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Computer Analysis of Zircon Morphology Data

(A contribution to geometrics)

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ABSTRACT

Analysis of zircon morphology is a useful petrologic tool. However, the calculations required for morphologic description and comparison are laborious and time consuming if done by hand. In order to facilitate these studies, automatic data handling techniques have been devised to process zircon morphology data with IBM 360 Model 40 electronic computers. Observations of crystal length and width are used to calculate a series of statistics, including means of length and width, standard deviations of the means of length and width, and the linear regression coefficients of the relation, crystal axial ratios vs. crystal length.

A systematic record format is described which allows for observations of faceting, degree of rounding, and color. Observations made on the prescribed record forms can be sent to a computer center along with a description of the comparisons desired on coded parameter card forms and the calculations can be made without further involvement by the experimenter.

Sample statistics can be calculated for one or a set of the faceting, rounding, and color subclasses to test for differences in shape within a given sample, or to compare shape for a given subclass between samples from different rocks. These calculations can be used in efforts to distinguish zircon of metasomatic granitic rocks from plutons of magmatic origin, as well as correlation of comagmatic igneous plutons.

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INTRODUCTION

The purpose of this paper is to present a time-saving method of statistically analyzing crystal morphology of accessory zircons.

Studies of zircon morphology can be useful in distinguishing meta-igneous rocks from metasedimentary gneisses, as well as in distinguishing comagmatic igneous bodies from those of different magma sources. Numerous recent papers have stressed the usefulness of zircon morphology studies in distinguishing these rock forming processes (Kalsbeek and Zwart, 1967; Kalsbeek, 1965 and 1964, Spotts, 1962). Zircon studies have a great advantage over other petrologic methods; they are inexpensive, simple, and relatively free of bias.

ZIRCON SEPARATION

The separation of zircon from disaggregated rock samples takes advantage of the high specific gravity and low magnetic susceptibility of the mineral. First, the grain size distribution of zircon should be roughly determined by thin-section study. Then, the rock sample is crushed to pass through a screen of mesh size just larger than the coarsest zircon expected. The size fraction which passes the coarse screen and remains on a 325 mesh screen is then poured into a separatory funnel filled with methylene iodide, S. G. 3.325. The rock forming minerals less dense than methylene iodide will float; zircon, most of the accessory minerals, and some dark minerals will sink. The heavy fraction is tapped out of the bottom of the separatory funnel into a filter. The light fraction is similarly recovered in a separate filter. After the heavy fraction is washed with acetone and dried, a hand magnet is used to remove highly magnetic minerals, such as magnetite.

The less magnetic portion of the heavy fraction is then passed through a Frantz Isodynamic Separator under successively increased amperage until approximately 1.5 amps is reached. The fraction which follows the less magnetic track at 1.5 amps should contain zircon, and pyrite, rutile, apatite, or other minerals of low magnetic susceptibility. By reversing the "back slope" to 2° forward slope on the Frantz track and reducing the "side slope" to 10°, the rutile can be taken off at the front collecting pan and zircon at the rear. By leaching the sample in hot HNO₃, the apatite and sulfides can be removed. After leaching, the residuum should be virtually pure zircon. This residuum should be carefully washed with water, then acetone, and dried in preparation for mounting and measurement.

MOUNTING FOR EXAMINATION

In preparing the zircon for measurement and description, it is convenient to make semi-permanent grain mounts on microscope slides. The mounting media should have a relatively high index of refraction, near that of zircon. A near, but not exact, match of the refractive index of the medium with that of zircon limits the refraction shadow at grain boundaries and allows more accurate measurement and description of the grains. Hyrax is a convenient mounting media having a refractive index of 1.823 near that of

zircon. Hyrax can be dissolved with xylene if recovery of the grains for other analyses is desired.

MEASUREMENT AND DESCRIPTION

The microscope slide is placed in a mechanical stage on a petrographic microscope. The magnified image of the grains is reflected down on a measuring surface by means of an objective drawing lens system such as that produced by Leitz. A convenient measuring surface is a piece of frosted mylar on graph paper. As grains in a field of view are measured, they can be checked off on the mylar using a pen with water soluble ink. The soluble ink marks are then wiped clean for measurement of the next field of view.

The length and width of the projected image of the crystals is measured with a ruler and recorded. Concurrent observation can be made of color, degree of rounding, fracturing, etc.

Figure 1 has proven to be a convenient form on which to record these observations and measurements. When the data are systematically recorded in this fashion, they can be readily adapted to computer analysis. The column numbers refer to columns on IBM 80 series punch cards as an aid to key punch operators in transcribing the data.

