A Demonstration of How To Calculate and Analyze the Grain Boundary Character Distribution Using the 'Full Domain" Stereology Codes

Gregory S. Rohrer

Feb. 1 2017

The data:

To illustrate the full domain code, we will analyze some old data from a Nb-doped titania ceramic. It has the tetragonal rutile structure. It must be noted, there are not nearly enough grain boundary observations in these data for a generally reliable five parameter analysis. Nevertheless, it provides a good illustration of how things work. As we go through the analysis, it will be apparent that there is a twin boundary in the system with a high concentration. We will focus the five-parameter analysis on this one boundary, for which there should be enough data to draw conclusions. These raw and analyzed data are archived at:
http://mimp.materials.cmu.edu/~gr20/Grain_Boundary_Data_Archive/rutile/rutile.html

The analysis starts with lists of grain boundary line segments produced by the TSL software. These lists are in text files. In the header, lines starting with '#' are ignored. One grain boundary line segment is described on each of the following lines. The data are 12 columns of real numbers. The first six are Euler angles. The final four are the coordinates of the grain boundary line segments, in units of microns. The other columns are ignored by my programs.

Note that at various times in the past, TSL has written these files in a 12, 14, or 21 column format. When extracting the line segments, you end up with one file for each field of view. The first step is to make a single file containing all of the line segments. This could be done manually by cut and paste. However, I use the program 'combine_segments' for this. For contemporary data, it is essentially mandatory to used combine_segments because TSL is currently writing it's line segments output in a 21 column format that will not be accepted by my programs. Combine segments writes the data in a 12 column format that is consistent with my programs.

Preparing the data

The data were collected as 32 separate fields of view. The TSL software was used to extract the grain boundary line segments, and one file was produced for each field of view (see full_domain_stereology_tutorial/segments/). To use combine_segs, the file names have to have a specific format. They must be named in the form: filename_NNN.txt. The string that starts the name is referred to as the 'base name'; in this case it is 'filename'. The base name must be eight characters. It could be any eight-character string, but I always use 'segments'. The last part of the name, NNN, is a set of sequential three-digit integers, such as 000, 001, 002, etc… So, a set of appropriate files would have names such as:
segments_001.txt
segments_002.txt

segments_004.txt
segments_004.txt, etc…
(see full_domain_stereology_tutorial/segments/, for examples)
There are some details about the limitations in the input file.
In practice, your data usually does not have these file names when you start. To change them to compatible file names, place the files in a single directory. They should be the only files in that directory. Then, in the terminal window, navigate to the directory. When in that directory, issue the following command on the command line (all one line).

```
find . -not -name '\.*' -type f | awk 'BEGIN{ a=0 }{ printf "mv \"%s\" segments_%03d.txt\n", $0, a++ }' | bash
```

This will re-label every file in that directory with a name that is compatible for combine_segs (thanks to my unix guru, Dave Crockett).

For the remainder of this description, I executed all of the steps and recorded the command line input and output, which can be found in terminal_I/O.txt. As you follow the description, you should get the same responses on your terminal.

To begin, move all of the segment files to the folder combine_segments.

Configure the input file (input.txt) with the appropriate parameters. Here, the base name is 'segments', the first file is '0', the last file is '31', the data are in a 14 column format and will be written as a single 12 column file. The final line is a comment that can be added to the resulting output file. I strongly recommend adding appropriate labels to your data.

After navigating to this directory in the terminal window, run combine_segs by typing 'combine_segs' on the command line

combine_segs will produce a single file, labeled 'all_segments.txt' that will have the header of the first file, with your comment line added, and a consecutive list of all of the grain boundary line segments in the 32 individual files.

Next, re-label the file 'all_segments.txt' to something more meaningful for your data. Here, I re-label it 'Nb_TiO2_segs.txt'.

With all of the grain boundary line segment data prepared in a single file, we are ready to begin the analysis.

Analyzing the data

1) Calculate the disorientation angle distribution

Move the list of line segments (Nb_TiO2_segs.txt) into the folder 'disor'.

Set the appropriate parameters in 'input.txt'. The parameters for the TiO2 demonstration data in this example are set appropriately. Instructions for the parameters are described in the input files.

After navigating to the directory 'disor' in the terminal window, run dis_calc by typing 'dis_calc' on the command line.

The results are written to a text file labeled:
report_[filename].txt (here: report_Nb_TiO2_segs.txt)
This is a text file and it can be read by standard graphics programs. A graph of this (I made this in Kaleidagraph, but I think any program that can read text will work) is shown in Fig. 1.

