

A SEARCH/MATCH COMPUTER PROGRAM FOR THE IDENTIFICATION OF MINERAL COMPONENTS OF MULTI-MINERAL X-RAY POWDER DIFFRACTOMETER PATTERNS

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ABSTRACT

A search/match computer program is presented to identify the mineral components of rocks and composite ores from x-ray powder diffraction patterns. This program aims to overcome the problems encountered when such identification is made visually through the A.S.T.M. cards.

INTRODUCTION

The x-ray powder diffraction method is one of the most widely used methods for the identification of minerals. The basic principle underlying the method is that each crystalline substance has its own peculiar atomic structure which diffracts x-rays in a characteristic pattern (Cullity, 1967).

A visual search through the J.C.P.D.S. manuals (or A.S.T.M. cards) establishes the name of the diffracting substance. However, when more than one mineral phase is involved in a sample pattern, the visual identification becomes difficult, time-consuming and error-prone.

The present system of mineral identification which was originally written for Textronix computers (Aral, 1986) consists of two files recorded on a floppy disc. The search/match program (MATCH) is recorded in the program file. The other file, the data base (DBASE), contains the d-values of the reference mineral data.

DATA BASE

In the data base, d-values of reference mineral patterns are stored. Each entry of the data base consists of eight d-values ordered in decreasing relative intensities, the name of the mineral and the pattern number (Table 1). In general, eight data items are found sufficient for a good match. In case of common major minerals, lower intensities are also introduced as a new entry. In such cases the match is based on up to 16 data items. The low intensity peaks are designated with a (LOW-INT.) sign next to the mineral name and placed immediately after the major entry (see Table 1). When two equally strong peaks are present in the reference mineral, the one with higher d-value is entered first. The creation of a data base in an orderly manner (i.e., decreasing I/I_0 intensity) is a major feature of this search/match system.

The data base enclosed with the main program includes 256 major reference minerals, the lines of which are taken from the university film archives. Additional files can be created in relation to the character of the problem. In general, it is advisable to organize the files into separate files according to their mineral groups such as oxides, sulphides, silicates, etc. Such an organization would reduce the search/match time. A correct data base is essential in order to obtain reliable results.

INPUT DATA

The input data consists of the following items:

- a) Sample number: Code name or number of the sample pattern.
- b) The d- or 2-theta or 4-theta value of major peaks whose relative intensities are greater than 50: Such major peaks are compared with the first two major peaks of the reference minerals.
- c) Total number of peaks to be entered: The number of peaks on the sample pattern has to be counted and entered.
- d) The d- or 2-theta or 4-theta value of each peak: An unlimited number of peak data can be entered into the program. Every single peak including those whose relative intensities are as low as 4 or 5 (out of 100) should be accounted for and entered into the program. This allows for the detection of minerals that may be present in small amounts. However, it should be realized that a large number of entries prolongs the search/match time.

Table 1. Part of the data base used in the search/match program.

	GRAPHITE 27
	3.36
	3.24
	3.29
	4.23
	3.48
	2.03
	1.80
	2.13
	EPIDOTE 17
	2.9
	2.68
	2.69
	8.04
	4.02
	2.6
	2.46
	3.4
	HARMATOME 116
	4.08
	3.13
	7.1
	8.19
	6.3
	4.99
	3.25
	2.94
	ARAGONITE 11
	3.4
	1.98
	3.27
	2.7
	2.37
	2.48
	2.34
	1.88
	ILVAITE 219
	2.71
	2.84
	7.28
	2.67
	2.44
	2.18
	2.11
	3.24

e) Some optional data such as maximum and minimum error percentages to compensate for poor chart/film readings and possible peak shifts are also used. It is known that the divisions of the d-scale are not uniformly spaced. Along this scale, higher values are more closely spaced and thus more liable to poor readings, therefore in the program, d-values greater than 6 are assigned to maximum error and those less than 6 to minimum error. The choice of the value 6 is based on personal experience. The program uses such correction values to define an "error window" around each peak. In general, a value between 0.015–0.02 is usually sufficient for maximum, and 0.005–0.01 for minimum error.