ANALYSIS OF MORPHOLOGY DATA

Standard methods of crystal morphometric analysis include calculation of mean length, standard deviation of length measurements, mean width, standard deviation of width measurements, mean axial ratio, the regression equation for width vs. length, and the correlation coefficient for the regression equation of width vs. length. The statistics are highly useful for comparison between zircon samples; however, they are very time consuming to compute. The hand calculation of the regression equation for a sample size of several hundred grains may easily require an entire afternoon. On an IBM 360 Model 40, electronic computer, the calculation takes less than 30 seconds. The measurements can automatically be converted from the arbitrary measuring units to micron units using a scale factor.

Additionally, the statistics: the regression equation of axial ratio vs. length, and the regression equation of axial ratio vs. volume can be quickly calculated.

A program for calculation of these statistics on IBM system 360 Model 40 electronic computers has been written by Hedberg and is available without charge by writing the Computer Center, University of Idaho, Moscow, Idaho.

The geologist can take advantage of this time and labor-saving method without having to learn computer languages, but he must provide the computer operator with certain procedural assistance and information. First, the measurements must be tabulated in a consistent and legible manner such as Figure 1.

Using dittoed copies of this form, it is a simple matter to record measurements as well as crystal habit, color, etc.

ZIRCON ANALYSIS

Magnification =
1 unit = Microns

Sample No.	Run No.	Crystal Form			Color	Width	Length	Ratio w/l	Obs. No.
		Roundness		Xtl faces					
		01 -	00 0%						
		02 +	01 1-20%						
03 brkn	02 20-90%	03	04	05	01 Char				
			03 90-100%		02 Brn				
					03 Blk				
					04 Pink				
					05 Hyacinth				
Col No. 1-8	9-10	11-12	13-14	15-16	17-18	19-22	24-26	29-30	76-80
									1
									2
									3
									4
									5
									6
									7
									8
									9
									10

Figure 1. Data Record Format

Figure 2

COMPUTER SERVICE REQUEST

Crystal Morphology

Investigator _____
Affiliation _____
Telephone _____ Date of Request _____
Estimated Completion Date _____

Set 1

Scale Factor

No. of obs.

Comparisons Desired

_____ vs. _____

_____ vs. _____

_____ vs. _____

Set 2

Scale Factor

No. of obs.

Comparisons Desired

_____ vs. _____

_____ vs. _____

_____ vs. _____

Set 3

Scale Factor

No. of obs.

Comparisons
Desired

_____ vs. _____

_____ vs. _____

_____ vs. _____

Second, the geologist must decide what comparisons he wishes to make. The comparisons desired will determine what statistics must be calculated. For example, he may decide to compare the means of length between two zircon samples. In such a case, the mean lengths and standard deviations of length must be calculated for each sample. After deciding what comparisons are desired, he should fill out a form similar to one shown in Figure 2. This form tells the computer operator what statistics he must calculate and what scale factor must be used to convert the data from arbitrary measurement units to microns.

Third, the researcher must be able to code his data and the parameter cards necessary to receive the desired statistics. The work load of computer centers is such that in order for the researcher to get his job done quickly and efficiently he should complete the control cards himself. Then, he must submit the completed forms to the computer center to be run on the specific program. Generally, in a couple of hours he then can have the output back from the computing center.

In the appendix is a write-up of the generalized Multiple Regression Analysis Program for use on IBM System 360 Model 40 computers. Also, a form for coding the parameter cards is provided. This will give the researcher sufficient information to code his problem for this program.

Two examples are included that relate to the specific problem of analyzing zircon morphology. These examples can be used as guidelines in writing up the parameter cards.

In these examples, a constant is used to convert the arbitrary measuring units into microns. This constant or scale factor is multiplied times each observation to make the conversion. The transformation card is used to calculate the axial ratio. A transformation card also could be used to calculate crystal volume or any other descriptive statistic desired by coding the desired transformations and making appropriate changes in the parameter card as indicated in the write-up.

SUMMARY

Zircon morphology comparisons are useful in petrologic studies. The separation of zircon and sample preparation is relatively simple and inexpensive. Measurement of crystal length and width can be easily done using a projected image and a ruler. The observation and measurements are recorded on a set data format to facilitate subsequent automatic data handling.

The desired comparisons are listed on a dittoed form. These forms can then be sent to a computer center for the necessary calculations. The program for these calculations is available from the Computer Center of the University of Idaho, Moscow, Idaho.

