CARNEGIE MELLON UNIVERSITY

DEPARTMENT OF
MATERIALS SCIENCE AND ENGINEERING

How to use Matlab

27-750

Texture, Microstructure & Anisotropy

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Last revised: 25th Feb. '14

In-Class Questions

- What is the procedure that one can follow to use Matlab+MTex to construct an orientation distribution from pole figure data?
- What is the procedure that one can follow to use Matlab+MTex to construct an orientation distribution from EBSD data?
- What else can one obtain from a Matlab+MTex analysis?

Installation of MTex

- Find MTEX by searching on "mtex google code"
- MTex has its own installation procedure. As detailed in the instructions found on-line, the steps include
  a) set the Matlab "path" to the folder/directory where the MTex package is located;
  b) in the Matlab command window, type "*startup_mtex*".
- Fortunately, this takes care of replacing any previous, older installations of MTex.
- The Matlab documentation will now include 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. *DO NOT* add it to the search 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

Navigating the file structure

>> pwd

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

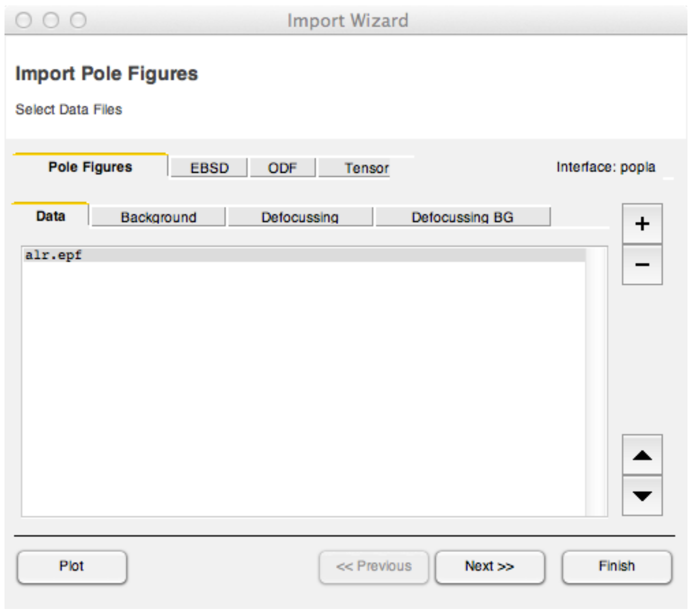
>> cd /directory-of-your-choice

will place you in whatever folder/directory you like, i.e. where you have your data.

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.

PF analysis

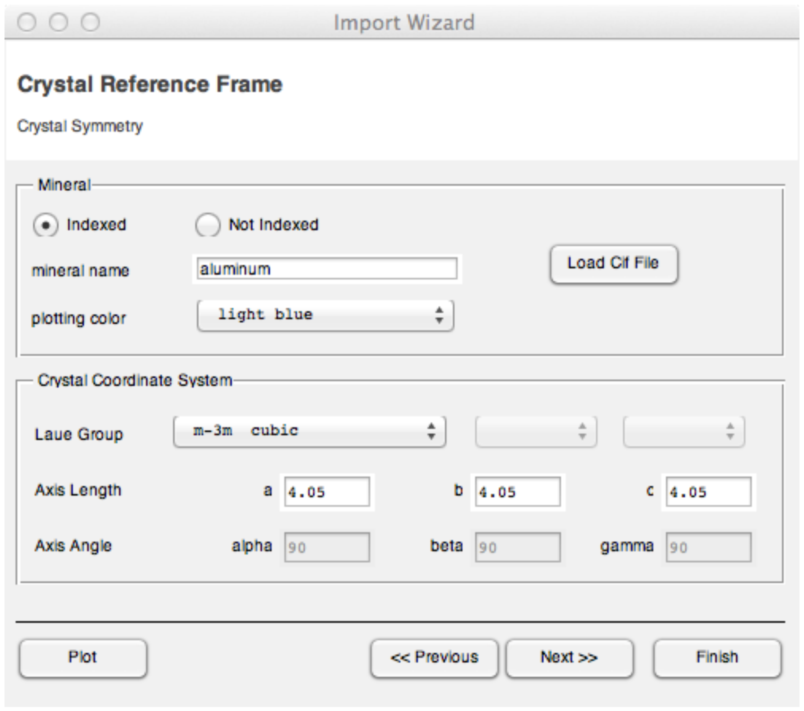
- Look in the "Mtex Toolbox" for "Short Pole Figure Analysis Tutorial". Do not use this!
- Instead, type import_wizard
- A new, small window will open. It should be set to the "Pole Figures" tab by default (but if not, click on that tab).
  Click on the "+" and navigate to where you have "alr.epf" stored.
  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” as the mineral name, it will recognize this material and make the appropriate entries for you.


Import Wizard

Crystal Reference Frame

Crystal Symmetry

Mineral

[● Indexed] Not Indexed

mineral name: aluminum

plotting color: light blue

Crystal Coordinate System

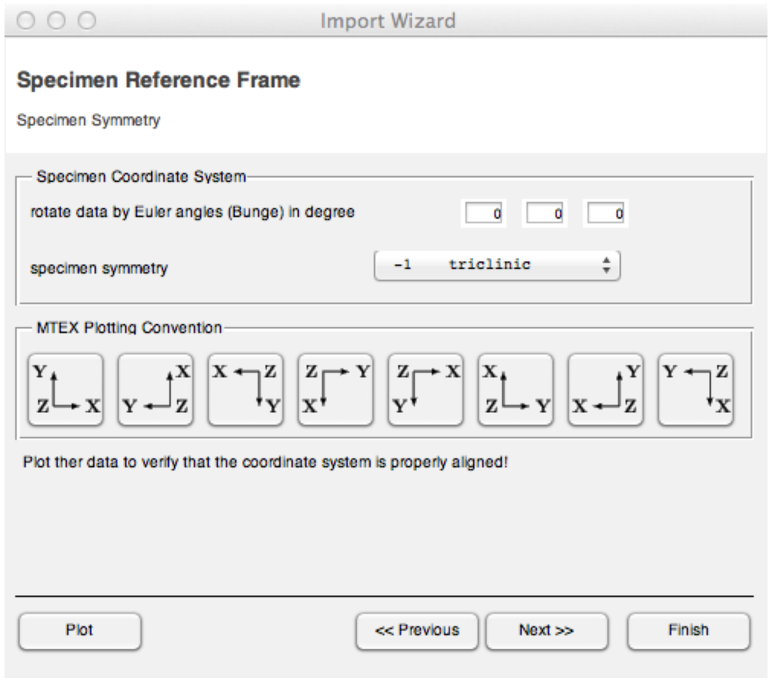
Laue Group: m-3m cubic

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”.



