be done with the command PlotDiff.

```
plotDiff(pf,odf)
```

Volume fraction

First we specify an texture component using “orientation”:

ori = orientation('Euler',phi1,Phi,phi2,cs,ss)

e.g. center = orientation('Euler’,0,55,45,CS,SS)

The function 'volume' returns the ratio of an orientation that is close to an orientation (center) by a misorientation tolerance (radius) to the volume of the entire odf.

Syntax:

v = volume(odf,center,radius,<options>)

Part 2: EBSD input

- Navigate with “cd” to wherever your data is; in this case, we will work with one or more of the CdTe datasets provided by Prof. Zaefferer’s group. You are recommended to place it in a folder/directory by itself so that you can store the images from running Matlab+MTEX. On the Macs, “Grab” is v handy for screen/window captures.
- Click on “Import EBSD data”, just as you did for the pole figure data and follow the steps to specify the material etc. **Make sure that you have CdTe.cif in the mtex-4.0.5/data/cif/ folder so that mtex knows about CdTe as a material**. It will very likely ask you about both the CdTe phase and about an unindexed phase. This latter is not a problem.
- This generates a dataset called “ebsd”. You can change this name in the script that was generated in the above step.
- Note that the mtex folder will have a version number (e.g. the 4.0.5 above) in the name but this version number may vary depending on when you downloaded the package.

EBSD: determine, plot grains

- We take input from: monomodGrainSize+Twins.ang
- Type "import_wizard" to get the interactive window for importing data.
- Click on the "EBSD" tab
- Navigate to the "monomodGrainSize+Twins.ang" file. The data will then be imported.
- Click "Next" several times to see the program recognize the phase(s) automatically until only "Finish" is available.
- You will then have a MatLab script in its own window. Save it under whatever name you prefer (you will see something like "myname.m" appear, in whichever folder/directory you choose).
- Click on "Run" (green arrow, pointing right). This will execute the script and import the dataset as an entity called "ebsd".
- Check the contents of the data by just typing the name "ebsd". If you do *not* see the phase "Cadmium Telluride" appear in the list (just a blank list) then edit the script to remove "not indexed" as a phase. In other words,

```
% crystal symmetry
CS = {...
  crystalSymmetry('432', [6.41 6.41 6.41], 'mineral', 'Cadmium Telluride', 'color', 'light blue'),…
  'not indexed'};
```

  should become:

```
% crystal symmetry
CS = {...
 crystalSymmetry('432', [6.41 6.41 6.41], 'mineral', 'Cadmium Telluride', 'color', 'light blue')};
```

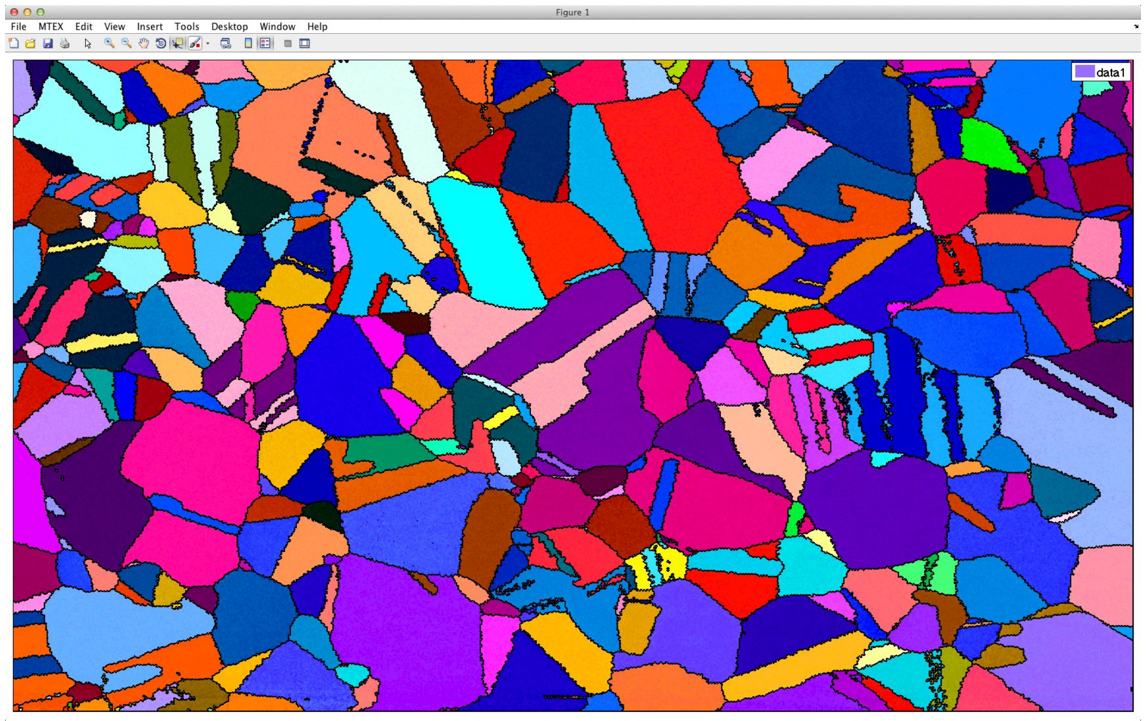
- Then repeat the importation by clicking on Run again, and again type "ebsd". You should see this:

```
>> ebsd
ebsd = EBSD (show methods, plot)
 Phase   Orientations            Mineral       Color  Symmetry  Crystal reference frame
     0  290700 (100%)  Cadmium Telluride  light blue       432
 Properties: ci, iq, sem_signal, x, y
 Scan unit : um
```

- This slightly odd procedure is required in order to account for the fact that MTEX gets confused if you tell it to look for both a real phase and non-indexed points when, in this particular dataset, every single point is indexed and belongs to the Cadmium Telluride phase. As of version 4.0.5, this problem appears to be fixed.