The required parameter cards are also coded on a dittoed form such as that one shown in Figures 3, 4, and 5 of the Appendix.

REFERENCES CITED

Kalsbeek, Feiko, 1964, Zircons from some metamorphic rocks in the Stavenger area (southern Norway): Norsk Geologisk Tidsskrift, vol. 44, pt. 1, p. 11 - 17.

_____, 1965, on the origin of some banded amphibolites and gneisses in the Belledonne Massif (French Alps): N. Jb. Miner. Abh., vol. 102, no. 2, p. 177-188.

_____, and Zwart, H. J., 1967, Zircons from some gneisses and granites in the Central and Eastern Pyrenees: Geologic on Mijnbouw, vol. 46, no. 1, p. 457-466.

Spotts, John H., 1962, Zircon and other accessory minerals, Coast Range batholith, California: Geol. Soc. America Bulletin, vol. 73, no. 10, p. 1221-1240.

Figure 3

PARAMETER CARDS FOR REGRESSION

1. // J O B _ _ _ _ _
2. RESIDUALS REQUESTED? YES _____ NO _____
3. // EXEC MULTREG R
4. _ _ _ _ _ (I D card)
5. 0 3 0 2 - 0 2 0 1 (col. 25) (parameter card)
 (#obs)
6. 0 7 0 2 0 3 0 2 0 9 0 1 0 1 0 1 (transformation card)
7. _ _ _ _ _ (scale factor)
- 8.* (T _ _ , F 5 . 0 , T 1 9 , F 5 . 0 , T 2 4 , F 5 . 0)
9. (data cards)
10. / *
11. 1 &

* On format card give beginning column of independent variable.

19 (width) or 24 (length)

Figure 4

EXAMPLE 1

PARAMETER CARDS FOR REGRESSION

1. / / JOB 9999234 REGRESSION BY IOER.
2. RESIDUALS REQUESTED? YES X NO _____
3. / / EXEC MULTREGR
4. WIDTH TO RATIO SCALE FACTOR = 1000 (I D card)
5. 030200780201
 (# obs) (col. $\frac{1}{25}$) (parameter card)
6. 0702030209010101
 (transformation card)
7. 1000. _ _
 (scale factor)
- 8.* (T19, F5.0, T19, F5.0, T24, F5.0)
9. (data cards)
10. / *
11. / &

* On format card give beginning column of independent variable.

19 (width) or 24 (length)

PARAMETER CARDS FOR REGRESSION

1. / / I O B 9 9 9 9 2 3 4 R E G R E S S I O N # 2 I O E R .
2. RESIDUALS REQUESTED? YES _____ NO X
3. / / E X E C M U L T R E G R
4. L E N G T H T O R A T I O , S C A L E = . 0 5 0 (I D card)
5. 0 3 0 2 0 1 0 3 0 2 0 1 (parameter card)
(# obs) (col. 0 25)
6. 0 7 0 2 0 3 0 2 0 9 0 1 0 1 0 1 (transformation card)
7. . 0 5 0 _ _ (scale factor)
- 8.* (T 2 4 , F 5 . 0 , T 1 9 , F 5 . 0 , T 2 4 , F 5 . 0)
9. (data cards)
10. / *
11. / &

* On format card give beginning column of independent variable.

19 (width) or 24 (length)

(MULTREGR)

THIS PROGRAM PERFORMS A STEP-WISE REGRESSION ANALYSIS ON UP TO 9999 SETS OF OBSERVATIONS ON ONE DEPENDENT VARIABLE AND UP TO 57 EXPLANATORY VARIABLES. THE PROGRAM ALLOWS FOR ELEVEN TYPES OF ALGEBRAIC TRANSFORMATIONS OF ORIGINAL DATA. OUTPUT CONSISTS OF MEANS, STANDARD DEVIATIONS, SIMPLE CORRELATION COEFFICIENTS, AND STEP-WISE RESULTS. STEPWISE RESULTS CONSIST OF THE STANDARD ERROR OF ESTIMATE, THE MULTIPLE CORRELATION COEFFICIENT, F, CONSTANT TERM, AND REGRESSION COEFFICIENTS AND THEIR STANDARD DEVIATIONS, STUDENT'S T'S AND BETA COEFFICIENTS. OUTPUT OF RESIDUALS IS OPTIONAL.