Import Wizard

Specimen Reference Frame

Specimen Symmetry

Specimen Coordinate System

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

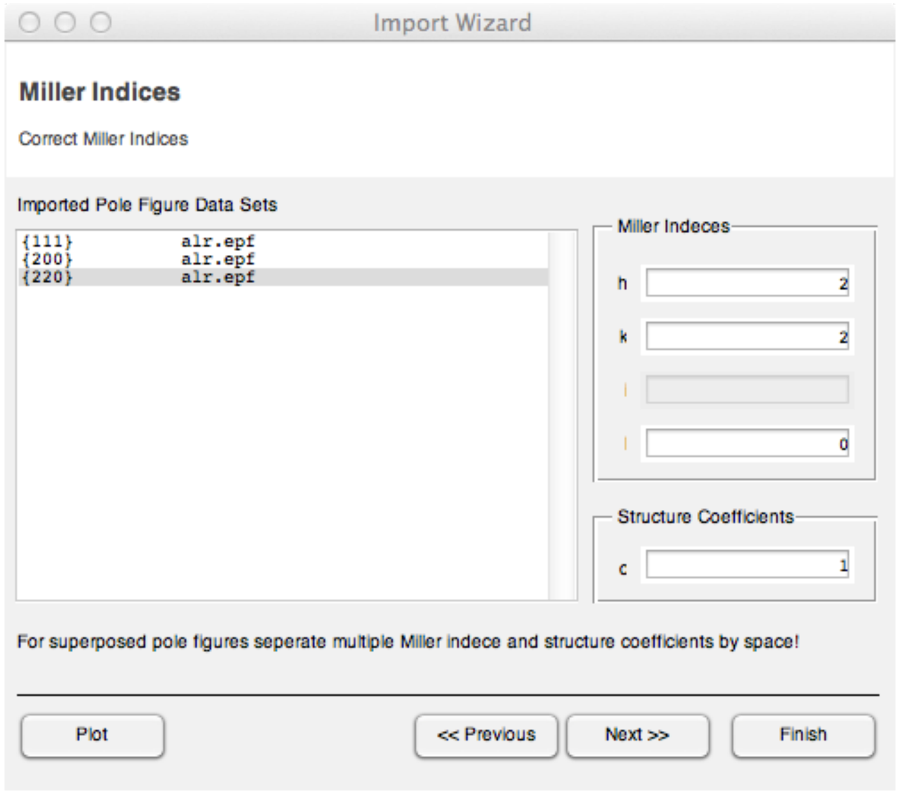
specimen symmetry -1 triclinic

MTEX Plotting Convention

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

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

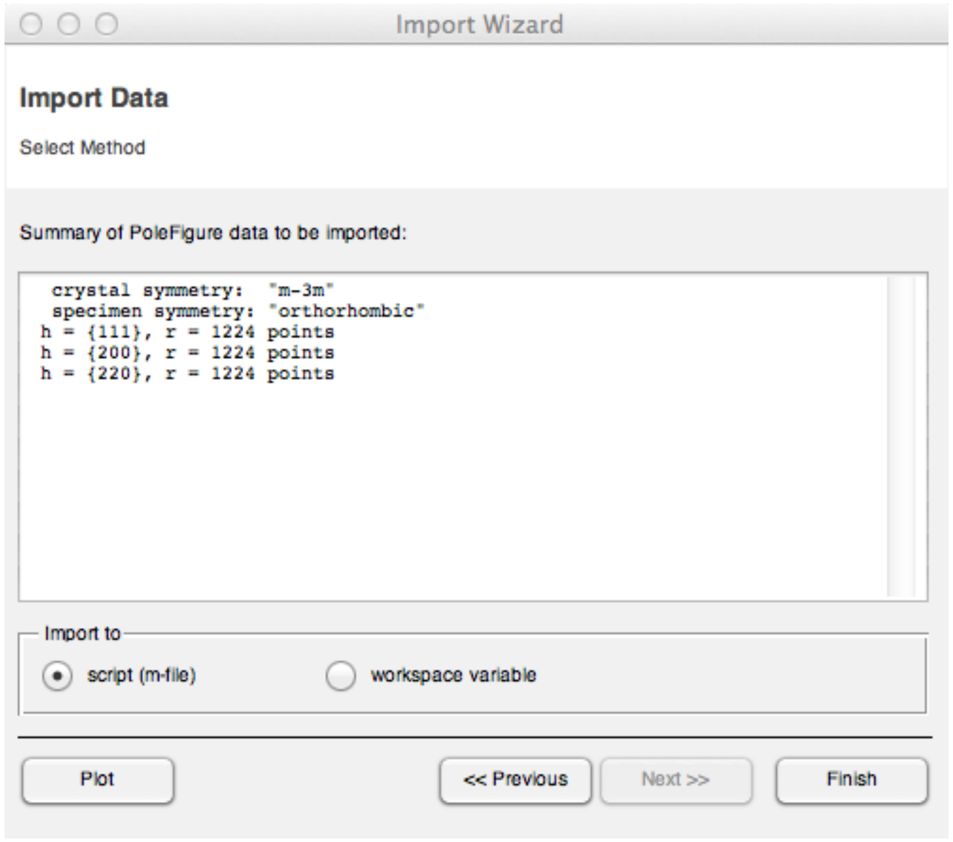
Structure Coefficients

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:

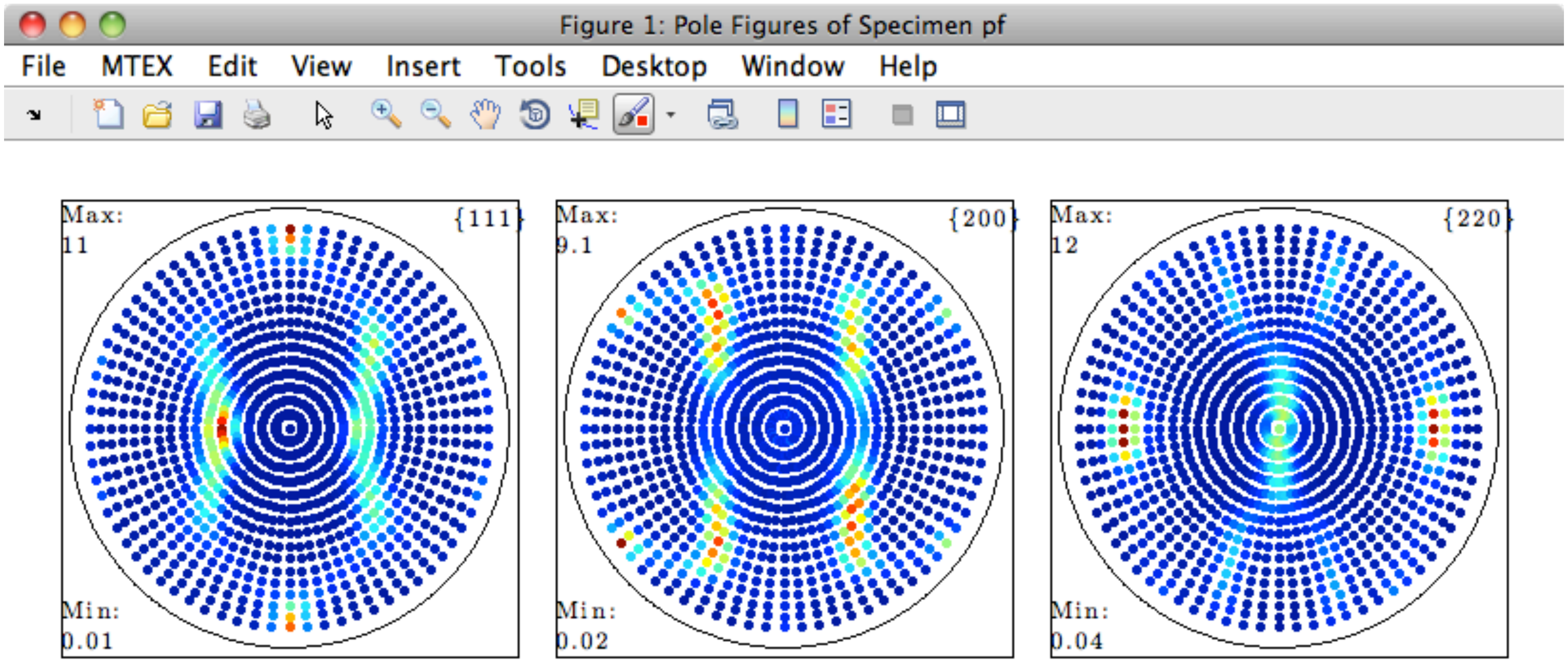
```
  crystal symmetry:  "m-3m"
  specimen symmetry: "orthorhombic"
 h = {111}, r = 1224 points
 h = {200}, r = 1224 points
 h = {220}, r = 1224 points
```

Import to

[✓ script (m-file)] workspace variable

Plot experimental PFs

- Plot(pf) should show you discrete pole figures; “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.