EBSD: determine, plot grains

- Type "grains_FMC = calcGrains(ebsd('Cadmium Telluride'),'FMC',… 3.5)" (takes a while to compute)
- Then compute inverse pole figure coloring with:
  oM = ipdfHSVOrientationMapping(ebsd('Cadmium Telluride'))
- Then plot the ipdfHKL map with
  plot(ebsd('Cadmium Telluride'),oM.orientation2color(ebsd('Cadmium… Telluride').orientations))
  and compute
  grain boundaries:
  gB=grains_FMC.boundary…
  ('Cadmium Telluride')
  hold on
  plot(gB,'linewidth',2.)
- This will provide a map with the GBs delineated (and "linewidth" controls the thickness).



ODF from EBSD

First, do this:

```
plot(ebsd)
```

This should be “boring” i.e. it should show only 1 phase.

```
odf = calcODF(ebsd('Cadmium Telluride').orientations)
```

.OR.

```
odf = calcODF(ebsd('Cadmium Telluride').orientations,'halfwidth',5*degree)
```

The second should show a few lines of output with details about the calculation.

The third is the calculation of the ODF (in v4, using “psi” as the 3rd argument does not work, hence the numerical value).

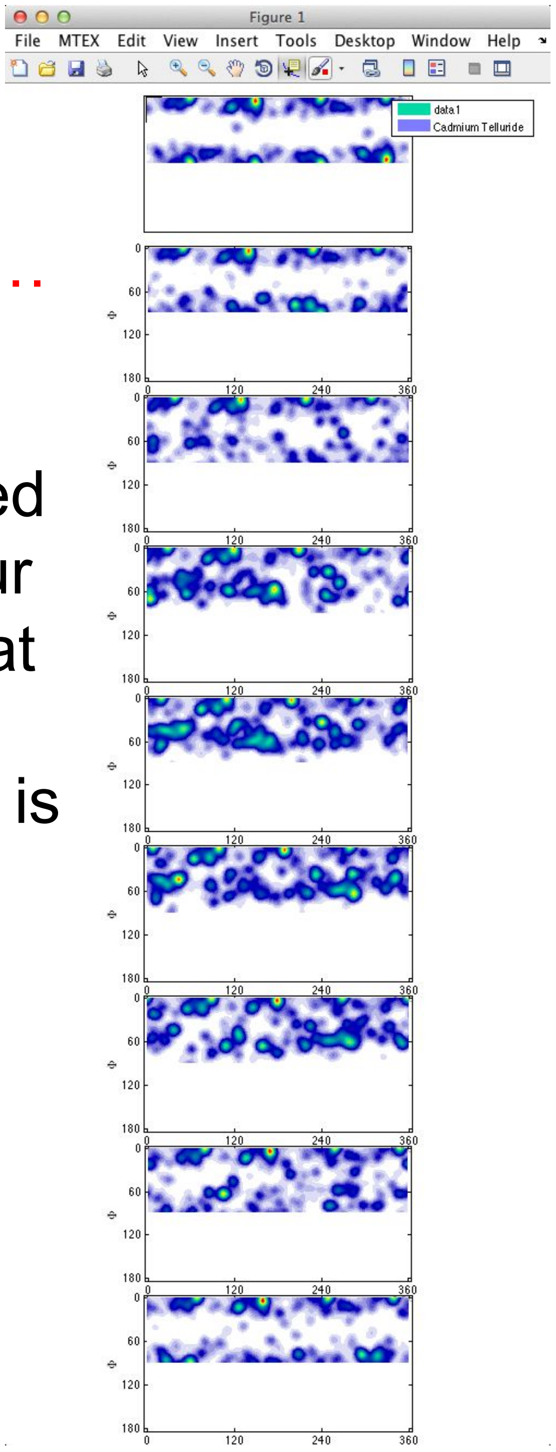
Plot ODF

h = [Miller(1,0,0,CS{1}),Miller(1,1,0,CS{1}),…
Miller(1,1,1,CS{1})]

