Homework 8: Various topics; *Solutions*
A.D. Rollett, 27-750, Texture, Microstructure and Anisotropy
30+30+20+20 = 100
Due date: 13th April, 2016

Q1. [30 points]
a) Certain 5-sided grains are observed to be just able to grow in a 2-dimensional microstructure. What are the dihedral angles likely to be found at the triple points?
b) What estimate can you make of the ratio of the energy of their perimeters (the GBs around their edges) to the energy of the GBs in the matrix around them?
c) Assume that these special grains are able to grow to a large size and preserve the difference in energy. If such a sample is annealed to develop surface grooves where the GBs intersect the surface, what do you expect to observe about the dihedral angles at the surface that associated with the special grains, versus the angles at GBs in the matrix? Assume that the surface energy is everywhere the same.

(a) By symmetry, the dihedral angles must be the same at every triple junction. Each segment of the perimeter must be straight if the 5-sided grain is only just able to grow. Therefore the turning angle between successive segments of the perimeter of the decahedron must be the same and equal to 1/5th of the complete circle. Divide 360° by 5 gives 72° as the turning angle. The dihedral angle inside the grain is therefore 180°-72° = 108°. The other two dihedral angles must be symmetrically disposed and equal to each other. The dihedral angles between a perimeter segment and the matrix boundary joined to each triple junction must be (360-72)/2 = 126°.
(b) Label the perimeter GB "A" and the matrix GBs "B". Applying Young's Equations, the ratio of the two energies must be equal to the inverse ratio of the sines of the dihedral angles. Therefore $(\gamma_A / \gamma_B) = \sin(126)/\sin(72) = 0.8090 / 0.9510 = 0.8506$.
(c) The surface dihedral angles of the GBs around the special (abnormal) grains will be larger than those of the matrix GBs because of the lower energy of those grain boundaries compared to general GBs.

Q2. [30 points]
a) Make diagrams or sketches to explain the point made on slide 45 in the Stereology notes about nearest neighbor distances being smaller than mean free paths (for a given particle volume fraction and size). Here we consider only particles as point objects (not, e.g., grains as defined by a network of boundaries).
a) The sketch should make the point that nearest neighbor distance in effect seeks the nearest neighbor in any direction. The mean free path is looking along a specific direction and therefore will likely "bypass" the nearest neighbor and strike a different neighbor.

b) Read Chapter 4 in the Underwood book. Derive the expression given in the notes on abnormal grain growth (see slide 16 about drag pressure) for the number of particles per unit area of boundary, $N_A = 3f/2\pi r^2$. Hint: the derivation is simple once you identify the correct expression.

(b) Start with the basic expression for the number of particles per unit area of test plane, $N_A$, which is equal to the product of the number per unit volume, $N_V$ and the projected height, H'. For uniformly spherical particles, the projected height is just the diameter, 2r. $N_V$ = volume fraction over volume per particle = $f / (4\pi r^3/3)$. Thus $N_A=2r*3f/4\pi r^3=3f/2\pi r^2$. QED.

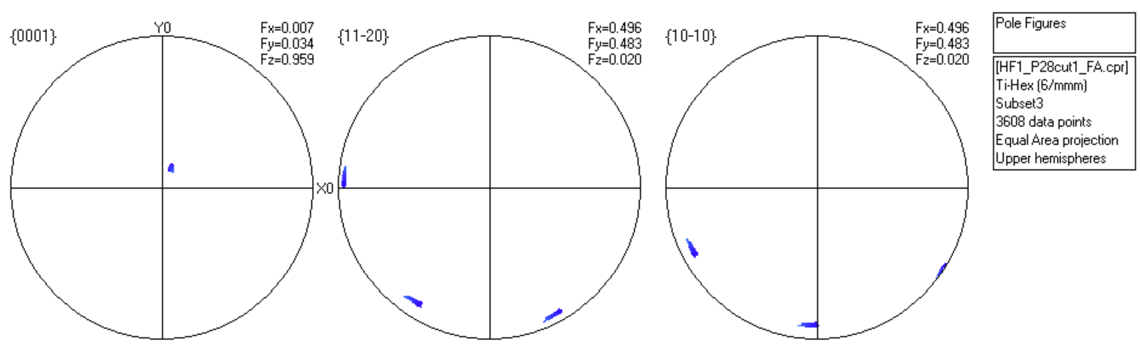
c) Based on the standard Smith-Zener analysis of particle pinning of grain growth, does variation in (anisotropy of) the grain boundary energy make any difference to the pinned grain size?

(c) No, the analysis balances the drag pressure against the growth pressure. The grain boundary energy enters the expression on both sides. Therefore the magnitude of the GB energy makes no difference.

Q3. [20 points]

Reference Frames

The figure below is taken from slide 27 in the EBSD Analysis lecture. From this set of discrete pole figures (ignore the spread in orientation that the streaks suggest), deduce the euler angles of the crystal assuming the reference frame is the default for HKL/Oxford (as indicated by the labels "X0" and "Y0" on the lefthand pole figure). Then repeat but with the assumption of the TSL/OIM system (as described in the lecture notes). You are strongly encouraged to make diagrams of the successive rotations starting from the reference position in order to verify that result is correct.