The major input data accuracy of which has a vital effect on mineral identification (items b and d above), is placed at the end of the program so that it can be inspected easily. In this way, wrong entries can be corrected by re-entering the correct data.

PROGRAM AND OUTPUT

The search/match is done in a FOR/NEXT loop between statement numbers 1030 to 1070 of the program (Appendix I). In this loop, the d-values of the A_i matrix is multiplied with the error values according to the criteria of $d \leq 6$ or $d < 6$ and stored as z. If the value of z is equal or smaller than the absolute value, obtained by subtracting the reference peak value (c) from the peak value of the sample diffractogram (A_i), the value of c is stored in the D_j matrix. If the absolute value of the difference is larger than z, then a new peak value is taken for comparison. As this process is based on the comparison of each c value of the data base to the peak values of the sample the search/match requires a small memory space and does not lead to the creation of large size matrices. If the first four elements of the D_j matrix are not matched the next four elements of the reference mineral are skipped (statement numbers from 1090 to 1210). This reduces the search/match time to a great extent.

After one complete run, an array with 8 d-values and corresponding name and reference pattern number appears for each mineral in the output (Table 2).

The computer's response "O" at the output indicates unmatched peaks. In the output, "flag" statements are printed when one of the major peaks of the sample is in agreement with the first or second peak of the reference pattern. The "flags" aim to attract the user's attention in the final selection (see below).

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10 FKEY OF
20 REM: APPENDIX
30 CLS
40 REM: A SEARCH/MATCH PROGRAM FOR THE IDENTIFICATION OF MINERAL
50 REM: COMPONENTS OF MULTI-MINERAL X-RAY POWDER
60 REM: DIFFRACTOMETER PATTERS
70 REM:
80 REM: BY H. ARAL
90 REM: DEPT. OF GEOLOGICAL ENG., HACETTEPE UNIVERSITY, ANKARA
100 REM:
110 REM: THIS PROGRAM WAS ORIGINALLY WRITTEN IN BASIC FOR TEKTRONIX
120 REM: 4051 AND 4054 COMPUTERS (ARAL, 1986)
130 REM:
140 REM: THIS PROGRAM ACCEPTS DATA FROM THE VALUES ENTERED TO THE
150 REM: END OF THE PROGRAM BY THE USER. THE TEST DATA ENCLOSED AT
160 REM: THE END FOR DEMONSTRATION MUST BE REPLECAD WITH YOUR OWN.
170 REM:
180 REM: TO RUN THIS PROGRAM THE DATA FILE DBASE IS NEEDEDFI.
190 REM: THE USER IS INTERESTED IN SPECIFIC CLASS OF MINERALS THAT
200 REM: ARE NOT INCLUDED IN THE DATA FILE, THEN, SUCH A FILE HAS
210 REM: TO BE CREATED BY THE USER.
220 SD=3.14/180!
230 A=O: B=O
240 REM:
250 REM: ..... INPUT .....
260 REM:
270 PRINT "ENTER sample No;"
280 INPUT O$
290 PRINT "How many major peaks do you have?"
300 INPUT K1
310 DIM B(K1)
320 FOR I=1 TO K1
330 READ B(I)
340 NEXT I
350 PRINT "How many peaks do you have?"
360 INPUT M
370 DIM A(M), D(8), C(8)
380 FOR I=1 TO M
390 READ A(I)
400 NEXT I
410 PRINT "Are the values dA-values or theta values?" (D/T);
420 INPUT M$
430 M$=MID$(M$, 1, 1)
440 IF M$="t" IOR M$="T" THEN 480
450 IF M$="d" OR M$="D" THEN 810
460 PRINT "Wrong Entry!"
470 GOTO 410