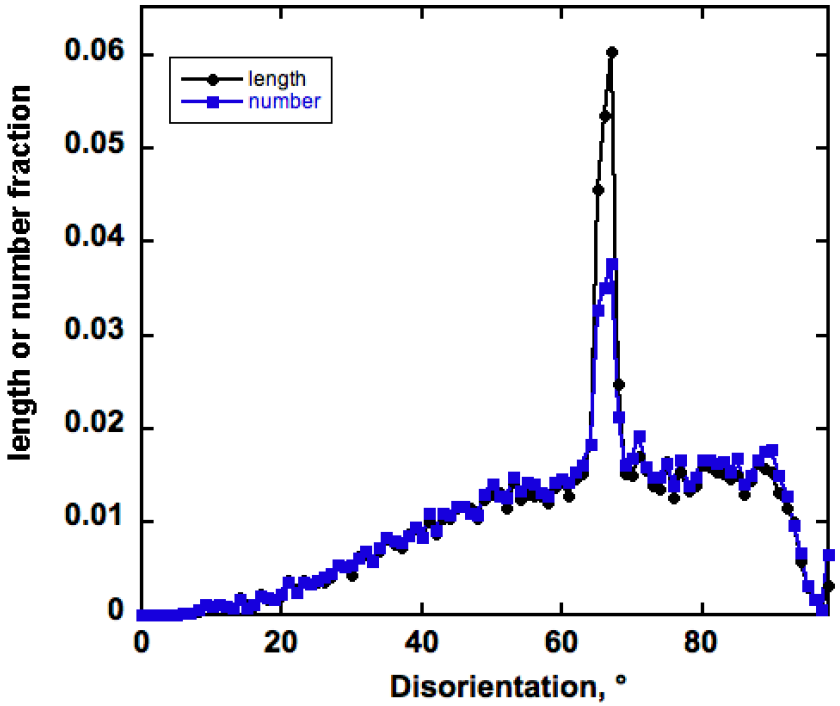

Figure 1. The disorientation angle distribution for Nd-doped TiO_2 (rutile). See: full_domain_stereology_tutorial/results/ disor_dist_TiO2_graph.tiff. The distribution was calculated discretely with a resolution of 1°.

The program dis_calc reports both the number fraction (counting each segment as one) and the length fraction. The results in Fig. 1 demonstrate that there is an unusual number of grain boundaries with a 66° disorientation. These boundaries make up roughly 6 % of the total grain boundary length.

For convenience, the disor folder also contains the random distributions for several symmetries, because you might want to add this to the graph. I generated these using a million boundaries with randomly selected Euler angles.

2) Calculate the Grain Boundary Character Distribution

Move the list of line segments ('Nb_TiO2_segs.txt) into the folder 'calc_gbcd_stereo_fd'.

Set the appropriate parameters in 'input.txt'. The parameters for the TiO2 data in this example are set appropriately. Instructions for the parameters are described in the input file. For the full parameter code, the resolution factor cannot be greater than 9.

After navigating to the directory 'calc_gbcd_stereo_fd' in the terminal window, run calc_gbcd_stereo_fd by typing 'calc_gbcd_stereo_fd' on the command line.

The results are written to a text file labeled: gbcd_[filename].txt . In this case, it is gbcd_Nb_TiO2_segs.txt.

This file contains a discrete five dimensional array, with one value on each line. The format is explained in notes at the end of the input file.

This file will serve as the input to the:
two parameter projection: gbpd_graph_fd
(here, all grain boundary planes are plotted in the crystal reference frame, ignoring misorientation)
three parameter projection: ax_ang_graph_fd
Here, the distribution of grain boundaries for all possible axes, at a single value of the disorientation angle, are plotted.
five parameter projection :gbcd_graph_fd
Here, the distribution of grain boundary planes at a fixed misorientation are plotted in the bicrystal reference frame.

3) Plot the grain boundary plane distribution

Here we plot the grain boundary plane distribution, in the crystal reference frame, ignoring misorientation.

Move the gbcd_Nb_TiO2_segs.txt, written by calc_gbcd_stereo_fd. to the folder gbpd_graph_fd.

Set the appropriate parameters in 'input.txt'. The parameters for these data are already set. For the cases of cubic and hexagonal, it is possible to plot the data in the fundamental zone (plot type = 4); for other symmetries, you must plot in the full hemisphere (plot type = 1). This is not a fundamental limitation, it is only that the scripts have not yet been coded to allow other symmetries.

After navigating to the directory 'gbpd_graph_fd' in the terminal window, run graph_gbpd_fd by typing 'graph_gbpd_fd' on the command line.

The program samples the gbcd and writes a new file that can be graphed by GMT (there is a more complete description in the text of the input file).