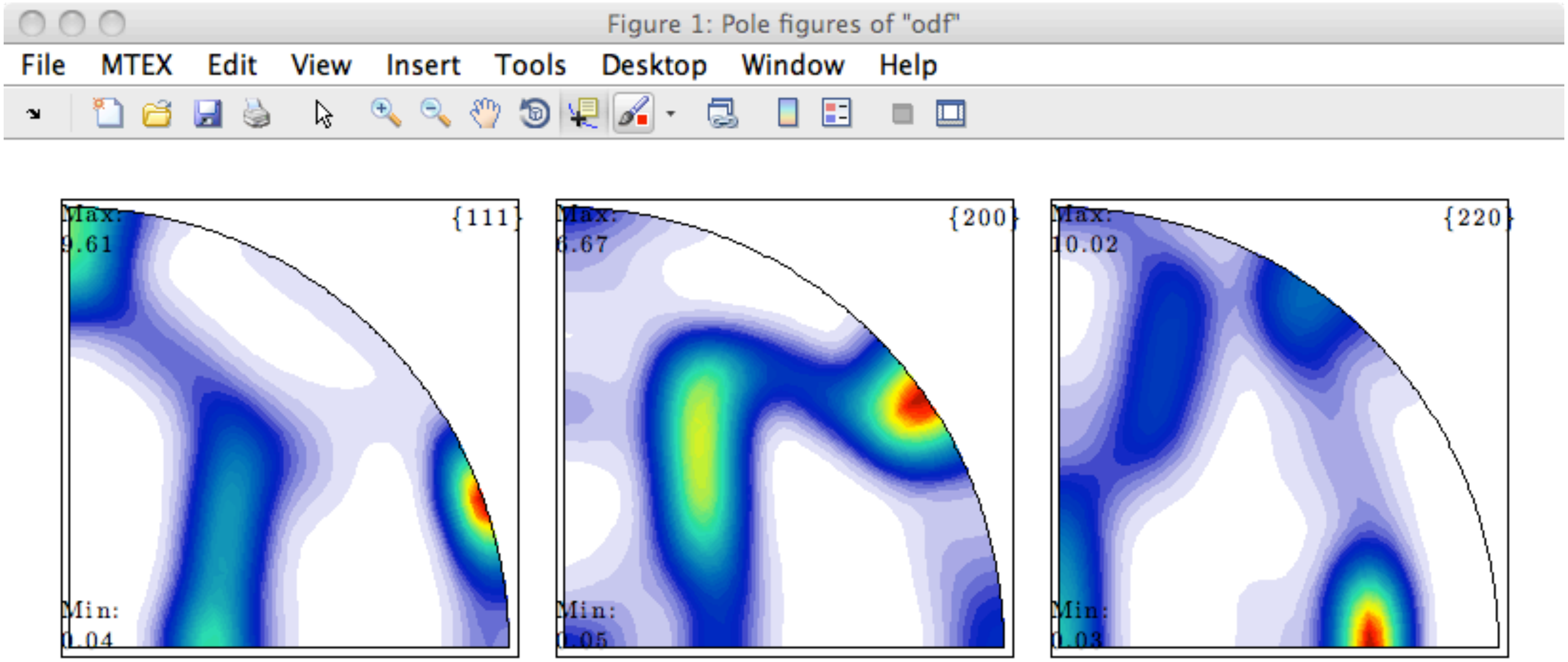
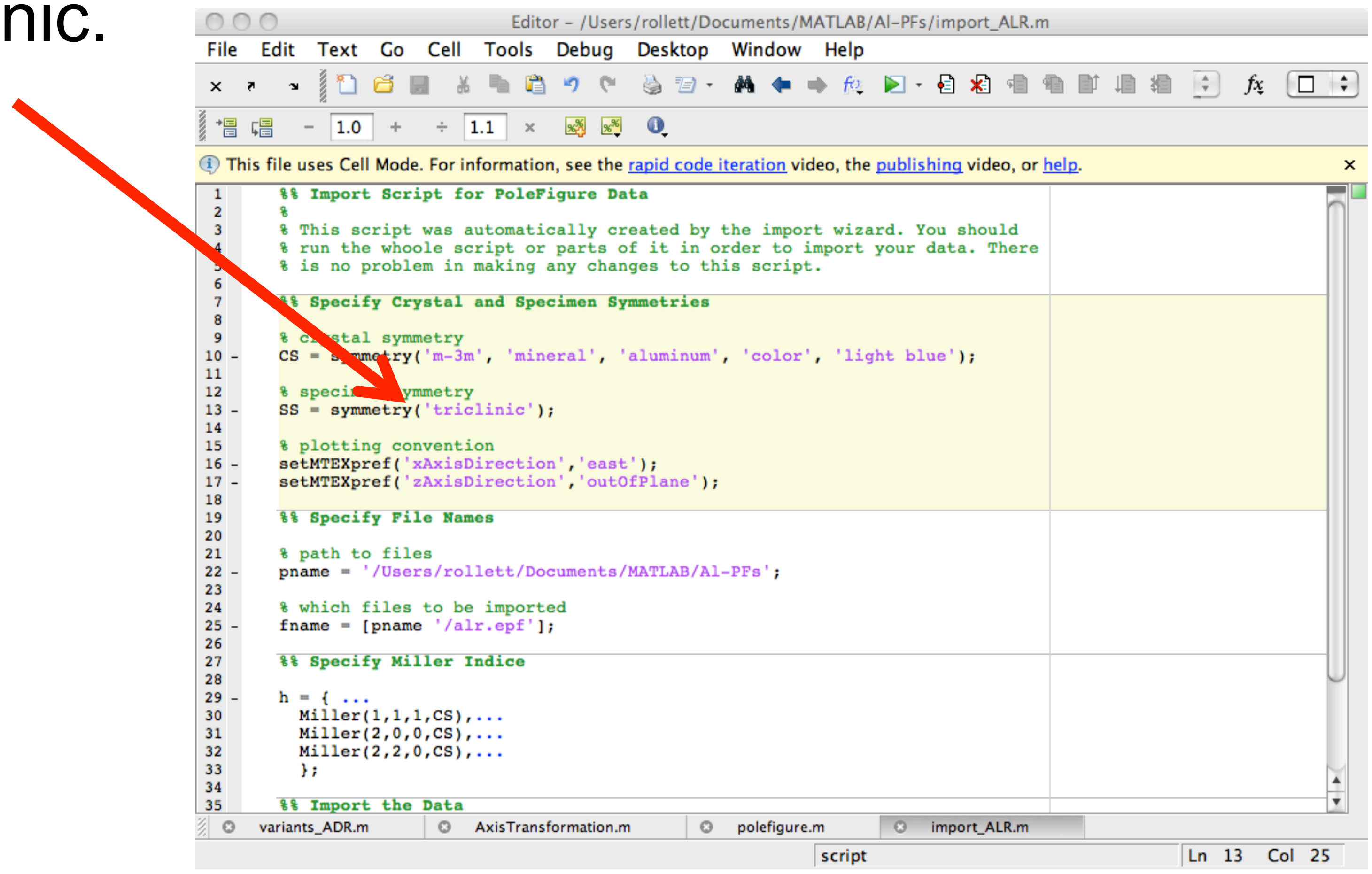


Figure 1: Pole figures of "odf"
File MTEX Edit View Insert Tools Desktop Window Help
{111}
Max: 9.61
Min: 0.04
{200}
Max: 6.67
Min: 0.05
{220}
Max: 10.02
Min: 0.03

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.

