Description of the program for indexing PDFs

To evaluate the data generated here, and to provide a tool for the community, we developed a web-based program for indexing PDFs. The program is designed to evaluate data from U-stage measurements to quickly assess the relationships between the c-axis and the various PDFs within a given grain. This evaluation is then compared to angles of known, typical, PDFs in quartz (as defined in Ferrière et al. 2009, and references therein). The presented approach simplifies the mathematical calculations required for indexing and allows removing errors related to some distortions that may be induced when representing information derived from a three-dimensional (3D) crystal on a 2D Wulff stereonet.

General description

To properly index PDF sets, two pieces of information are mandatory: 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 the a-axis cannot be determined with the U-stage (although this is possible with an Electron Back-Scatter Diffraction-system), an approximation is typically used, namely the angular relationship between two (or more) sets of non-basal PDFs are compared, which can then be used to determine the orientation of the a-axis.

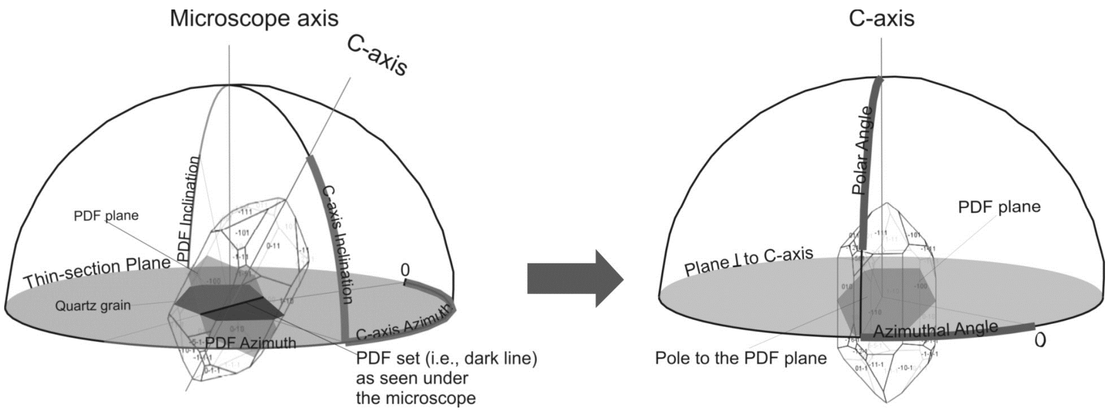

Figure 1. Illustration of the process of transformation of the coordinates from "microscope-oriented" (left) to "crystal structure-oriented" (right) coordinates. To avoid confusion, after transformation to the "crystal structure-oriented" coordinates, the PDF (or the c-axis) azimuth becomes an "azimuthal angle", and the inclination angle a "polar angle".

For each quartz grain, U-stage measurements provide angular coordinates (azimuth and inclination) of the c-axis and of all visible PDFs. The program is based on a set of equations that allow the transformation of the coordinates for each grain, from microscope-oriented coordinates to crystal structure-oriented coordinates (Figure 1). The program essentially "rotates" a grain to have the c-axis coincide with the central axis of the sphere used for the indexing (i.e., the c-axis' inclination angle becomes 90º) and corresponding transformations are applied to all planar features determined in the given grain (Figure 1), mathematically mimicking the manual process that would be performed with the Wulff stereonet.

The following equations were used to transform the coordinates systems, related to the cosine and sine rules of a spherical triangle:

$$(1)\ \sin(\delta) = \sin(a)*\sin(\varphi)+\cos(a)*\cos(\varphi)*\cos(A)$$

$$(2)\ \sin(H) = -\sin(A)*\cos(a)/\cos(\delta)$$

$$(3)\ \cos(H) = [\sin(a)-\sin(\delta)*\sin(\varphi)]/\cos(\delta)*\cos(\varphi)$$

Where δ is 90° minus the polar angle of the measured planar feature; a is the measured inclination of the planar feature, φ is the measured inclination of the c-axis, A is the azimuthal distance between the c-axis and the planar feature, and H is the azimuthal angle of the planar feature. After performing the transformation described above on the measured PDFs, the relative angular relationships of the PDFs within a grain can be read directly from their coordinates.

