

Homework 3: Pole Figure Analysis with popLA

Due Date: 18th Feb '08

The *purpose* of the homework is for each student to learn how to perform analysis of pole figure data by using popLA. The preferred data set will be one that you have generated from your own sample(s). Many new concepts will be introduced which we will then discuss and explain during the course. Later on, we will ask you to interpret your results as part of your term project.

Each question requires you to perform a certain action in the analysis package, to make a plot, and to comment on the result(s). The purpose of the comments is for you to understand that the analysis involves some degree of operator judgment (and experience).

popLA practice

Required for Question 3:

- (i) Access to a working copy of popLA*. If you have not had your own copy of popLA, please write to popla@lanl.gov and request an official copy so that you can receive notices of updates etc. (If you do not have time to obtain an official copy from Los Alamos, try downloading the set of files from neon.materials.cmu.edu/rollett/popLA.)
 - (ii) The popLA manual (download from the 27750 website) – this is *required reading!*
 - (iii) A set of pole figure data, preferably based on a specimen of your own material. This should be in the form NAME.RAW where “NAME” is whatever identifier you assigned to that specimen and “.RAW” indicates that it contains measured intensities. You will also need a defocusing correction file; this is the type of file that has extension “.DFB”. If you are uncertain as to how to obtain this, talk to your local x-ray expert, or generate a theoretical set using popLA, but read the Kocks book and the popLA manual first.
- If you made your measurements on the CMU Phillips (now Panalytical) XPert system then you will need some assistance to convert the data into popLA format; I can send you a copy of the conversion program, along with notes about how to correct the output .RAW file so that popLA will read it.
 - If you do not have your own data set (or cannot get one in time) then please download the data file for an iron specimen that you will find on the course website called “RAW data file of pole figures from an iron specimen”. You will also need to generate a theoretical .DFB file, so use the appropriate option in page 2 to do this. I suggest that you use a 1mm slit width and a 1mm beam width as your first guess.
 - Note on POD and Windows-XP: in contrast to older systems (Windows 98, NT etc.) XP does not permit screen capture from a DOS window (supposedly to cut down on illegal copying) which means that POD is only useful for displaying results, but not for producing report-ready images. I have been told (but not tried it for myself) that DOSBOX is a program that allows you to run DOS-based programs in a traditional way. The alternative for now is to use the program PF2PS to generate a postscript file (a .ps file) that you can convert to some other format such as PDF or JPG with your own choice

of program (on a Mac, you can simply double-click on a .ps file; on unix, use “convert” to do it, assuming that you have a package called “Imagemagick” installed). If you are into doing things for yourself with open source software, try using the General Mapping Tools (GMT) package with the script available at the URL just below. You will need to download and install this package in order to plot with it, obviously.

URL: neon.materials.cmu.edu/rollett/texture_subroutines/plotting_with_GMT

Note that there is also a small Fortran program called pf2GMT.f that you need in order to convert the popLA format files into a format suitable for use by the GMT script. If someone would like to convert this to c++, that would be welcome.

Objective for #1: comprehend a pole figure as a map of diffracted intensity as a function of direction with respect to sample axes. Always keep in mind that a pole figure is a display of (hemi-)spherical intensity data projected (stereologically, e.g.) onto a flat page (plane figure).

1a) Use ‘POD’ on p6 to plot the pole figures as received. There are 3 pole figures. I suggest that you start with a maximum contour value of 400, with 2 values below 1 (where 1 represents a random intensity). Explain what your reasons were for your choice of contour levels.

1b) Explain what you would expect to see in your plot if there was *no* preferred orientation (texture) in the material.

Objective for #2

Learn how to rotate a data set around the projection plane normal (or, north pole of the hemisphere, following the usual convention). Relate the result to the (statistical) sample symmetry apparent in the data (i.e. the set of 3 orthogonal mirrors expected for plane strain compression). A secondary objective is to familiarize students with the convention for specimen axes in metal processing of rolling direction (RD), transverse direction (TD), and normal direction (ND, or rolling plane normal). Numerically, we typically (although not necessarily!) assign RD//1, TD//2 and ND//3.

2) Use the ‘rotate pole figures’ (p2) to optimize the alignment of the pole figures with the specimen axes. “Optimize” means to maximize the degree to which you can reflect the data in a mirror plane perpendicular to the rolling direction (or, perpendicular to the transverse direction). The program should suggest a rotation of -4° . Try using different values and describe what you think of the result. Plot both one of your own choices (and label it) and the ‘standard’ -4° rotation result. Each time you rotate, you will generate a new version of ISGB.RPF.