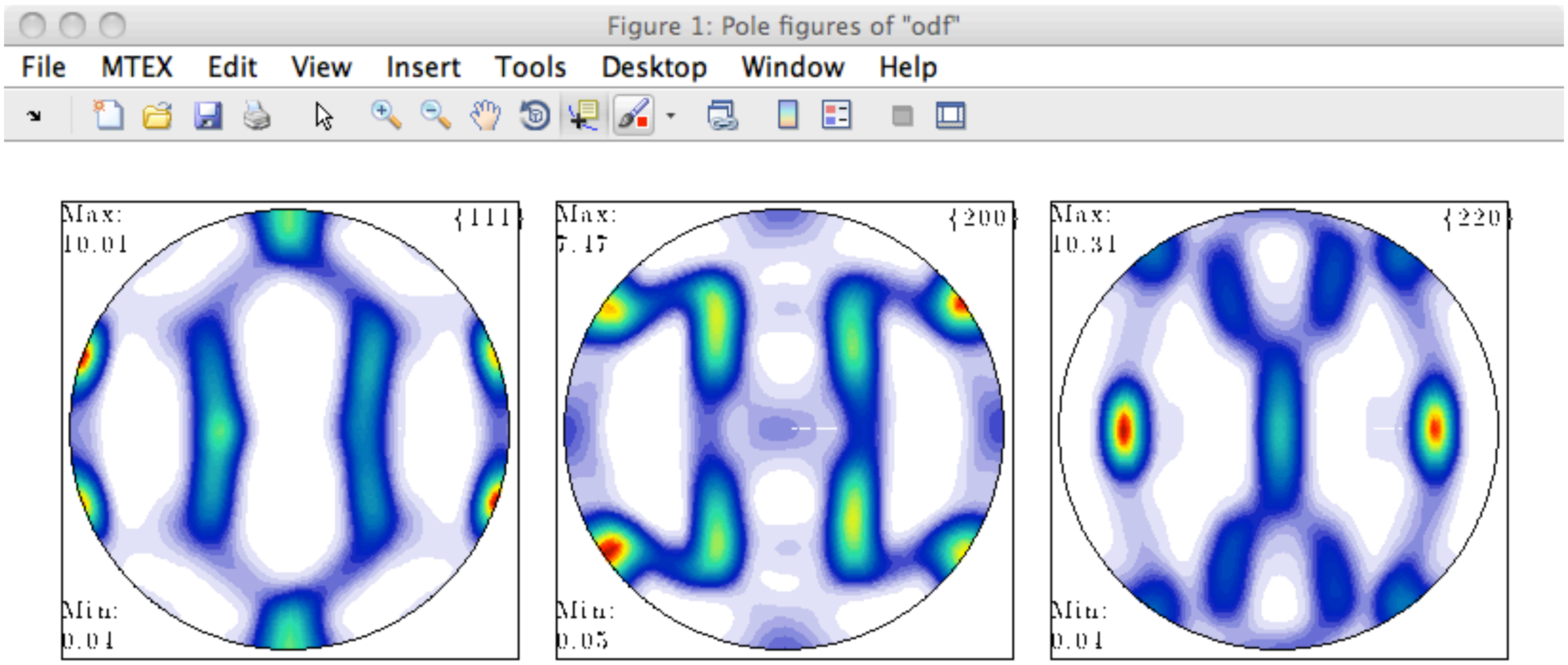
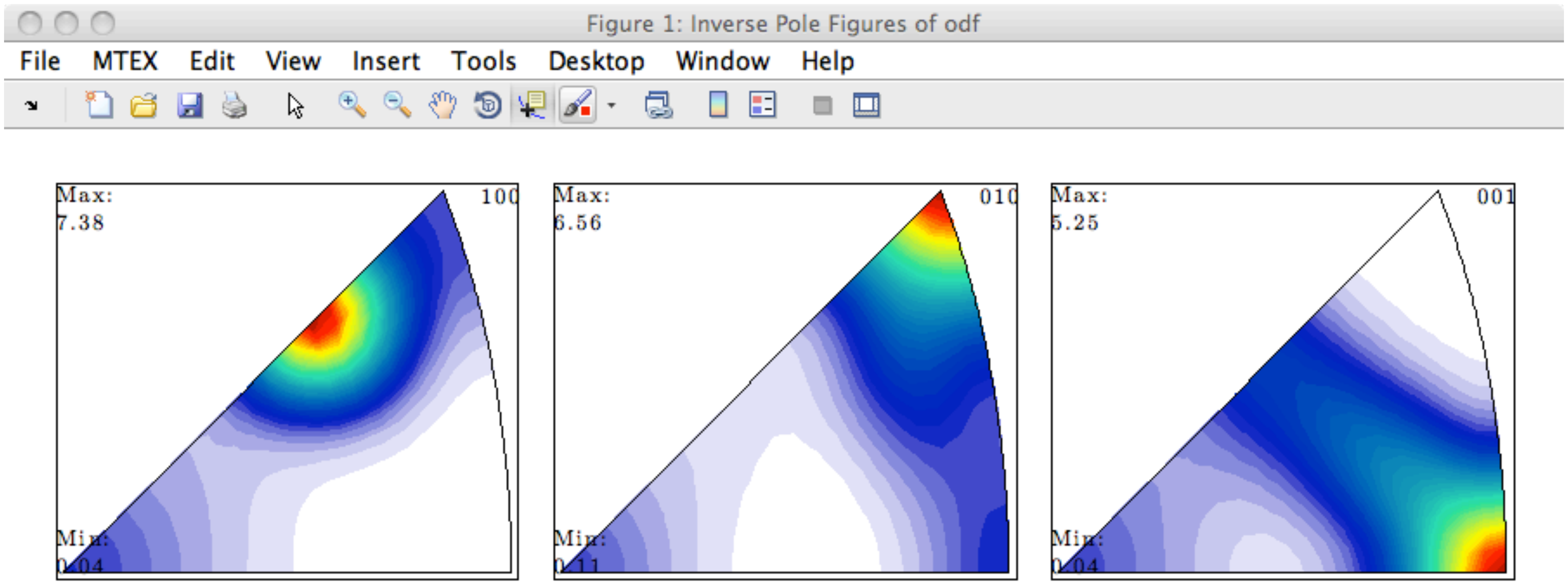


Figure 1: Pole figures of "odf"
File MTEX Edit View Insert Tools Desktop Window Help
Max: 10.01
{111}
Min: 0.04
Max: 7.47
{200}
Min: 0.05
Max: 10.31
{220}
Min: 0.04

Inverse PFs

- To get a complete set of 3 inverse pole figures, type "plotipdf(odf,[xvector,yvector,zvector],'antipodal')". The 3 sample directions are specified by the built-in "xvector", "yvector" and "zvector".



