

A WEB-BASED PROGRAM FOR INDEXING PLANAR DEFORMATION FEATURES IN QUARTZ.

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Introduction: Planar deformation features (PDFs) in quartz grains are the most commonly used diagnostic features of hypervelocity impact structures. PDFs are straight, parallel sets of planes of amorphous material that are less than 2 μm wide and spaced 2-10 μm apart [e.g., 1,2]. Specific combinations of PDF orientations provide information on the peak shock pressure recorded by samples, within the range of ~5 to 35 GPa [e.g., 1,3].

The determination of PDF orientations is usually done using a universal-stage (U-stage)-equipped petrographic microscope, followed by indexing measurements to crystallographic orientations in relation to the c-axis [e.g., 4]. Currently, indexing of PDFs is done manually using a Wulff net and a stereonet and following a strict procedure [4], which is both time consuming and error-prone. Because of limitations of the manual indexing method, only information about polar angles and Miller-Bravais indices of PDFs were recorded and used in previous studies. The angular relationships between PDF sets were in most cases ignored. Here, we present a web-based program for indexing PDFs that also allows for analysis of azimuthal angles between PDFs in a given quartz grain. The study of combinations of PDF orientations can be useful for a better understanding of impact processes (see companion abstract [5]). Our program is available from: <http://lithosphere.univie.ac.at/impactresearch/>. The source code (i.e., implementation in Java programming language) will be made available.

Program description: *Input data:* Data input is in the form of a .csv file (comma-delimited) (an example of an input file with detailed instructions is available online together with our program). Every line of the input file is a set of numbers describing a single grain. The measured angles can be entered as a range of values (minimum and maximum measured values; “min-max”). There are no limitations on the number of grains in the dataset, or on the number of determined features per grain. If there is an error in the input data (e.g., inappropriate number of PDFs in relation to number of input columns), an error message will be displayed.

Options: *Error handling:* There are three modes of error handling for the dataset: (1) “Average”: the algorithm calculates the average value of the entire measured interval, and indexing is performed using this “av-

erage value”. (2) “Min-max”: values from the entire interval are considered. Using this setting, a PDF will be indexed if any part of the measured interval matches a known crystallographic orientation. (3) “Manual equivalent” (will be added soon to the program): this approach is very similar to the “min-max” option, but with the c-axis calculated as an average point and PDFs indexed using the range of measured values. This approach is closest to manual indexing with the stereonet.

Error level: It is possible to specify the desired error level used in the calculation. However, it is strongly recommended to use a 5° error, as this is the value used in previous stereographic projection templates [1, 4].

Processing: First, the program “rotates” a grain to have the c-axis coincide with the central axis of the sphere used for indexing (i.e., the c-axis’ inclination angle becomes 90°) and corresponding transformations are applied to all planar features determined in this grain. Such a transformation is used to simplify subsequent calculations.

As mentioned above, to properly index a PDF set, two pieces of information are needed: (1) the polar angle between the c-axis and the measured feature, and (2) the azimuthal angle between the a-axis and a PDF set. As information about the a-axis is not available, we use an approach that does not require deriving its position: Information on the azimuthal relationship of at least two PDFs is sufficient to index them (when neither is a basal PDF).

The algorithm used for the indexing of PDFs consists of four steps. First, measured planar features are indexed using only polar angle data. This eliminates some sets from further computation when no known PDF orientation can be assigned. For the remaining features, one or more known PDF orientations are assigned. Then, all possible combinations of feature-index pairs (indices assigned based on their polar angle) are organized into configurations that represent all possible solutions for a given grain. These solutions are verified to check if their mutual azimuthal relationships are consistent. Inconsistent configurations are excluded from further analysis. Finally, the total error (i.e., the sum of all angular differences between known PDFs orientations and determined features orientations) is calculated. The combination with the lowest error is chosen.

Output: Results are available in a variety of formats, including .csv or .jpg files. The results can be presented as a table with input and output data together, or as a set of graphics and tables similar to those commonly presented in literature [e.g., 2,4]. Additionally, a detailed log of performed computations is available for each grain, including detailed information on polar angle, compared azimuthal angles, and all possible combinations of PDF indices.