1. THE NUMBER OF VARIABLES IS LIMITED TO ONE DEPENDENT AND 57 EXPLANATORY. THE DEPENDENT VARIABLE IS THE VARIABLE ON THE LEFT-HAND SIDE OF THE EQUAL SIGN OF THE REGRESSION EQUATION. EXPLANATORY VARIABLES ARE THOSE ON THE RIGHT-HAND SIDE OF THE EQUAL SIGN.

2. THE NUMBER OF OBSERVATIONS IS LIMITED TO 2,000 WHEN THE PRINTING OF RESIDUALS IS REQUESTED. OTHERWISE, THE NUMBER OF OBSERVATIONS IS LIMITED TO 9999.

3. THE NUMBER OF OBSERVATIONS MUST EXCEED THE NUMBER OF EXPLANATORY VARIABLES BY AT LEAST 2.

4. THE SPECIFIED F LEVEL OF INCOMING VARIABLES MUST NOT BE LESS THAN THE SPECIFIED F LEVEL FOR OUTGOING VARIABLES.

1. JOB CARD

COLS 1 - 72 // JOB XXXXXXXX (PROJECT NAME OR OTHER ID)
WHERE XXXXXXXX IS THE JOB NUMBER
ASSIGNED BY THE COMPUTER CENTER.

2. CONTROL DECK FOR RESIDUALS (OPTIONAL)
IF RESIDUALS ARE REQUESTED GET THIS DECK FROM THE
COMPUTER CENTER IT WILL LOOK LIKE THIS:

```
// VOL SYSOO8, UOUT
// DLAB 'REGRESSION INPUT DATA
//          0001,68010,68010,'
// XTENT 1,000,000001000,000003009,'111112',SYSOO8
// EXEC CLRDSK
// UCL B= (K=0,D=60),X'00',DY
```

```
// END
// VOL SYSOO8, IJSYSO8
// DLAB 'REGRESSION INPUT DATA          1111112',      C
//          0001,68010,68010,'
// XTENT 1,000,000001000,000003009,'111112', SYSOO8
```

3. EXECUTE CARD

COLS 1-16 // EXEC MULTREGR

THIS CARD CALLS THE PROGRAM FROM DISK WHERE IT IS STORED.

4. ID CARD

COLS 1-72 ANY ALPHANUMERIC INFORMATION DESCRIBING THIS REGRESSION RUN

COLS 78-80 IF BATCH PROCESSING SEVERAL REGRESSIONS PUT ANY POSITIVE NUMBER (SUCH AS 9 IN COL 80) IN THIS FIELD AND THE PROGRAM WILL COME BACK AND START READING THE SECOND REGRESSION STARTING WITH THIS ID CARD. IF ONLY ONE RUN IS TO BE MADE LEAVE THIS FIELD BLANK.

5. PARAMETER CARD

COLS 1-2 THE NUMBER OF VARIABLES OBSERVED (INCLUDING THE DEPENDENT VARIABLE). MAXIMUM IS 58. THIS ENTRY MUST BE AT LEAST AS LARGE AS THE ENTRY IN COLUMNS 3-4 OF THE PARAMETER CARD. IF THE NUMBER OF VARIABLES TO BE USED FOR THE REGRESSION EQUATION EXCEEDS THE NUMBER OBSERVED (E.G. AS IN POLYNOMIAL CURVE FITTING). ADD DUMMY VARIABLES TO THE OBSERVATION SET BY INSERTING ADDITIONAL FIELDS IN THE FORMAT CARD.

COLS 3-4 THE NUMBER OF VARIABLES TO BE USED FOR THE REGRESSION EQUATION (INCLUDING THE DEPENDENT VARIABLE; THIS IS ALSO THE NUMBER OF THE DEPENDENT VARIABLE. IT SHOULD BE READ INTO THIS POSITION OR TRANSFORMED INTO IT.) MAXIMUM IS 5 8

COLS 5-8 NUMBER OF OBSERVATIONS

COLS 9-10 NUMBER OF DATA TRANSFORMATIONS (SEE TRANSFORMATION CARD). MAXIMUM IS 60

COLS 11-12 NUMBER OF CONSTANTS (SEE CONSTANT CARD). MAXIMUM IS 12.

COLS 13-18 F LEVEL FOR ENTERING VARIABLES. THIS FIELD ESTABLISHES A CRITERION OF SIGNIFICANCE FOR ENTERING VARIABLES INTO THE REGRESSION EQUATION. IF CODED ZERO ALL VARIABLES WILL BE ENTERED. THIS ENTRY MUST NOT BE LESS THAN THE F LEVEL FOR DELETING VARIABLES. DECIMAL IS ASSUMED BETWEEN COLUMNS 15 AND 16.