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.

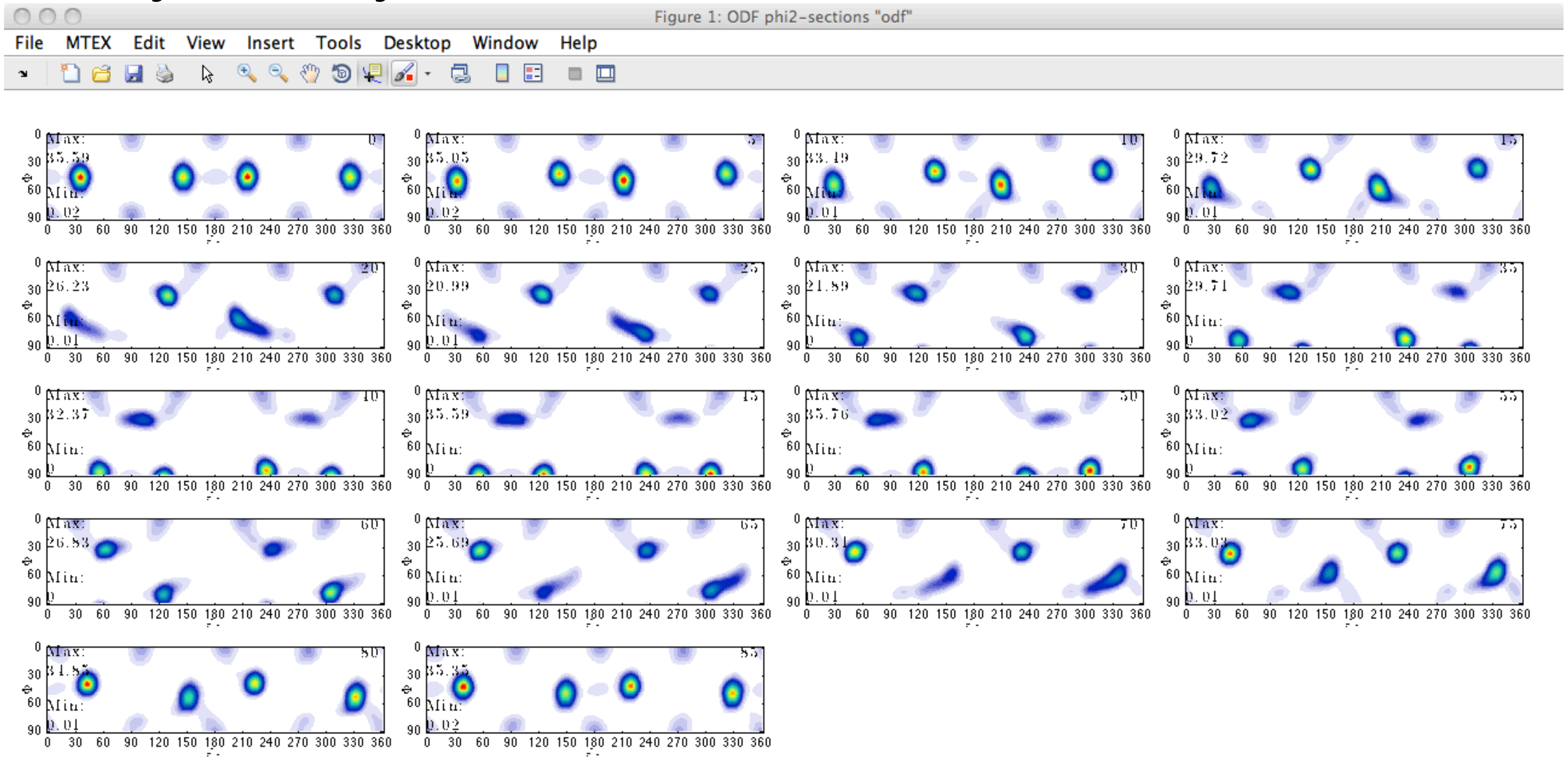


Figure 1: ODF phi2-sections "odf"
File MTEX Edit View Insert Tools Desktop Window Help

3D view

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

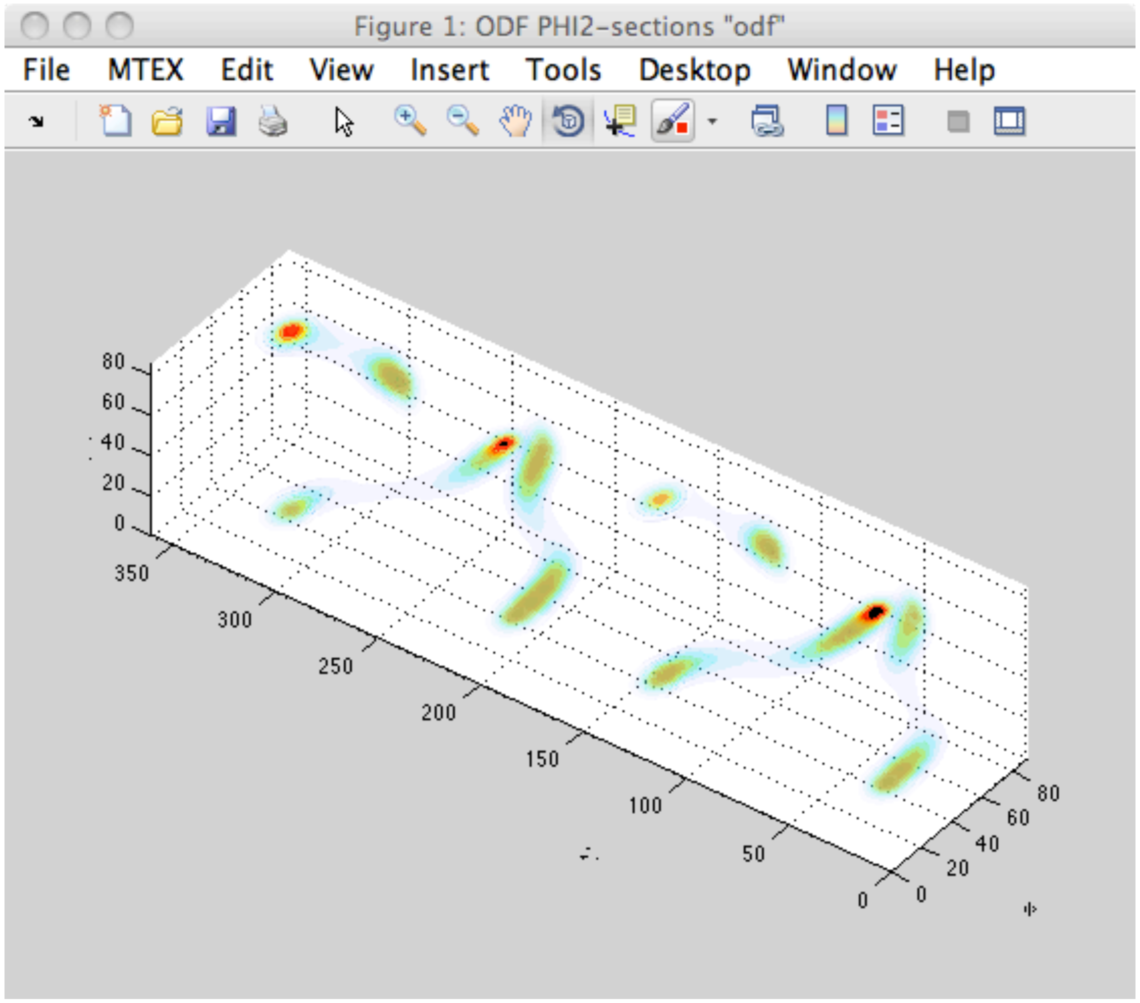


Figure 1: ODF PHI2-sections "odf"
File MTEX Edit View Insert Tools Desktop Window Help
80
60
40
20
0
350
300
250
200
150
100
50
0
0
20
40
60
80

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.