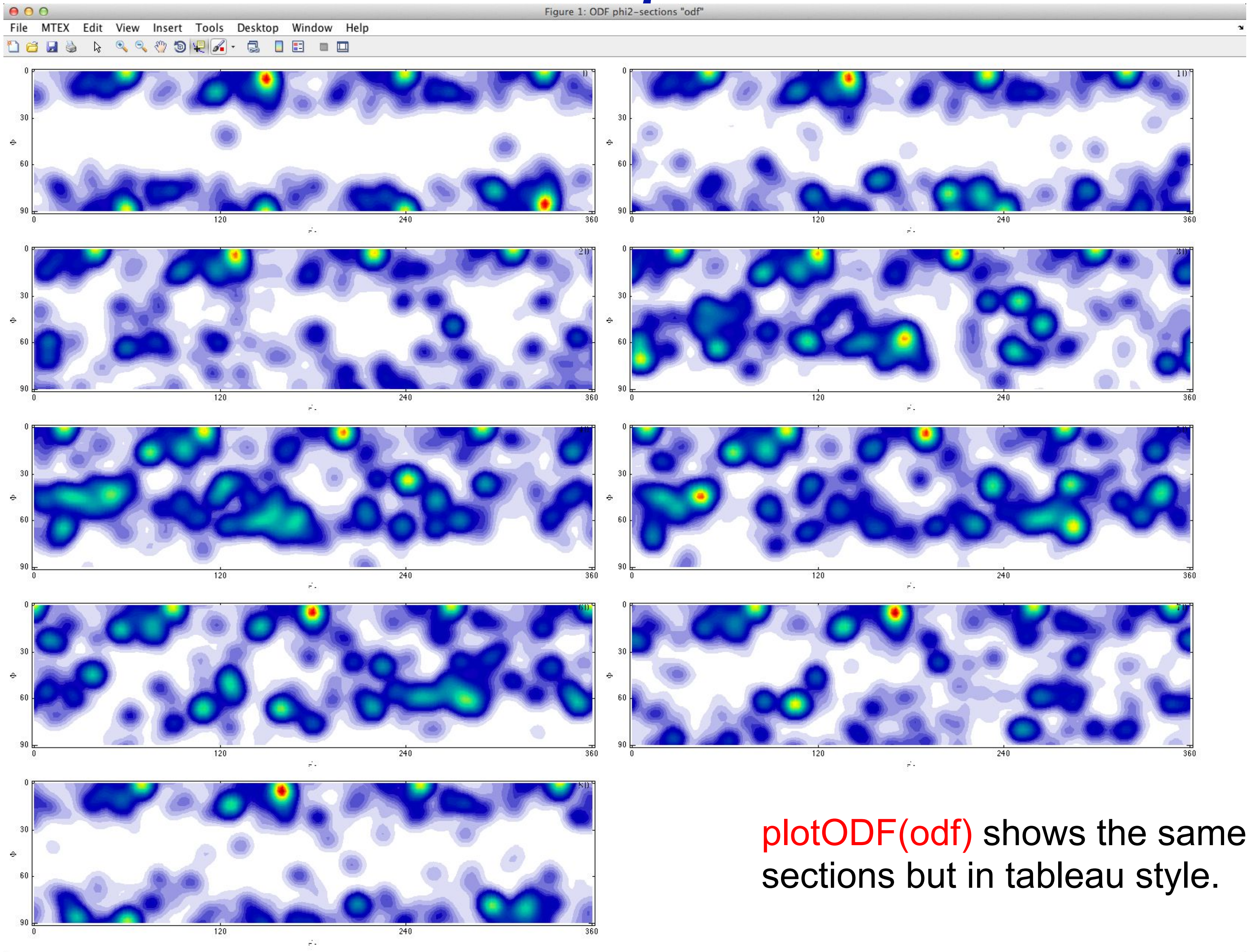
This defines a set of pole figure indices.
CAUTION: the above assumes you specified two phases in the input script, so check your input script as to which phase is the one that you want. For example, you may need to replace "{1}" by "{2}" if the phase of interest is the second one.

plotODF(odf,h,'antipodal')

This shows a set of sections based on the calculated ODF.



ODF plot



plotODF(odf) shows the same sections but in tableau style.