HKL/Oxford.

The righthand (RH) pole figure (PF) for {10-10} shows that the 1st Euler angle is approximately -30°, which is equivalent to 330°, i.e. clockwise rotation from the position marked "X0" in the lefthand (LH) PF for {0001}. The pole in the LH PF shows that the second Euler angle is approximately -20°, which is equivalent to 160° (since the 2nd angle repeats in 180°), i.e. a clockwise rotation about the 10-10 axis. No further rotation is needed so that 3rd Euler angle is 0. The result is an orientation of {-30°, -20°, 0°}.

TSL/OIM/EDAX.

First one must remember that the Euler X-axis is opposite to the direction marked "Y0" in the LH PF. Via similar arguments therefore, the 1st Euler angle is about +60°. The second angle is the same, about -20°. Now we have to subtract 30° for the third Euler angle because in the TSL default setup, the Cartesian x-axis is aligned with 2-1-10. The result is an orientation of {60°, -20°, -30°}, or {330°, 160°, 330°}.

Q4. [20 points] Learning how to make probability plots
This exercise is included mainly to convince you that making probability plots is not difficult and can produce interesting results.
Firstly, download the "R" project from www.r-project.org and install it on your computer.
Secondly, figure out how to install the package e1071 that allows you to draw probability plots.
Thirdly, read in the data from the list given below, e.g., by storing the numbers in a text file and using the *read.table* command.

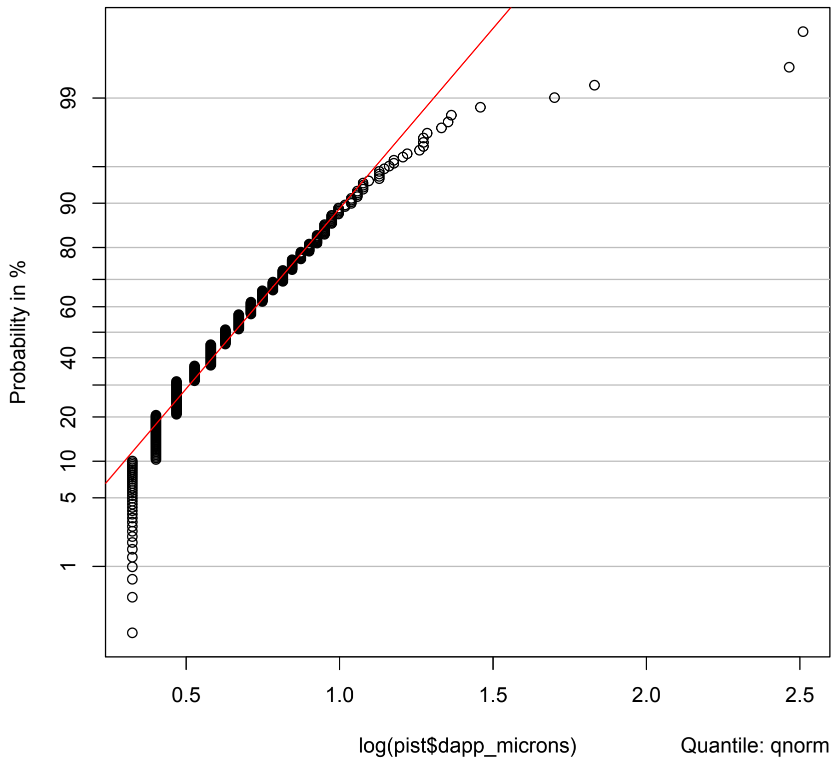
Submit a screenshot (or copy of the transcript) that shows that you have read in the data, taken the log of each datapoint, and made a probability plot, along with a copy of the plot. Indicate on the plot which parts of the distribution conform to a normal distribution (bell curve) and which parts do not. If you observe divergence from log-normal, does the result indicate more large grains/particles than you would predict from the log-normal part of the data, or fewer?

Hints:
- Once you have read in the data, you should type "summary" to see what R thinks it has.
- Try using the probability plot directly on the data.
- Then make a probability plot of the log of the data.

There are many guides and introductions to R on the web. Google is your friend!
[As an extra exercise, see if you can figure out how to normalize each column of points by their mean; look at the "summary" command above which provides a mean value and create a new dataset from the existing column of data.]

It turns out that probplot can operate directly on the data read in with data.table. Thus:
Pist = data.table("filename.txt")
Probplot(pist$dapp_microns)
Followed by:
Probplot( log(pist$dapp_microns) )

The result should look something like the following figure. The parts of the distribution that follow the straight line conform to a normal distribution. Where the distributions diverge, they are not part of a bell curve. Basically, most grain size distributions are log-normal but only in the central part of the distribution. These results diverge strongly towards larger particles/grains at the upper end.




Data for probability plot question.

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