When graph_gbpd_fd runs, it writes the following output to your screen.

……

I am graphing data in the file labeled: gbcd_Nb_TiO2_segs.txt
The data will be in the format for gmt
you have specified the symmetry as tetragonal
The [001] direction will be normal to the plane of the drawing.
The average value is 0.93 MRD.
The minimum value is 0.65 MRD.
The maximum value is 1.99 MRD.

to initiate the gmt script, enter ./Draw_stereograms 1 [filename]_2d_gmt 2d rainbow [min] [max] [interval]
For example: ./Draw_stereograms 1 gbcd_Nb_TiO2_segs_2d_gmt 2d rainbow 0.65 1.99 0.13

……

This output is important, because you need it too instruct the script that controls GMT. To draw a plot in the simplest possible way, copy the line:
./Draw_stereograms 1 gbcd_Nb_TiO2_segs_2d_gmt 2d rainbow 0.65 1.99 0.13
onto your clipboard, and then paste it on the next command line. This will initiate the Draw_stereograms script that issues the necessary commands to GMT. Note that this line is a reasonable 'hint' and will draw a plot for you, but you can always do better. Mainly, the last three numbers are simply the max value, the min value, and the difference divided by 10. I practice, you would rather have rational bounds on your graph, so I would change these to 0.6 2.0 0.2. Also, the script defaults to cubic. If the material is not cubic (for example, here it is tetragonal), then you would prefer not to have great circles on the stereogram corresponding to cubic symmetry. Unfortunately, the GMT script only coded at this time for cubic, hexagonal, and orthorhombic lines. Orthorhombic is the best match for this particular case. So, the best command to draw the plot is:

./Draw_stereograms 1 gbcd_Nb_TiO2_segs_2d_gmt 2d rainbow 0.6 2.0 0.2 stereo ORT

If you would prefer no lines on the plot, replace 'ORT' with anything other than 'CUBIC' or "HEX' and the section of the script that draws these lines will be skipped.

The Draw_stereograms script is text file and you can read some instructions within, in case you would like a projection other than stereographic or a coloring other than rainbow.

When you run the script, GMT will produce the graph in both .ps and .tif formats. They should be identical, it just gives you a choice if you like one or the other. [note, it might be necessary to install the free code, ImageMagick, for complete functionality.]

The results for this case are illustrated in Fig. 2, which suggest that the most common grain boundary plane orientations are (110).