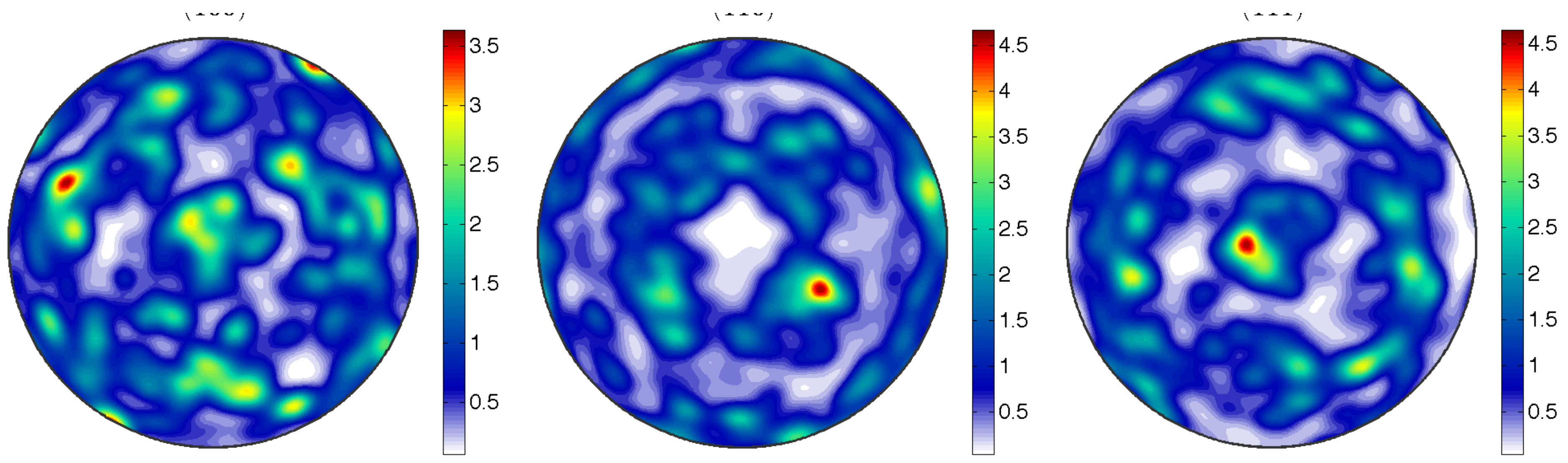
Pole figures

Try this first: `plotPDF(odf,h,'antipodal’)`

This longer version should equalize the contour levels:

```
plotPDF(odf,h,'antipodal','minmax', 'off', 'contour', 0:0.5:4)
colorbar
set(gcf,'PaperPositionMode','auto');
print(w1,'-dpng’,'filename');
```

This shows a set of PFs based on the calculated ODF. As you can see, the texture is nearly random. Make sure that MatLab is pointed to your local directory/folder with the data.



Discrete PFs

- This command will show discrete pole figure plots, where the argument “500” controls how many individual orientations are included in the plot: plotPDF(ebsd(’Cadmium… Telluride').orientations,h,'points',500,'antipodal')

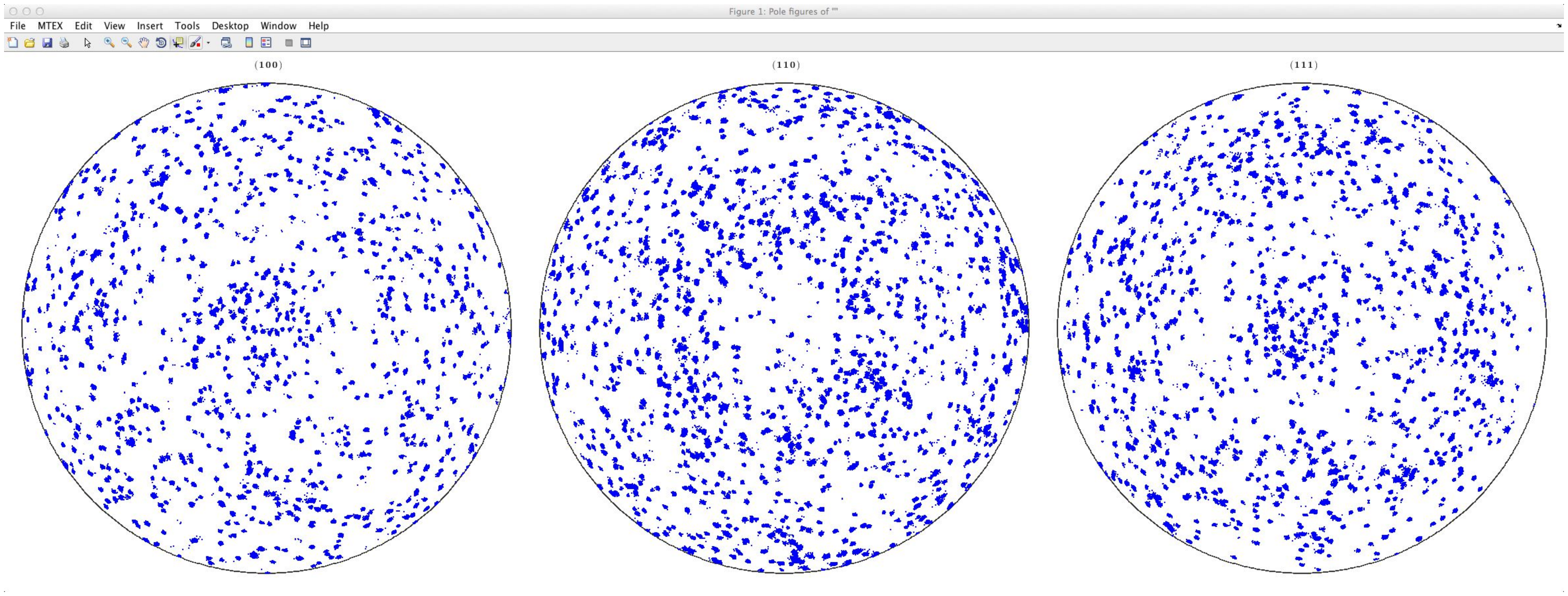
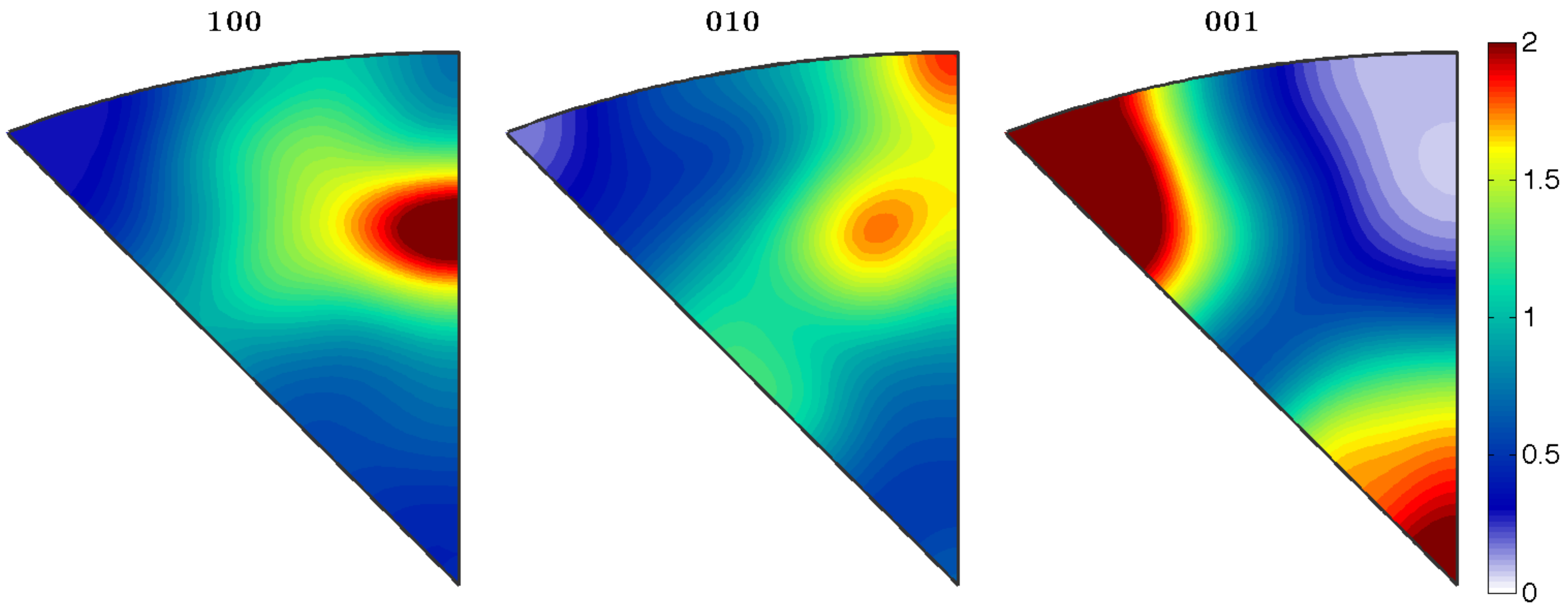