COLS 19-24 F LEVEL FOR DELETING VARIABLES. THIS FIELD ESTABLISHES A CRITERION OF SIGNIFICANCE FOR VARIABLES IN THE REGRESSION EQUATION. VARIABLES NOT SATISFYING THIS CRITERION ARE DELETED FROM THE EQUATION. DECIMAL IS ASSUMED BETWEEN COLUMNS 21 AND 22.

COL 25 ENTER 1 IF RESIDUALS (ACTUAL MINUS ESTIMATED FOR EACH OBSERVATION) ARE DESIRED; OTHERWISE ENTER 0 OR LEAVE BLANK.

6. TRANSFORMATION CARDS

EACH TRANSFORMATION ON ORIGINAL DATA IS REPRESENTED BY AN 8 DIGIT CODE. NINE TRANSFORMATIONS CAN BE CODED ON A SINGLE CARD STARTING IN COLUMN 1 AND ENDING IN COLUMN 72. THE MAXIMUM NUMBER OF TRANSFORMATIONS IS 60, THE MAXIMUM NUMBER OF TRANSFORMATION CARDS IS 7. THESE CARDS ARE OMITTED IF THERE ARE NO TRANSFORMATIONS.

ASSUME THE 8 DIGIT TRANSFORMATION CODE TO BE OF THE GENERAL FORM IJJKKLL. II DEFINES THE TYPE OF TRANSFORMATION. JJ IS THE NUMBER OF THE TRANSFORMED VARIABLE WHICH RESULTS FROM THE TRANSFORMATION. KK IS THE NUMBER OF AN ORIGINAL VARIABLE THAT IS TRANSFORMED. LL IS THE NUMBER OF AN ORIGINAL VARIABLE THAT IS TRANSFORMED OR THE NUMBER OF A CONSTANT USED IN THE TRANSFORMATION. LL IS NOT ALWAYS USED AND SHOULD BE CODED 00 WHEN NOT USED.

THE FOLLOWING TABLE DESCRIBES THE ELEVEN AVAILABLE TRANSFORMATIONS.

TYPE (II)

- 01 VARIABLE (JJ) = VARIABLE (KK), LL NOT USED.
- 02 VARIABLE (JJ) = - VARIABLE (KK), LL NOT USED.
- 03 VARIABLE (JJ) = LOG VARIABLE (KK), LL NOT USED.
- 04 VARIABLE (JJ) = 1/VARIABLE (KK), LL NOT USED.
- 05 VARIABLE (JJ) = VARIABLE (KK) + VARIABLE (LL).
- 06 VARIABLE (JJ) = VARIABLE (KK) * VARIABLE (LL).
- 07 VARIABLE (JJ) = VARIABLE (KK) / VARIABLE (LL).
- 08 VARIABLE (JJ) = VARIABLE (KK) + CONSTANT (LL).
- 09 VARIABLE (JJ) = VARIABLE (KK) * CONSTANT (LL).
- 10 VARIABLE (JJ) = SIN (VARIABLE (KK)), LL NOT USED.
- 11 VARIABLE (JJ) = COS (VARIABLE (KK)), LL NOT USED.

* 7. CONSTANT CARD

* CONSTANTS WHICH ARE USED IN TRANSFORMATION TYPES
* 08 AND 09 ARE CODED IN A CONSTANT CARD. EACH CON-
* STANT IS 6 DIGITS WITH THE DECIMAL ASSUMED BETWEEN
* DIGITS 3 AND 4. CONSTANT 01 IS ENTERED IN COLUMNS
* 1-6, CONSTANT 02 IN COLUMNS 7-12, ETC. THE MAXI-
* MUM NUMBER OF CONSTANTS IS 12. THIS CARD IS OMITTED
* IF THERE ARE NO CONSTANTS.

* 8. FORMAT CARD

* COLS 7-72 FORTRAN TYPE FORMAT VARIABLES IN FLOATING POINT
* EXAMPLE:
* (3X,F6.3,2X,F7,4,3F6.0,T1,F3.0,T50,F6.3)

* THE NUMBER OF VARIABLES IN THE FORMAT SHOULD EQUAL
* THE NUMBER IN COL 1-2 OF THE PARAMETER CARD.

* 9. DATA CARDS

* 10. REPEAT 4-9 IF BATCH PROCESSING

* 11. END OF DATA

* COLS 1-2 /*

* 12. END OF JOB

* COLS 1-2 /&

/&