ANIE: A MATHEMATICAL ALGORITHM FOR AUTOMATED INDEXING OF PLANAR DEFORMATION FEATURES IN SHOCKED QUARTZ. M.S. Huber[1], L. Ferrière[2,3], A. Losiak[1], and C. Koeberl[1,3], [1]Department of Lithospheric Research, University of Vienna, Althanstrasse 14, A-1090 Vienna, Austria (matthew.huber@univie.ac.at), [2]Department of Earth Sciences, University of Western Ontario, 1151 Richmond Street, London, ON, N6A 5B7, Canada, [3]Natural History Museum, Burgring 7, A-1010 Vienna, Austria.

Introduction: Planar deformation features (PDFs) in quartz grains are considered one of the most reliable indicators of shock-metamorphism for the confirmation of hypervelocity impact structures (see [1-5]). PDFs are regularly spaced, thin, planar, and generally oriented parallel to rational crystallographic planes, and formed at shock pressures exceeding 5-10 GPa in quartz grains [2]. Certain crystallographic planes are known to accommodate shock deformation [6], thus, suspected PDFs can be measured using a universal stage (U-stage) and indexed by comparison to known shock orientations. The manual process of converting raw measurements from the U-stage to orientations of PDFs has traditionally only been possible using a graphical method based on a Wulff (equal-angle) stereonet and a stereographic projection template [6], and can be significantly time-consuming. Manually determining the Miller-Bravais indices using the graphical method may also introduce some additional errors to the measurement. We have determined the mathematical basis for indexing PDFs and have developed an algorithm for indexing, named Automated Numerical Index Executor (ANIE), designed for use in Microsoft Excel. Automatically indexed PDF data from three samples, BOS (a meta-greywacke from the Bosumtwi impact crater), M8 (a biotite-gneiss from the Manson impact structure), and AUS (a sandstone from the Gosses Bluff impact structure), are compared to results obtained by hand (i.e., using the stereographic projection template) in order to demonstrate the veracity of our mathematical method.

Mathematical method: The mathematical method of indexing PDFs follows the same steps as are used in the graphical method [6]. Data from the U-stage are first adjusted so that the c-axis is centered on a sphere, using the law of sines for spheres to correct the inclinations and the law of cosines for spheres to correct the azimuths of each measured PDF. The angles between the PDFs are then calculated using the law of cosines for spheres. Once the angle between the PDFs is calculated, the polar angle (great circle distance between a PDF and the c-axis) is compared to the polar angles of known PDFs, and then the angle between PDFs is used to determine if the PDF sets are all oriented parallel to typical PDF crystallographic planes.

Automated Numerical Index Executor: A Microsoft Excel macro (working with Excel 2007 and later on a PC, but not on a Mac) has been produced for automated indexing of PDFs and will eventually be made available for distribution. This program is appreciably more efficient for indexing PDFs than the manual, graphical method, allowing large datasets to be indexed in a matter of seconds. The program can index any number of grains with up to 10 measured PDF planes. The program allows for control of angular error used for indexing (5º in stereographic projections used for the graphical method). Grains with a single PDF set can be excluded from measurements. Because data can be input as a full range of values, the program can be set to either index based on an average value or the full range of values. The program automatically indexes data upon command, generating a table of each individual PDF, a summary table displaying how many of each PDF are found, and graphs of the frequency percent of each crystallographic index and the frequency percent of polar angle of the poles to PDFs.

Comparison of ANIE to graphical method: The data for three samples (AUS, BOS, and M8, all containing more than 65 grains with PDFs) have been processed mathematically using the ANIE program under four sets of conditions: (1) with a 5° error and using average values from U-stage data; (2) with a 5° error and using the full range from reported U-stage data; (3) with a 6° error and using average values from U-stage data; and (4) with a 6° error and using the full range from reported U-stage data. The reason for testing the mathematical method with a 6° error was to account for the potential additional errors introduced in the graphical method. Note that all PDFs were indexed by hand using the graphical method by an experienced user (see [6] for the exact methodology and procedure). Results using ANIE with average values from U-stage data, with both 5° and 6° error, are noticeably different compared to results obtained with the graphical method. However, very similar results are found between the graphical and mathematical results for 5° error using ranges of values, and near-identical results are found when 6° error is used with ranges of values.