The details of indexing algorithm

The algorithm is designed to find if relative angular relationships between measured features are consistent with the model angular relationships of PDFs as described by Ferrière et al. (2009). This operation consists of four steps (Figure 2). First, the measured planar features are indexed using only the polar angle data by comparing calculated values of polar angles with values of polar angles of known PDFs. If no typical orientation corresponds to a known PDF for a calculated polar angle, the measured planar feature is rejected and not used for further computation, and marked as "UNX". For all of the remaining features, one or more known PDF classifications are assigned (this is called here the initial classification). If a single planar feature was measured within a given grain, or also in the case that only one other planar feature was indexed as a set of basal

PDF (0001) based on its polar angle, the program will already achieve the calculation for this grain at this step. The final display will then indicate that this set of PDF was indexed only based on its polar angle.

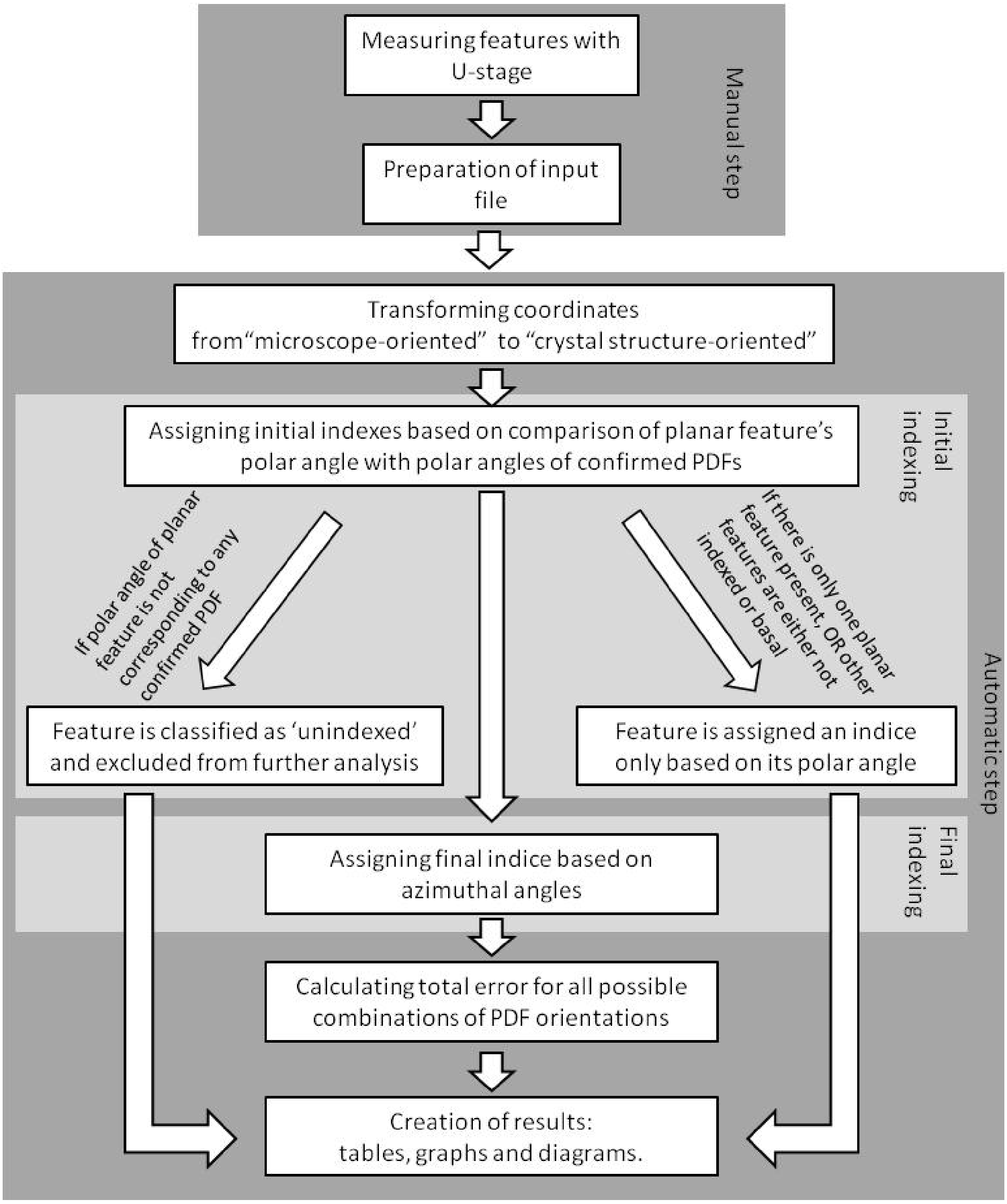

Figure 2. Flowchart showing the algorithm of the web-based PDF indexing program presented in this paper.