Figure 1: Pole figures of ""
File MTEX Edit View Insert Tools Desktop Window Help
(100)
(110)
(111)

Inverse Pole Figures (IVPs)

```
plotIPDF(odf,[xvector,yvector,zvector],'antipodal','minmax', 'off',…
'contour', 0:0.25:2)
>> hold on
>> colorbar
```

Note how the 001 inverse pole figure shows a maximum at the <111> position. Annotate can be used to label the corners.



Grain Boundaries

To compute the grain boundaries:

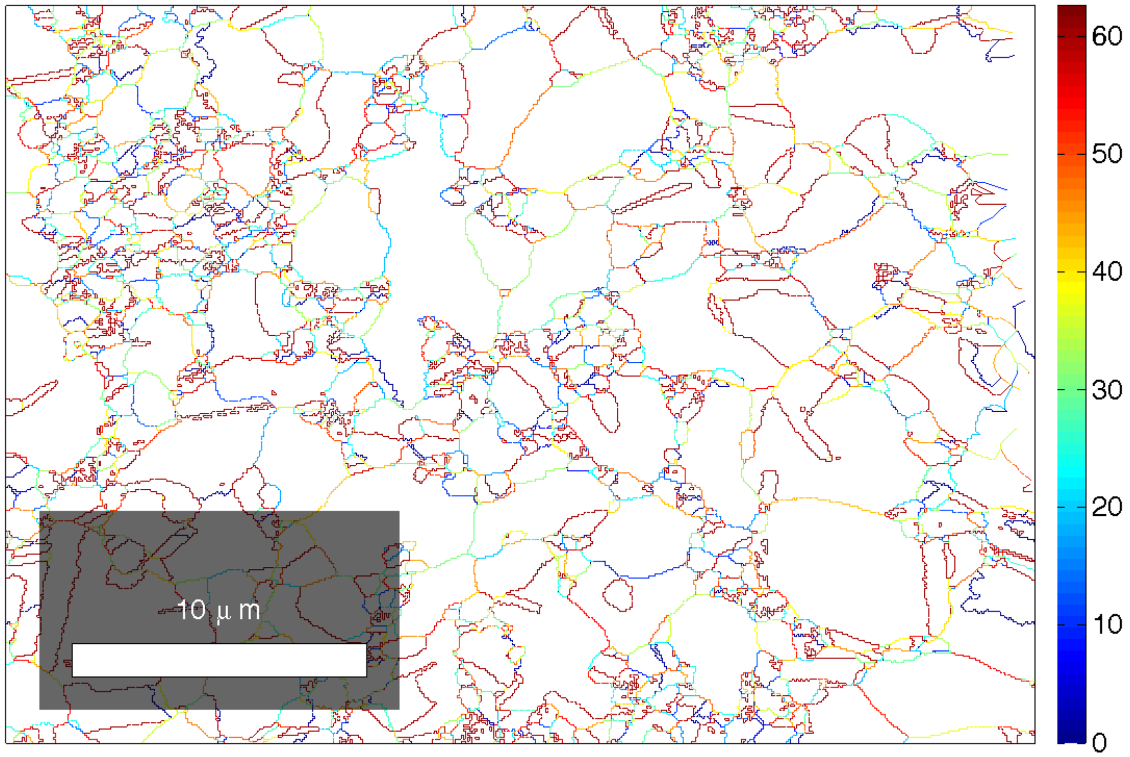
gB = grains_FMC('Cadmium Telluride') .boundary