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>)
```

EBSD input

- Navigate with “cd” to wherever your data is; in this case, you need to download fw-ar-IF1-avtr12-corr.ctf from the CMU box for 27-750. 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.
- This generates a dataset called “ebsd”.
- Type “plot(ebsd,'colorcoding','ipdfHKL')”
- This will give a map of the material that is colored by the crystal plane exposed at the surface.

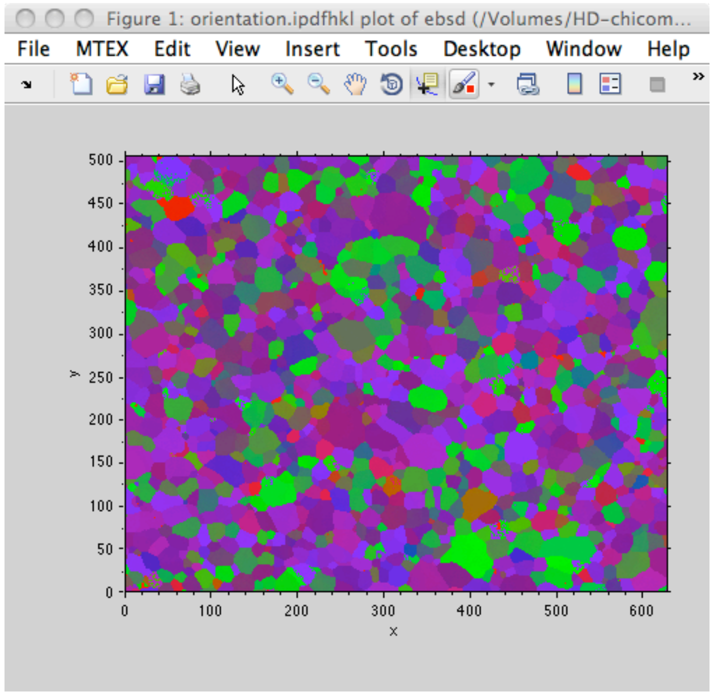
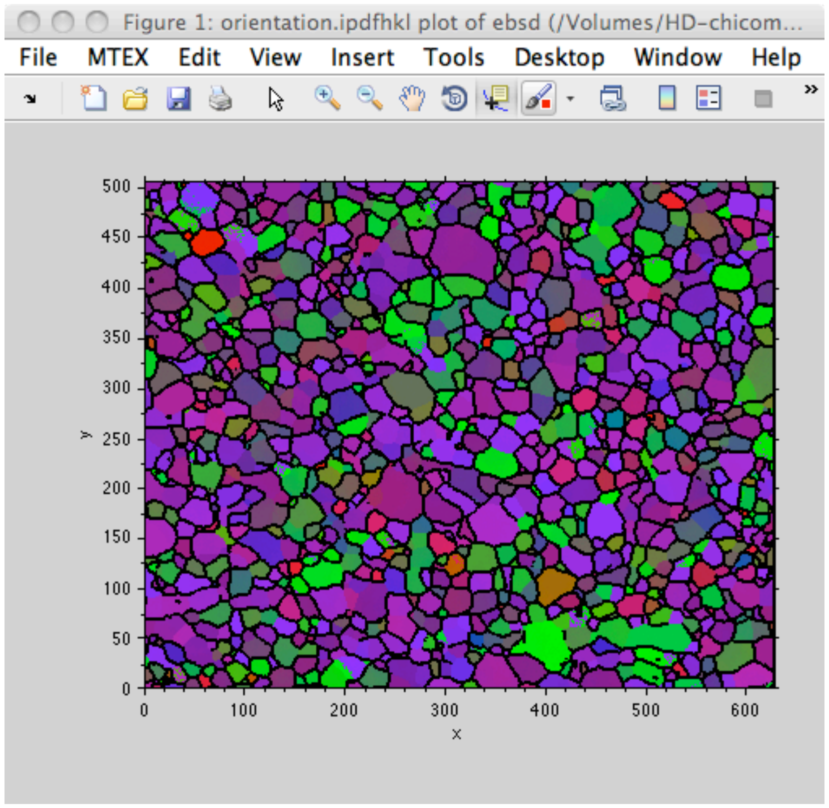


Figure 1: orientation.ipdfhkl plot of ebsd (/Volumes/HD-chicom...
File MTEX Edit View Insert Tools Desktop Window Help
500
450
400
350
300
250
200
150
100
50
0
y
0
100
200
300
400
500
600
x

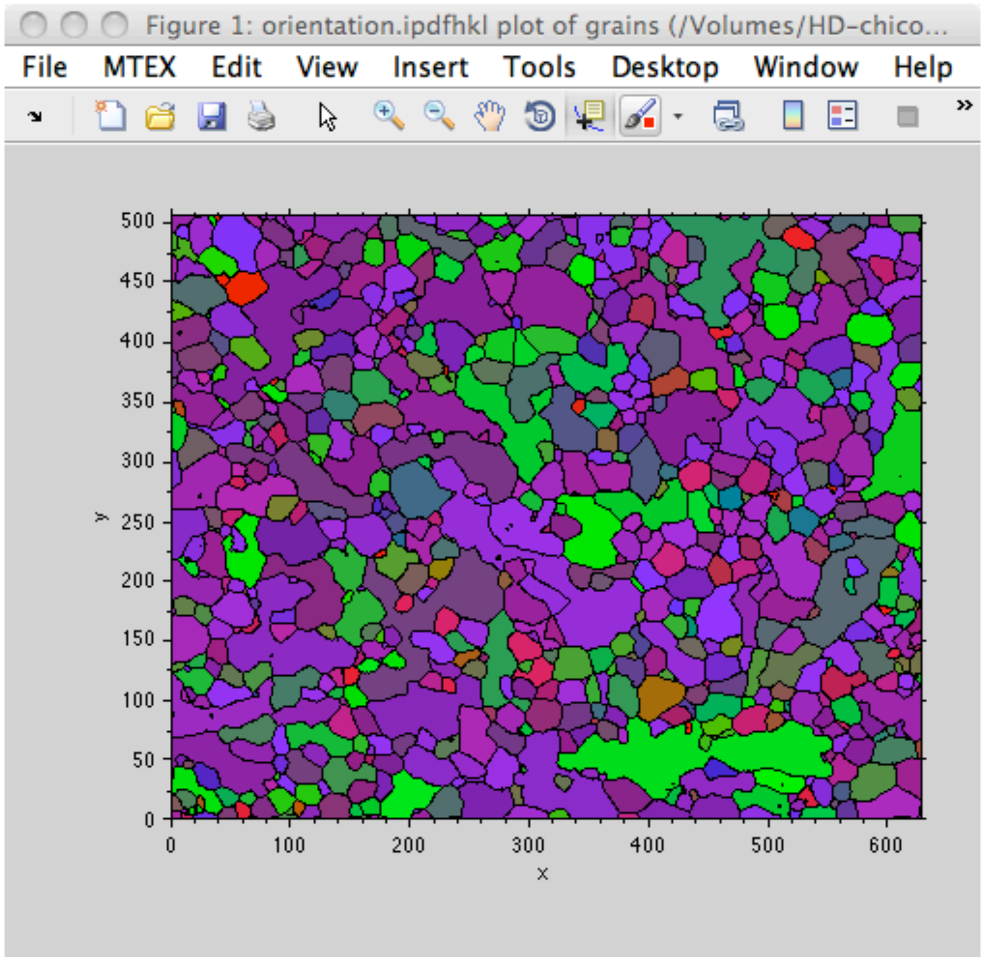
EBSD: get grains

- Type "grains = calcGrains(ebsd)"
- Then re-plot the ipdfHKL map and add grain boundaries:
  plot(ebsd,'colorcoding','ipdfHKL')
  hold on
  plotBoundary(grains,'linewidth',1.5)
- This will provide a similar map but with the GBs delineated.



Average grain orientations

- plot(grains,'colorcoding','ipdfHKL')



ODF from EBSD

First, do this: `plot(ebsd,'property','phase')`