During the second step, the program compares the angle between measured sets of PDFs in the grain to known typical PDFs. The expected classification of measured PDFs based on the polar angle (step 1) is used to generate the possible and expected azimuthal angles between two sets of PDFs. For example, if two measured features were classified as $\{10\bar{1}3\}$ and $\{10\bar{1}2\}$ orientations in the first step, the only possible azimuthal differences between them are: 60°, 120°, 180°, 240°, and 300° (± error size). If the program finds that the measurements do not fall within these expectations, then, only one set of PDF (i.e., the one with the smaller polar angle error) is indexed, while the other set of PDF is considered to be unindexed. In many cases, more than one combination of indexed PDFs is possible; e.g., some PDFs can be indexed either as $\{10\bar{1}3\}$ & $\{10\bar{1}3\}$ orientations or as $\{10\bar{1}3\}$ & $\{10\bar{1}4\}$ orientations. In this specific case, the program takes into account all possible combinations of PDF sets.

The third step of the algorithm consists in the calculation of the errors for each of the possible classifications by summing up all angular differences between known PDF orientations and measured orientations of PDFs.

Finally, the combination of PDF sets with the lowest error is chosen as the proper indexed orientation; however, all other possible combinations are also listed in the detailed results table.

Input file

For the data input, the user has the choice between a .csv file (coma-delimited) or a .txt file. An example of an input file, with detailed instructions, is available online together with our program. Each line of the input file corresponds to a set of numbers describing a single quartz grain (Figure 3). The measured angular data can be entered as a range of values (minimum and maximum measured values; “min-max”). If the c-axis was determined to be vertical during measurements it should be converted manually to the horizontal position (e.g., by "subtracting" 90º from the inclination and by correcting the azimuth by 180º; or the easiest is to change W to E (or E to W) and to "subtract" 90º from the inclination; the corresponding PDFs measurements should, in any case, be altered). There are no limitations on the total number of grains in the dataset, or on the number of features/PDFs per grain. If there is an error in the input data (e.g., an inappropriate number of PDFs in relation to the number of input columns), an error message describing the type of problem will be displayed.

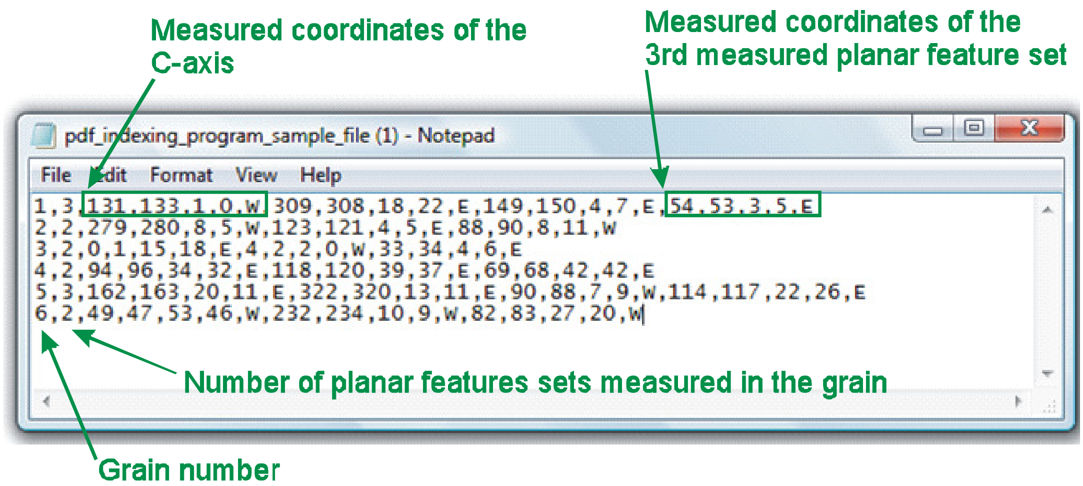

Figure 3. Example of the input file.

Calculation options: “Error rate” and “Error handling method”

In addition, two different types of options are available for the calculation, the so-called "error handling" and "error level". “Error handling” specifies how the program interprets data input with a range of values for the c-axis and the sets of PDFs in a given grain. There are two modes of "error handling" for the dataset: 1) “Average”: the algorithm calculates the average value of the entire measured interval, and the indexing is performed using this “average value”; 2) “Min-max”: values from the entire interval are considered in the subsequent computations. Using this second setting, a PDF will be indexed if any part of the measured interval matches a known, typical, PDF orientation. "Error level" describes the distance from a classified PDF orientation that will still be counted as properly indexed. It is recommended to use a 5° error level, as it is thought to be a level of error inherent to the optical microscopic measurements and have been typically used when plotted manually with the stereographic projection templates (e.g., Engelhardt and Bertsch 1969, Stöffler and Langenhorst 1994, Ferrière et al. 2009).