Then to get a map of just the GBs:

plot(gB)

To map GBs by misor angle [note that in v4.0.4, one has to add a double phase specification]:

plot(gB('Cadmium Telluride', 'Cadmium Telluride'),gB('Cadmium Telluride', 'Cadmium Telluride').misorientation.angle/degree,'linewidth', 1.5)



Note that you restrict the GBs examined to a particular phase by specifying the two phases in the command about GBs that you are using, just as you see here.

Grain Boundaries: 2

You can make a basic analysis of the grain boundaries in your map by making a histogram of the misorientation angles.

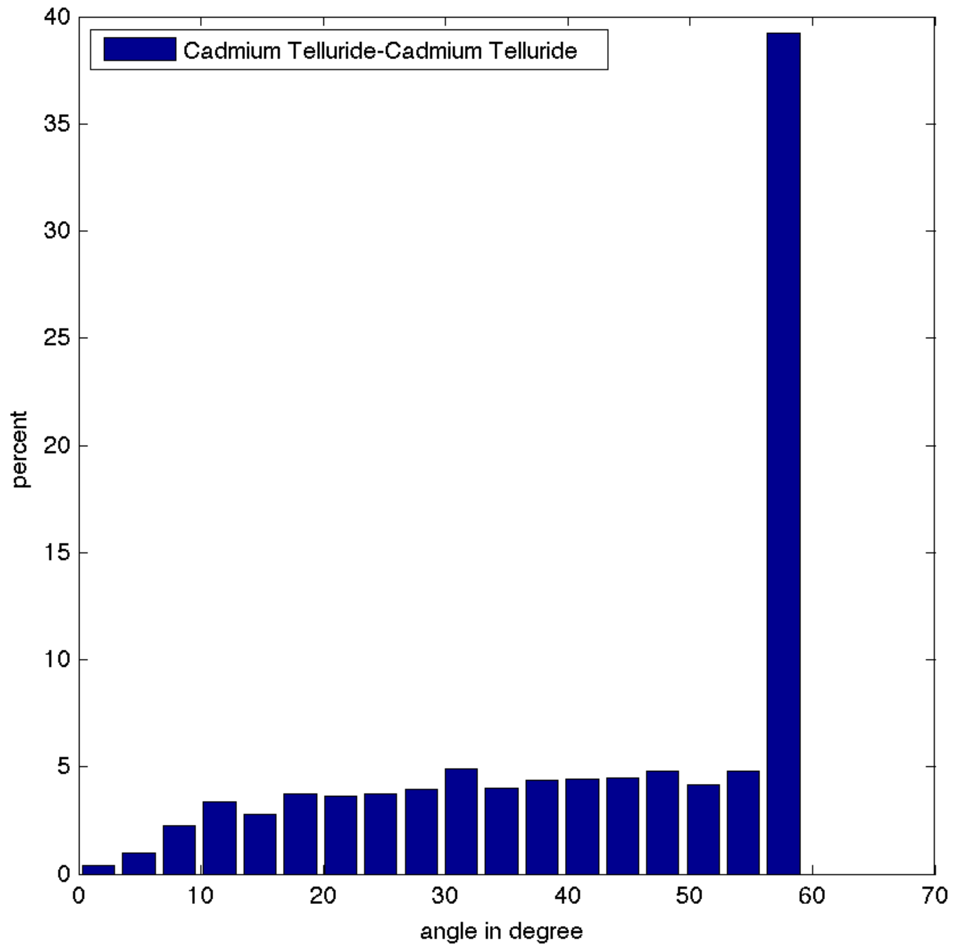
```
plotAngleDistribution(gB
('Cadmium Telluride’
,'Cadmium Telluride'));
```

To export the figure directly, here’s a new trick. You can save the figure as a MatLab object:

```
w1 = figure(1);
```

Then you export it in, say, PNG format thus:

```
set(gcf,'PaperPositionMode','auto')
print(w1,'-dpng',
’path_to_your_directory’);
```



The clumsy thing here is the need for the complete pathname. This can be structured by saving the path to the relevant directory in a MatLab variable and then concatenating with an actual (local) filename.