```
psi = calcKernel(grains('Fe'))
odf = calcODF(ebsd('Fe'),'kernel',psi)
```

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

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

The third is the calculation of the ODF.

Plot pole figures

```
h = [Miller(1,0,0),Miller(1,1,0),Miller(1,1,1)];
```

This defines a set of pole figure indices

```
plotpdf(odf,h,'antipodal')
```

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

ODF plots

plot(odf,'PHI2','surf3')

This shows a 3D view of the ODF; 2 views shown

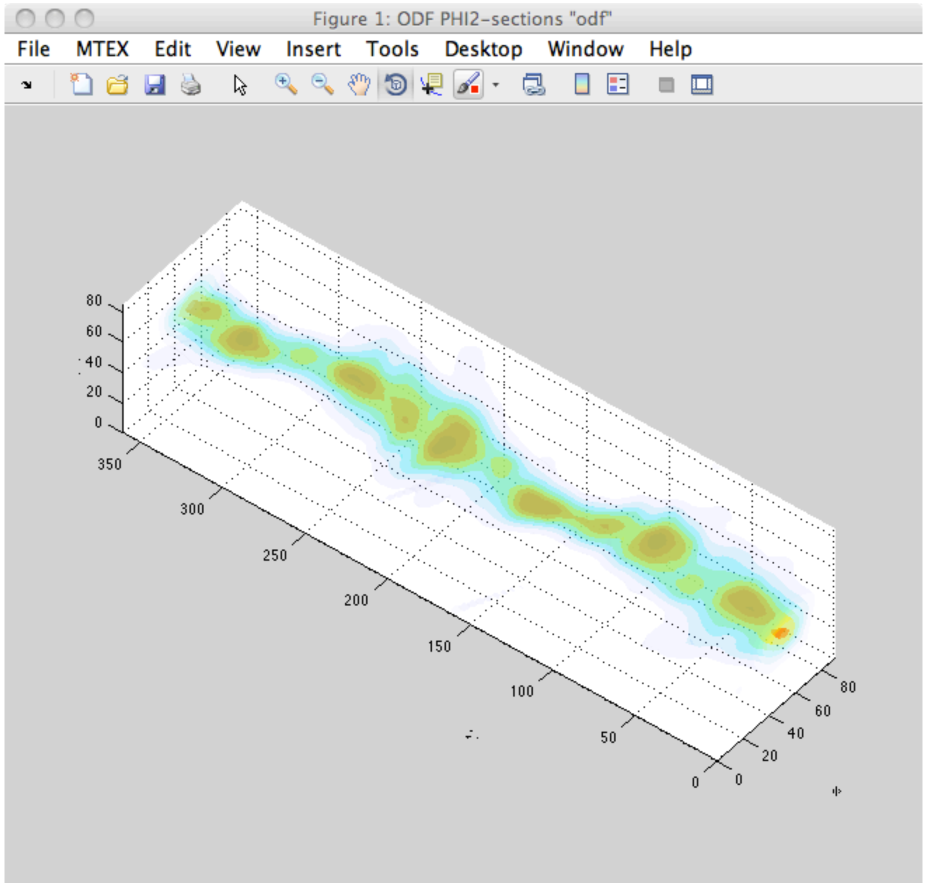


Figure 1: ODF PHI2-sections "odf"
File MTEX Edit View Insert Tools Desktop Window Help
80
60
40
20
0
350
300
250
200
150
100
50
0
0
20
40
60
80