The comparison between the produced results using the different "error handling" options is shown in Figure 4 and in Table 1. Table 1 shows that, no matter which method is used, the relative abundance of the different indexed PDF orientations does not change significantly. Additionally, the larger the error level, the more similar are results of the computing using different error handling options. Increasing the "error level" results in a significant decrease of the number of unindexed PDFs. For example, when applying an “average setting" and changing the "error level" from 3°, 5°, to 7°, the number of unindexed PDFs decreases from 43 % through 19 % to only 9 % (see Table 1). Furthermore, the proportion of unindexed features/PDFs strongly depends on the error handling method that is used for the calculation; for example, the proportion of unindexed features will increase from 5 % to 19 % just by changing the error handling method used, from the “Min-max” to the “Average” method. Results obtained using the "Min-max" method with a 5° error level and the "Average" method with a 7° error level are usually very similar. This suggests that the average uncertainty on the measurements in this study using the U-stage is at least of 4°.

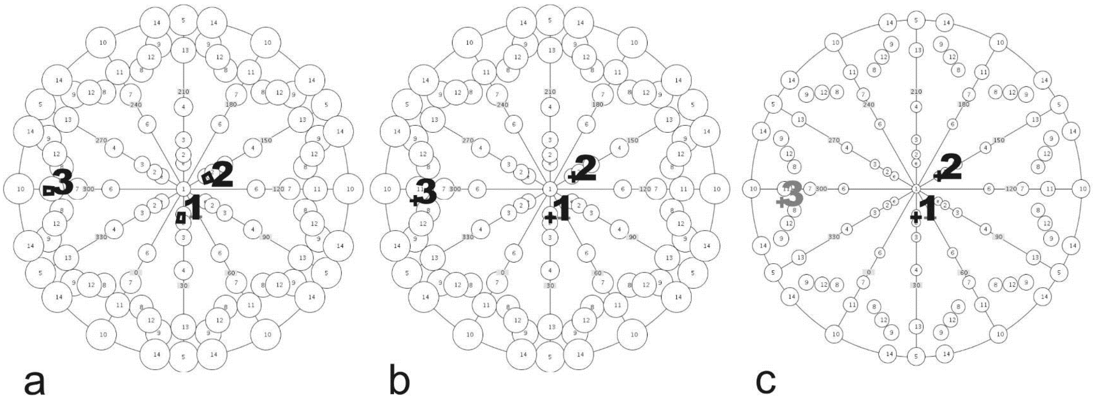

Figure 4. Stereographic projection templates (after Ferrière et al. 2009) with the c-axis in the center and the circles representing the positions of the most common poles to PDF planes. These plots show a comparison of the resulting diagrams for a quartz grain with three planar features (marked as 1, 2, and 3, respectively) as produced using different program parameters: a) using the “min-max” method and a 5° error, b) using the “average” method and a 5° error, and c) using the “average” method and a 3° error. Note that in c) feature “3” is unindexed.

Table 1. Comparison of results for a sample from the Bosumtwi crater (sample BOS-3; data previously published in Ferrière et al. 2009) indexed with our web-based program, using the two available error handling methods; i.e., the "min-max" method (the algorithm uses values from the entire interval) and the "average" method (the algorithm calculates the average value of the entire measured interval, and the indexing is performed using this “average value”) and three different error rates (distance from a classified PDF orientation that will still be counted as properly indexed), 3°, 5°, and 7°. Data is given here as number of PDFs.

Method	Error rate	(0001)	$\{10\bar{1}4\}$	$\{10\bar{1}3\}$	$\{10\bar{1}2\}$	$\{11\bar{2}2\}$	$\{10\bar{1}1\}$	$\{11\bar{2}1\}$	$\{21\bar{3}1\}$	$\{22\bar{4}1\}$	$\{31\bar{4}1\}$	$\{40\bar{4}1\}$	$\{51\bar{6}1\}$	$\{10\bar{1}0\}$	$\{11\bar{2}0\}$	$\{51\bar{6}0\}$	Un-indexed
min-max	3°	0	28	51	28	2	6	2	2	6	3	1	3	1	1	0	11
min-max	5°	0	29	53	29	2	8	2	2	7	3	1	2	1	1	0	5
min-max	7°	0	30	54	30	1	9	2	3	7	4	0	1	1	1	0	2
average	3°	0	27	37	20	2	4	0	1	2	4	3	1	1	0	0	43
average	5°	0	30	45	24	2	7	1	4	5	3	2	2	1	0	0	19
average	7°	0	30	50	28	2	7	2	5	6	2	1	1	1	1	0	9

Output

Results can be exported as csv and/or jpg files. The results are presented as follows: 1) a main result table with the best possible combination of PDFs orientations for each grain, 2) a detailed results table with input and output data together with all possible combinations of PDFs orientations, 3) aggregated result tables, 4) diagrams for all measured PDFs and also for each grain. The presentation of the results is similar to what is commonly presented in the literature (e.g., Grieve et al. 1996, Ferrière et al. 2009). Additionally, a detailed log of the performed computations is available for each single grains, including detailed information on polar angle, compared azimuthal angles, and all possible combinations of PDF indices.