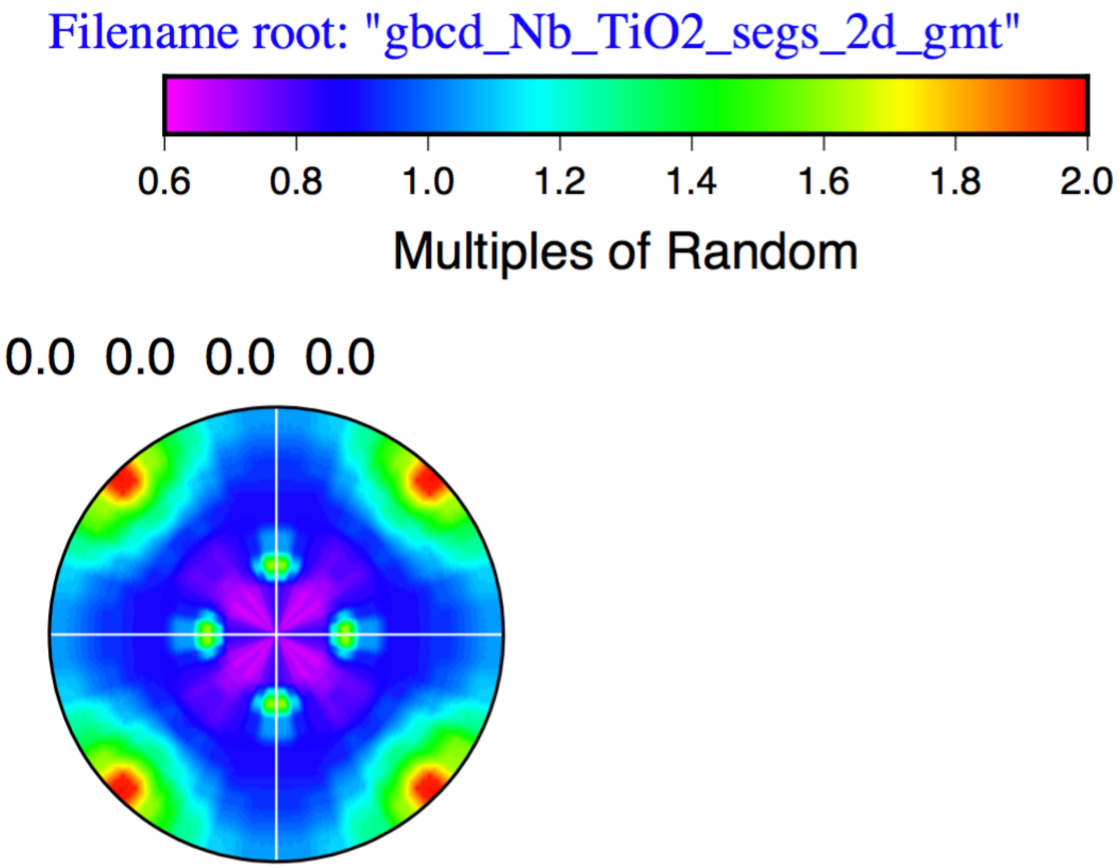

Figure 2. The grain boundary plane distribution, ignoring misorientation. The maximum occurs for the {110} orientation. Note that the distribution has the symmetry of the crystal and eight fundamental zones are repeated.

4) Plot the distribution of grain boundaries in axis angle space

Here we plot the distribution of grain boundaries, at fixed disorientation angles, as a function of the disorientation axis in the crystal reference frame.

Move the gbcd_Nb_TiO2_segs.txt, written by calc_gbcd_stereo_fd. to the folder ax_ang_graph_fd.

Set the appropriate parameters in 'input.txt'. To decide which angle or angles we want to fix, we refer back to the disorientation angle distribution (Fig. 1). The only peak that is significantly above random is at 66° (this is a well known twin in TiO_2 rutile). The parameters for these data are set. For the cases of cubic and hexagonal, it is possible to plot the data in the fundamental zone (plot type = 4); for other symmetries, you must plot in the full hemisphere (plot type = 1). This is not a fundamental limitation, it is only that the scripts have not yet been coded to allow other symmetries.

After navigating to the directory 'ax_ang_graph_fd' in the terminal window, run graph_ax_ang by typing 'graph_ax_ang' on the command line.

The program samples the gbcd and writes a new file that can be graphed by GMT (there is a more complete description in the text of the input file).

When graph_ax_ang runs, it writes the following output to your screen.

……
I am planning to make 1 plots
plot number= 1
  66.0000000
 now plotting: 66.0000000
  1.15191734
For this misorientation, the average value is 1.66 MRD.
For this misorientation, the maximum value is   41.17 MRD.
For this misorientation, the minimum value is   0.61 MRD.

to initiate the gmt script, enter ./Draw_stereograms [Number of plots] [filename]_gmt_ 5d rainbow [min] [max] [interval]
For example: ./Draw_stereograms 1 gbcd_Nb_TiO2_segs_gmt_ 5d rainbow 0.61 41.17 4.06
  1.15191734
……

As above, this information guides you in providing a good command to Draw_stereograms. As written, it will work. But, it will be better if we choose more rational bounds and do not draw cubic lines. The following will work:

./Draw_stereograms 1 gbcd_Nb_TiO2_segs_gmt_ 5d rainbow 0 40 5 stereo ORT

When you run the script, GMT will produce the graph in both .ps and .tif formats. They should be identical, it just gives you a choice if you like one or the other. For example, the result is found in the file: gbcd_Nb_TiO2_segs_gmt_.ps, which is plotted in Fig. 3. Note that at this angle, the distribution is strongly peaked at the {100} axis. Taken together with Fig. 1, this means the most common boundary in the system

has a 66°/[100] misorientation. This is consistent with what is known about twinning in rutile.

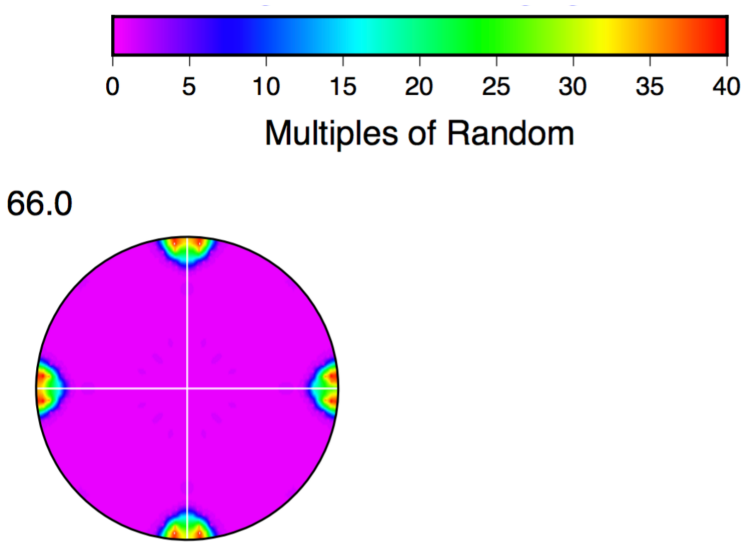

Figure 3. The distribution of grain boundary axes of disorientation, at a 66° disorientation angle. Peaks occur at the {100} positions.