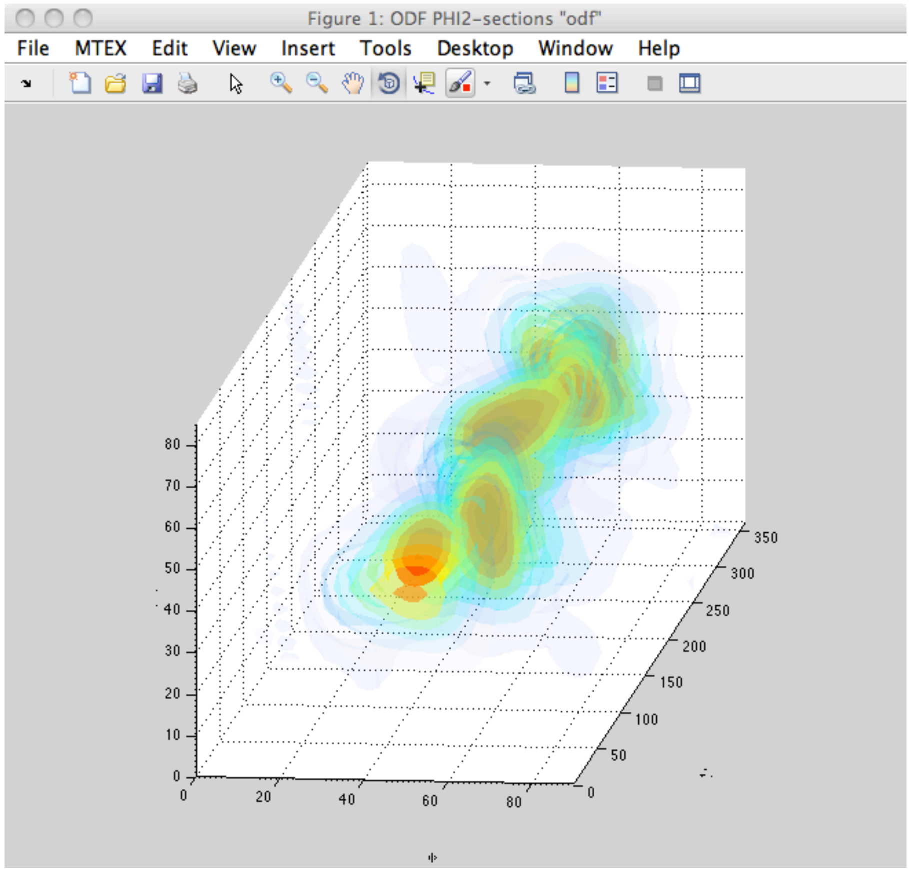
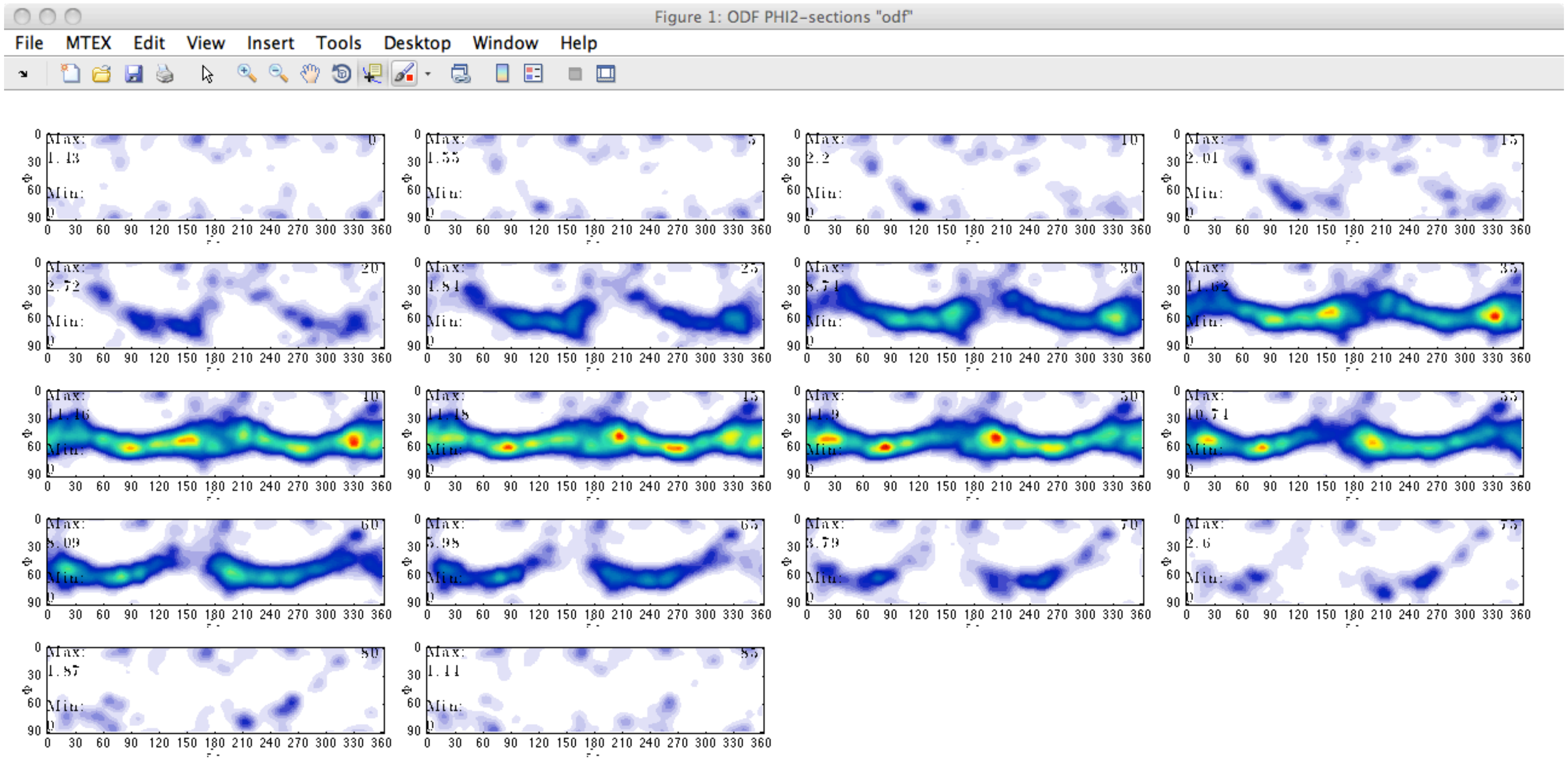


Figure 1: ODF PHI2-sections "odf"
File MTEX Edit View Insert Tools Desktop Window Help
80
70
60
50
40
30
20
10
0
0
20
40
60
80
0
50
100
150
200
250
300
350

ODF sections in ϕ_2

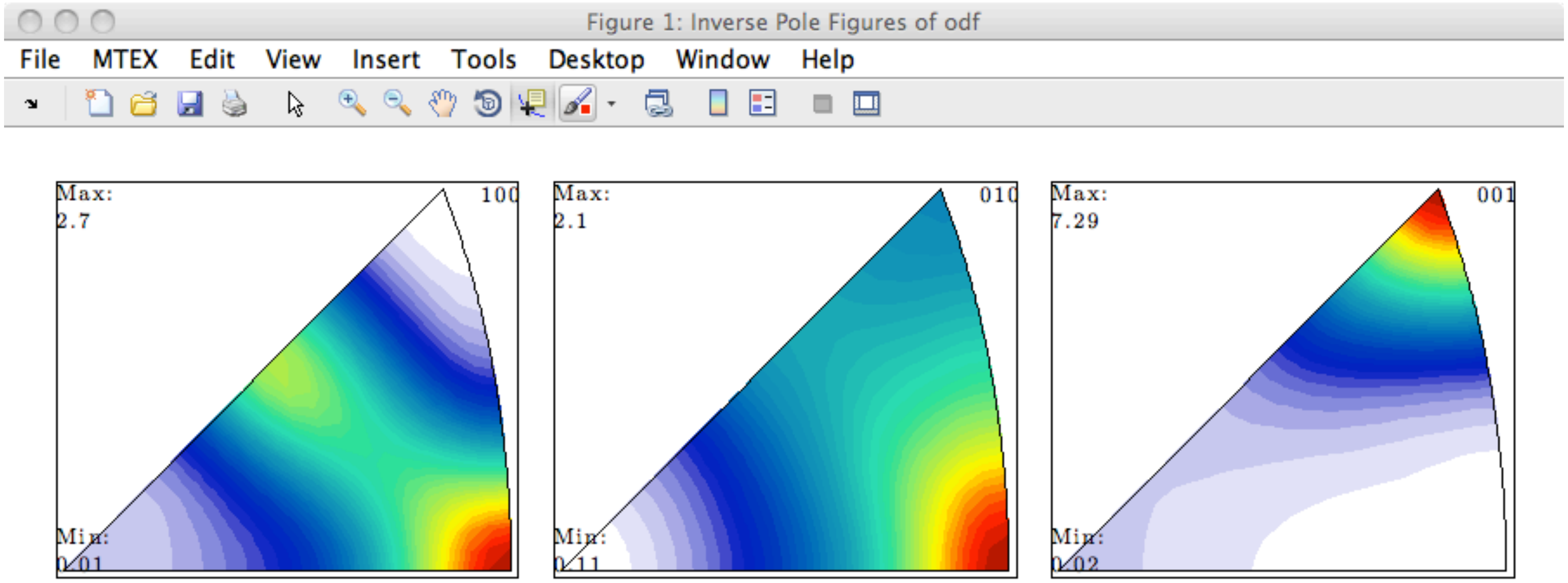
These show a clear gamma fiber, albeit imperfect. This is characteristic of a rolled bcc metals.



Inv. PFs

plotipdf(odf,[xvector,yvector,zvector],'antipodal')

Note how the 001 inverse pole figure shows a strong maximum at the <111> position.



Additional Steps

- Eliminate small grains:

```
% correct for too small grains
grains = grains(grainSize(grains)>5);
```

Summary

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