Comparison between the "manual” and "automatic” methods for PDF indexing

To test and validate our program we compared the results generated by our program (using the "Min-max" method and 5° error level) with those obtained with the manual (graphical) method. For this purpose, we have used data obtained from five samples from different impact structures (see Table 2).

Table 2. Comparison between manually (by L. Ferrière) and automatically indexed PDFs (using our web-based program) from five samples from five different impact structures (from: [1]Ferrière et al. 2009, [2]Ferrière et al. 2011, [3]Ferrière et al. 2010). Data is given here as number of PDFs.

Crater, lithology	Method	(0001)	$\{10\bar{1}4\}$	$\{10\bar{1}3\}$	$\{10\bar{1}2\}$	$\{11\bar{2}2\}$	$\{10\bar{1}1\}$	$\{11\bar{2}1\}$	$\{21\bar{3}1\}$	$\{22\bar{4}1\}$	$\{31\bar{4}1\}$	$\{40\bar{4}1\}$	$\{51\bar{6}1\}$	$\{10\bar{1}0\}$	$\{11\bar{2}0\}$	$\{51\bar{6}0\}$	Un-indexed	Total
Gosses Bluff[1], sandstone	program	59	39	70	2	2	13	1	2	2	2	1	2	1	0	1	11	208
	manual	59	110		2	5	10	0	3	0	3	2	1	1	1	1	10	208
Bosumtwi[1], meta-greywacke	program	0	29	53	29	2	8	2	2	7	3	1	2	1	1	0	5	145
	manual	0	81		28	4	5	2	3	6	3	2	1	1	1	0	8	145
Manson[1], biotite-gneiss	program	4	46	117	4	2	15	0	5	10	2	1	0	0	0	1	5	212
	manual	4	166		2	3	13	0	3	10	2	2	1	0	0	1	5	212
Luizi[2], sandstone	program	12	45	116	8	0	0	0	0	1	0	0	0	0	0	0	3	185
	manual	12	163		5	0	0	0	0	0	0	0	0	0	0	0	5	185
Keurusselkä[3], ortho-gneiss	program	0	61	66	1	0	0	0	0	0	0	0	0	0	0	0	1	129
	manual	0	124		1	0	0	0	0	0	0	0	0	0	0	0	4	129

The results obtained using the program (“automatic”) and the manual method are almost identical. The differences in absolute frequency percentage are negligible and too insignificant to influence inferences on the shock pressure during impact cratering (e.g., Stöffler and Langenhorst 1994). These minor discrepancies between the manual and automatic methods can have several origins. First, a human operator is more prone to index a feature that is near the boundary (i.e., almost indexed), while the program is very strict. Second, the human operator and the program can choose different Miller-Bravais indices for certain grains, for example, when two PDF sets can be indexed either as $\{10\bar{1}1\}$ & $\{22\bar{4}1\}$ orientations or as $\{11\bar{2}2\}$ & $\{40\bar{4}1\}$ orientations. Due to the lack of a-axis data, it is in fact impossible to differentiate between these two combinations, and the program will choose the option with the smallest cumulative error. Third, it seems that the projection that is used for the manual indexing tends to over-index PDFs with low polar angles. In addition, the manual method does not take into account the full measured interval for the c-axis orientation (Ferrière et al. 2009), while our program does. Finally, even the most accurate and precise human operator will make mistakes due to the wearisome nature of the manual indexing method. The comparison of the PDFs indexed by hand and using the program (Tab. 2) shows that the automatic method of indexing gives very comparable results to the ones obtained by an experienced researcher (L. F.); however, based on the nature of the automated algorithm, the results are more precise and reproducible.

The program that was developed for this study is available online at: www.MeteorImpactOnEarth.com/ustage/program.html.

The source code (i.e., implementation in Java programming language) is also available upon request from the authors.

In case of any questions or noticed errors please contact Ania Losiak (anna.losiak@univie.ac.at or ann.losiak@gmail.com).

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