Comparison with the manual method: To test our program we compared the program results with those obtained with the manual (graphical) method. Here we present the evaluation for AUS sample previously analyzed by [4] (Table 1). Results from the “manual” and “min-max” methods (both with 5° error) are almost identical. Differences in absolute frequency percent are less than 3%. This difference is too small to influence inferences about shock pressure. The program, using the “min-max” and 5° error settings, results in a slightly higher number of unindexed PDFs. In about 90% of the cases, discrepancies are due to the fact that a human operator is more prone to index a feature that is near the boundary, while the program is strict. In a few cases, the human operator and the program choose different Miller-Bravais indices for certain grains, e.g., when two PDF sets can be indexed either as $\{10\bar{1}1\}$ & $\{22\bar{4}1\}$ or as $\{11\bar{2}2\}$ & $\{40\bar{4}1\}$ orientations. Due to the lack of a-axis data, it is impossible to differentiate between these two combinations, and the program chooses the option with the smallest cumulative error.

When comparing results obtained using different options of the program, it is obvious that percentage of unindexed features strongly depends on the error handling method used. Applying the “average” option with a 5° error results in a significant increase in the proportion of unindexed sets (see Table 1). However, no mat-

ter which method is used, the relative abundance of the different indexed PDFs do not change significantly.

Choosing the best program options: None of the options is perfect; the “min-max” option minimizes the number of unindexed PDFs. It is also the option most consistent with the manual method. However, especially if the measurement error is large, in particular for the c-axis, it allows almost all measured features to be indexed, including those that are not PDFs. Additionally, because every measured feature and c-axis has a different individual range of angular values, the cumulative error changes for every feature in every grain. Thus, the assigned 5° error should be treated as a minimum error used for indexing. The error may not only be higher than the assigned 5°, but also is highly variable within the dataset. The use of the “average” option results in a significant increase in the number of unindexed features (Table 1), but the error rate remains the same for the entire dataset.

Conclusion: It is our hope that the web-based program will become a valuable tool for PDF indexing, as it saves time, significantly decreases the number of errors, and makes the entire process much more predictable and comparable among different operators. Note that an Excel version of this program is presented in [6].

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References: [1] Stöffler D. and Langenhorst F. (1994) *Meteoritics & Planet. Sci.*, 29, 155–181. [2] Grieve R.A.F. et al. (1996) *Meteoritics & Planet. Sci.*, 31, 6–35. [3] Barker L.M. et al. (1993) *High-pressure Shock Compression of Solids*, Springer, 43–74. [4] Ferrière L. et al. (2009) *Meteoritics & Planet. Sci.*, 44, 925–940. [5] Losiak A. et al. (2011), *LPSC XLII* (this volume). [6] Huber M.S. et al. (2011), *LPSC XLII* (this volume).

Table 1. Comparison of results as obtained with the manual method vs. our web-based program (using two different settings and assigned 5° error) for AUS sample. Percentages are calculated using absolute frequency including unindexed features [see 4].

| Miller-Bravais indices | | (0001) | {10-14} | {10-13} | {10-12} | {10-11} | {10-10} | {11-22} | {11-21} | {21-31} | {51-61} | {11-20} | {22-41} | {31-41} | {40-41} | {51-60} | UnX |
|------------------------|----|--------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|-----|
| manual | no | 59 | 36 | 74 | 2 | 10 | 1 | 5 | 0 | 3 | 1 | 1 | 0 | 3 | 2 | 1 | 10 |
| | % | 28% | 17% | 36% | 1% | 5% | 0% | 2% | 0% | 1% | 0% | 0% | 0% | 1% | 1% | 0% | 5% |
| min-max | no | 59 | 38 | 69 | 2 | 12 | 0 | 2 | 1 | 2 | 2 | 2 | 1 | 3 | 1 | 0 | 14 |
| | % | 28% | 18% | 33% | 1% | 6% | 0% | 1% | 0% | 1% | 1% | 1% | 0% | 1% | 0% | 0% | 7% |
| average | no | 53 | 28 | 60 | 2 | 8 | 0 | 2 | 0 | 2 | 2 | 2 | 1 | 3 | 1 | 0 | 44 |
| | % | 25% | 13% | 29% | 1% | 4% | 0% | 1% | 0% | 1% | 1% | 1% | 0% | 1% | 0% | 0% | 21% |