Kernel Ave. Misorientation

To see gradients in orientation, one can calculate and then map thus:

```
kamvalues = KAM(ebsdmonotwins,'threshold',5*degree);
plot(ebsd,ebsd.KAM./degree);
```

to control the color range

```
setColorRange([0,1]) ;
```

And include a color bar (legend):

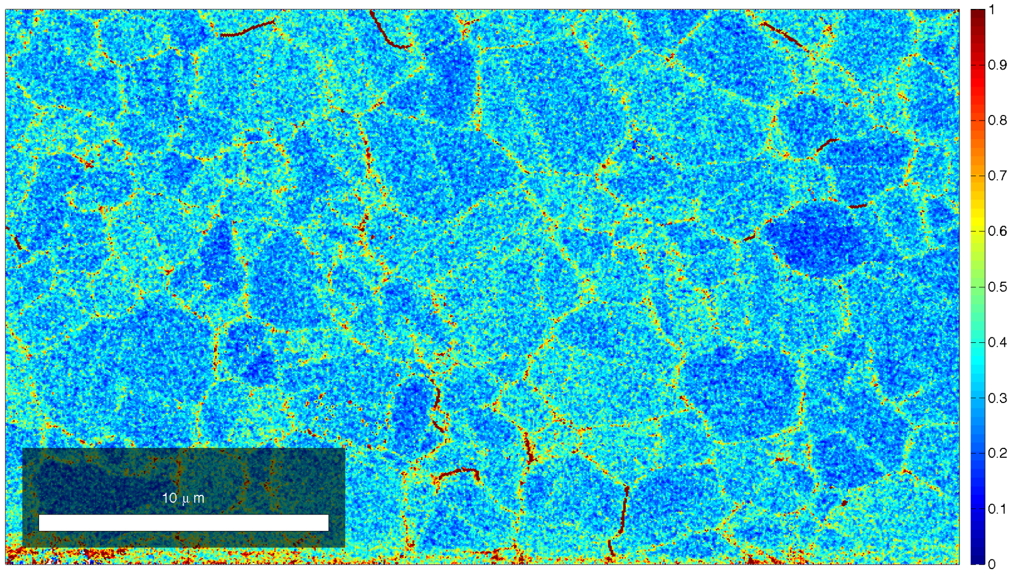
```
colorbar
```

And then capture the figure thus:

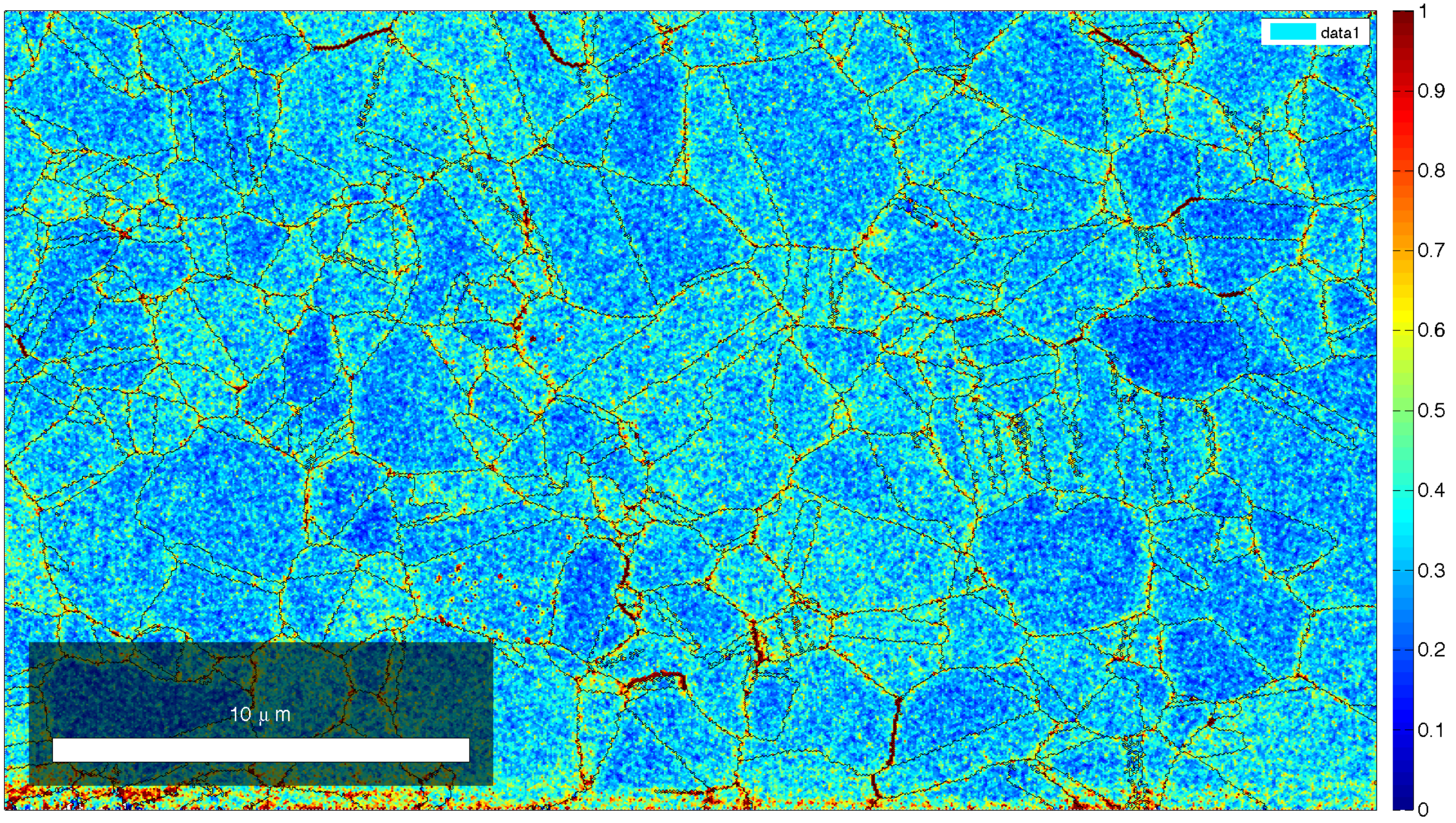
```
w2=figure(1);
```

this ensures that the framing of the figure is correct (tends to cut off large aspect ratio figures unless you do this):

```
set(gcf,'PaperPositionMode','auto')
print(w2,'-dpng',
'path_to_your_directory');
```