5) Plot the distribution of grain boundary planes at a fixed misorientation.

Move the gbcd_Nb_TiO2_segs.txt, written by calc_gbcd_stereo_fd. to the folder gbcd_graph_fd.

Set the appropriate parameters in 'input.txt'. In general, you might want to survey a range of axes and angles. Here, as mentioned before, there is a twin with a misorientation of 66°/[100]. So, we will use this axis and angle. The parameters for these data are set. For these distributions, you must plot in the full hemisphere (plot type = 1).

After navigating to the directory 'gbcd_graph_fd' in the terminal window, run graph_gbcd by typing 'graph_gbcd' on the command line.

When graph_gbcd runs, it writes the following output to your screen.

```
……..
I am planning to make 1 plots
plot number= 1
now plotting:  1.00   0.00   0.00   66.00
For this misorientation, the average value is 44.11 MRD.
For this misorientation, the maximum value is  816.61 MRD.
For this misorientation, the minimum value is    0.00 MRD.
```

to initiate the gmt script, enter ./Draw_stereograms [Number of plots] [filename]_gmt_ 5d rainbow [min] [max] [interval]
For example: ./Draw_stereograms 1 gbcd_Nb_TiO2_segs_gmt_ 5d rainbow 0.00 816.61 81.66
……

As above, this information guides you in providing a good command to Draw_stereograms. As written, it will work. But, it will be better if we choose more rational bounds and do not draw cubic lines. The following would be a reasonable start:

./Draw_stereograms 1 gbcd_Nb_TiO2_segs_gmt_ 5d rainbow 0 800 100 stereo ORT

Using this command you will see some regions of the plot are colored black. I do not know why this happens, be it is common whenever 0.0 is used as a lower bound. My 'work around' is to change the lower bound to a negative number that is small compared to the upper bound. Here, -0.4 works:

./Draw_stereograms 1 gbcd_Nb_TiO2_segs_gmt_ 5d rainbow   -0.4 800 100 stereo ORT

The result is illustrated in Fig. 4. Note the very strong peak at the (0-11) orientation. This is the known twin plane for rutile.

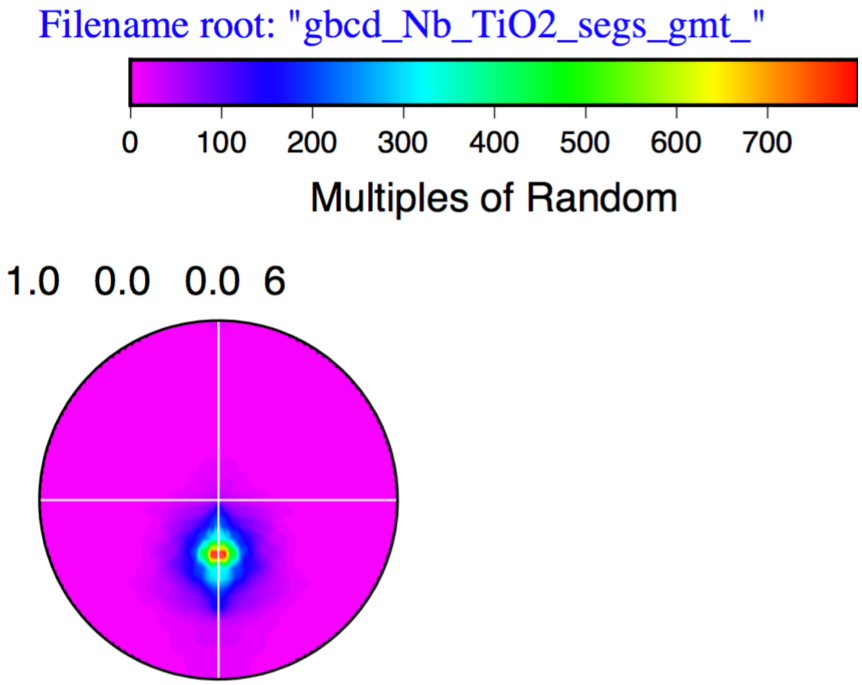

Figure 4. The grain boundary plane distribution for the misorientation of 66°/[100]. The maximum is at the (0-11) orientation.