Sample AUS has 74 grains and 208 measured PDF sets. By hand, it was found to have 10 unindexed planes, whereas when using ANIE and average values from U-stage data, with 5° and 6° error, 49 and 38 unindexed PDF sets were found respectively. However, using the ranges of values resulted in 21 unindexed

PDFs for 5° error, but 10 unindexed PDFs in 6° error. The graphically measured polar angles for AUS were similar to those found using ANIE, though with some minor discrepancies, such as PDFs identified as being basal PDFs when plotted by hand, but unindexed using the mathematical method. This results from the angular distance between the c-axis and the PDF set being slightly above the error limit. The majority of differences between the graphical and mathematical method are the result of imprecision in the graphical method on the order of less than half a degree. Similar problems occur when the angle between PDF sets is not actually within error. For example, one grain in AUS contains 6 PDF sets, all of which were found by hand to correspond to either $\{10\bar{1}3\}$ or $\{10\bar{1}4\}$ orientation. However, using ANIE, one of the PDF sets has an angle of 47° from another set, which falls just short of the 50° angle needed for the plane to be uniquely indexed.

Regarding the sample with the fewest grains, BOS, with 145 PDF sets measured in 65 grains, only 8 unindexed PDF sets were found when processed with the graphical method. Using ANIE with 5° error, 21 PDFs are unindexed when using averages, and 9 PDFs are unindexed when using ranges of values. When using 6° error, 12 PDFs are unindexed using averages, and 6 are unindexed when using ranges of values. No major differences in the measured polar angles were found for this sample between the two methods of indexing. Note that this sample differs from the two other samples in that it contains no basal PDFs.

Finally, in the case of sample M8, 211 PDF sets were measured in 71 grains. This sample shows the largest discrepancy between the results obtained with graphical versus mathematical method. Graphically, M8 was found to have only 5 unindexed planes. Using ANIE with 5° error and with averages, 42 PDFs are unindexed, whereas using ranges of values, 16 planes are unindexed. With 6° error and with averages, 25 PDFs are unindexed, whereas using ranges of values, 12 PDFs are unindexed. The majority of the discrepancy of results between the two methods is due to the fact that data plotted for the poles of these PDFs were close to the values required for indexing, but are just outside of the error limit. A few differences can also be explained by errors in manually plotting the data.

When PDFs are indexed with ANIE using ranges of values and 6° error, there are 46 differences (of 564 PDFs evaluated) from the graphical method. Twenty-two of these differences are a result of multiple possible solutions that allow all measurements to fit within known PDF crystallographic orientations. A graphical user estimates the best fit visually (i.e., using eyes and "intuition"), while the mathematical method determines which set of Miller-Bravais indices has the lowest error and, thus is the most likely. Another twenty-two differences are from PDF sets that are close to a known PDF crystallographic orientation but that fall just outside of the defined error limit. The remaining differences in the methods result from other discrepancies between graphical versus mathematical method, such as errors in plotting data. Thus, very similar results are obtained when using the range of measured values and an error of 6°.

Conclusions: Our comparison of indexing PDF sets using the mathematical method (i.e., the ANIE program) versus the "old" graphical method reveals that the best fit between the two methods is found when using 6° error and the full ranges of values (as opposed to the average value of measurements) in the ANIE program. For the 564 PDFs evaluated in the present study, a total of 46 differences were found between indexing with the mathematical method versus the graphical method, which corresponds to a difference of ~8%. Our study suggests that the graphical method, although designed with a 5° envelope of measurement error, is closer to 6° error in reality. However, it is recommended to users to define a 5° error when using ANIE program. If a 6° error is used, the error envelopes of the PDF pole traces for some orientations will overlap. Anyone presenting PDF data indexed with the ANIE program is asked to state clearly the error used in the calculation, as well as whether the average value of measurements or the ranges of values was used for indexing.

A web-based multi-platform program using the same mathematical method as this program is presented in [7].

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