KAM Misorientation with GBs



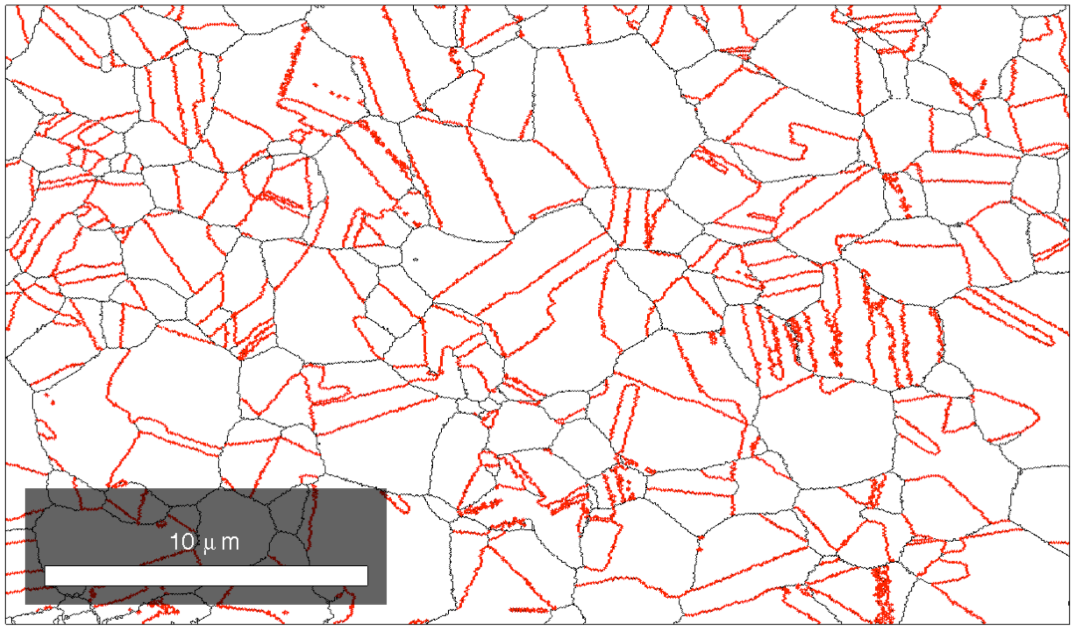
Grain Boundary types

As an example, let's emphasize sigma-3 boundaries; first we have to specify the boundary type as an axis-angle pair.

```
rot = rotation('axis',vector3d(1,1,1),'angle',60*degree);
gB = grains_FMC.boundary('Cadmium Telluride','Cadmium Telluride')
ind = angle(gB.misorientation,rot)<10*degree;
```

Then to make the map:

```
close all
plot(gB)
hold on
plot(gB(ind),'linewidth',1.5,…
'linecolor','r')
```



Plot shows general GBs in black and twin boundaries in red selected as Σ3

[Works as of 5-Nov-14 in v 4.0.5]

Misc.

- These notes from the workshop in Belo Horizonte, Brasil, Sept. 2015.
- Look for a folder called workshops-BeloHorizonte-2015.1 with “15-brasil” inside, with “matlab” inside that.
- There are example scripts in the folder, each of which contains many procedures to do various things.

Extra for Grain Boundaries

- Note that you restrict the GBs examined to a particular phase by specifying the two phases in the command about GBs that you are using, just as you see here.
- The general Matlab command "struct" will show you what's inside a variable/container.
- To smooth grain boundaries (and you can use a different name to avoid over-writing the previous, unsmoothed dataset):
  grains = smooth(grains)
- To get the list of boundaries in the different phases:
  grains.boundary [I think …]
- (Note that "grains" is the name of your current set of grains and boundaries) The coordinates of the segments (F for segment) are in a list like this where the 1st column is the 1st vertex and 2nd column is the 2nd vertex (at the end vertex); the list is as long as the number of segments:
  grains.boundary.F
- The actual coordinates of each vertex (V for vertex) is given by
  grains.boundary.V
- If you type the following, you get the two IDs on either side of the boundary segment:
  grains.boundary.grainID
- The index into the orientations of the adjacent pixels can be found thus:
  grains.boundary.edsdID
- The list of point/pixel orientations:
  Edbsd.rotations (grains.boundary.edsbID)

Homework

- The homework is simple to state but will require thought, in addition to processing the datasets with MTEX:
  Four datasets are provided. Investigate the differences between them and report on what you (or your group) believe those differences are.

Summary

- The sequence provided up to this point illustrates how to read in and perform standard analysis on pole figures and EBSD maps.