Objective for #3:

Here the objective is to introduce students to the procedure for fitting generalized spherical harmonic functions to orientation data (i.e. pole figures). Although this is equivalent to calculating a Fourier transform, the details are considerably more complicated. These are the same functions used to describe electron orbital shapes! We will, however, not graph the functions themselves, or even the values of the coefficients

multiplying each function, but just use the results in terms of re-normalized pole figures. A secondary objective is to stimulate thought about what normalization means.

3) Use ‘harmonic analysis’ with cubic crystal symmetry and orthorhombic sample symmetry to perform a first analysis on the data. Plot the data that have been re-normalized from the file ISGB.FUL. Compare with the original data (ISGB.EPF) and describe the comparison in words (qualitatively). Explain, as best you can, what *normalization* means in the context of pole figures.

4a. If step 4b below does not work because ‘CUBIC.WM3’ is not present, you will have to generate this. Ask for help on this one. You can generate your own pointer matrix that connects locations in a pole figure to locations in an orientation distribution by using the appropriate option on the WIMV page, p3.

Objective for #4: to introduce students to a procedure for numerically fitting a discrete (three dimensional) orientation distribution (OD) to pole figure data. “Discrete” means that a value for the intensity of the OD is calculated at every point in 5 degree steps in Euler space. The point of this (as with the spherical harmonic calculation above) is to solve the classical texture problem. Solving this problem made Hans Bunge famous.

4b) Use ‘WIMV’ (option 4 on page 3) to calculate an orientation distribution, using ISGB.FUL as the data input, CUBIC.WM3 as the “pointer matrix” file and no sample symmetry (triclinic sample symmetry). Write down and describe the progress of the (iterative) calculation in terms of the texture index and the error value reported. Later on, we will discuss the error value and its meaning. Plot the resulting pole figures that are calculated from the OD (ISGB.WPF). Compare to the original data, best of all by combining the .WPF and the .FUL files (copy ISGB.FUL+ ISGB.WPF ISGB.CMB) and plotting them on the same page.

Objective for #5:

This is to show you how to re-organize the OD data resulting from a WIMV calculation. One can think of taking a box full of numbers and slicing it two different ways – one gives an SOD and the other a COD.

5) Convert the SOD to a COD (Conversions page). No notes are required here.

Objective for #6: use a standard tool for plotting the sections in OD data.

6a) Use SODCON to generate an OD plot: although you can run this program in command-line mode with arguments (for unix types), I suggest that you simply start it up and answer the questions as they come. The output of SODCON is a postscript file (a .ps file) that you can convert to some other format such as PDF or JPG with your own choice of program (on a Mac, you can simply double-click on a .ps file; on unix, use “convert” to do it). Once you have a result, compare it to the somewhat similar plot shown as an example in the first lecture (in the sense that the lecture example was also a rolled fcc metal). The source code (Fortran) is sodcon.f and can be found in my texture_subroutines directory on my website. You will also need psplot.txt, which is available from www.nova.edu/ocean/psplot.html. Note that I’ve also provided sod4con.f,

which can be used to plot SOD and COD files that do not have any sample symmetry (first Euler angle has range 0-360°).

Objective for #7: this is another useful step for plotting to make it easier to plot OD data, i.e. by eliminating every other section.

7) Select sections for plotting by using the “PARE” option (in p5) with the standard choice of one section each 10° (i.e. you pick out every other section in orientation space). Use the name ‘ISGB.SOS’ for the pared-down version of ISGB.SOD and ‘ISGB.COS’ for the pared-down version of ISGB.COD. Again, no notes are required, but look at the contents of the file in order to understand what the pareing accomplished.

Objective for #8: to show students how to use the plotting tools provided to graph sections from OD data.

8) Again, using POD, plot the pared-down orientation distributions. Comment on what you observe.

Objective for #9: to familiarize students with the procedure for calculating inverse pole figures and to illustrate the differences with pole figures. One way to explain the difference is to see that pole figures portray texture data from the perspective of an observer standing on sample axes: inverse pole figures, by contrast, show texture information from the perspective of an observer standing on crystal axes (and plotting the relative frequency of a certain sample direction). Both are 2D projections of 3D information.

9) Go back to the WIMV page (p3) and calculate a set of inverse pole figures. Go ahead and plot them using POD. Comment on what you observe. What is the significance of the numbers (indices) associated with each plot? What is being plotted, exactly?