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480 PRINT "Are theta values 2-theta or 4-theta? ENTER 2 or 4"
490 INPUT T7
500 IF T6=2 THEN 680
510 IF T7=4 THEN 580
520 PRINT "Wrong Entry!"
530 GOTO 480
540 REM:
550 REM: CALCULATION OF D-VALUES FROM 4-THETA VALUES:
560 REM: BASED ON BRAGG'S EQUATION
570 REM:
580 FOR I=1 TO M
590 H1=1.5405/(2!*SIN(SD*A(I)/4))
600 A(I)=H1
610 NEXT I
620 REM:
630 FOR I=1 TO K1
640 H2=1.5405/(2!*SIN(SD*B(I)/4))
650 B(I)=H2
660 NEXT I
670 GOTO 810
680 REM:
690 REM: CALCULATION OF D-VALUES FROM 2-THETA VALUES:
700 REM: BASED ON BRAGG'S EQUATION
710 REM:
720 FOR I=1 TO M
730 H3=1.5405/(2!*SIN(SD*A(I)/2))
740 A(I)=H3
750 NEXT I
760 REM:
770 FOR I=1 TO K1
780 H4=1.5405/(2!*SIN(SD*B(I)/2))
790 B(I)=H4
800 NEXT I
810 PRINT "ENTER your MAXIMUM reading+instrumental error for d-value"
820 PRINT "NOTE that a value between 0.015-0.02 is usually sufficient."
830 INPUT Z1
840 PRINT "ENTER your MINIMUM reading+instrumental error for d-value"
850 PRINT "NOTE that a value between 0.005-0.01 is usually sufficient."
860 INPUT Z2
870 CLS
880 REM: ..... PROGRAM .....
890 PRINT "..... LIST OF MINERALS IDENTIFIED ....."
900 PRINT
910 PRINT "Sample No: "; O$
920 PRINT "MAX. error window: "; Z1;" MIN. error window: "; Z2
930 PRINT
940 F$="DBASE"
950 OPEN "I", Ć1, F$

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960 J=0
970 IF EOF (1) THEN 1440
980 INPUT Ć1, N$
990 J=J+1
1000 IF J>8 THEN 1220
1010 INPUT Ć1, C
1020 D(J)=0
1030 FOR I=1 TO M
1040 IF A(I)>=6 THEN Z=1Z*A(I) ELSE Z=A(I)*Z2
1050 IF ABS (A(I)-C)> Z THEN 1070
1060 D(J)=C
1070 NEXT I
1080 REM: ..... OUTPUT .....
1090 ON J GOTO 1110, 1130, 1150, 1170, 1180, 1180, 1180, 1180
1100 GOTO 990
1110 IF D(1) =0 THEN 1190
1120 GOTO 990
1130 IF D(2) =0 THEN 1190
1140 GOTO 990
1150 IF D(3) = 0 THEN 119a
1160 GOTO 990
1170 IF D(4) =0 THEN 1190
1180 GOTO 990
1190 FOR =1 TO 8-J
1200 INPUT Ć1, C
1210 NEXT I
1220 FOR J=1 TO 8
1230 IF D(1)<> 0 AND D(2)<> 0 AND D(3)<> 0 AND D(4)<> 0 THEN PRINT D(J);
1240 IF J<> 8 THEN 1260
1250 IF(1)<> 0 AND D(2)<> 0 AND D(3) <> 0 AND D(4)<> 0 THEN PRINT N$
1260 NEXT J
1270 FOR I=1 TO K1
1280 IF B(I)=> 6 THEN Y=Z1*B(I) ELSE Y=Z2*B(I)
1290 IF ABS(B(I)-D(1))> Y THEN 1310
1300 IF D(1)<> 0 AND D(2)<> 0 AND D(3)<> 0 AND D(4)<> 0 THEN PRINT "****
1st Major line"; D(1); "agree with"; B(I);)"
1310 IF ABS(B(I)-D(2))> Y THEN 1330
1320 IF D(1)<> 0 AND D(2)<> 0 AND D(3)<> 0 AND D(4), THEN PRINT "**** 2nd Ma-
jor line "D(2);" "agree with"; B(I);)"
1340 GOTO 960
1350 REM: ..... TEST DATA .....
1360 REM ** Major peak values of the TEST DATA 5 peaks *****
1370 DATA 7.05, 3.52, 4.72, 14.1, 3.18
1380 REM*** This is a TEST DATA; Number of peaks = 46 *****
1390 DATA 14.1, 8.37, 8.05, 7.05, 6.38, 5.02, 4.72, 4.6, 5.2, 4.02, 3.76
1400 DATA 3.67, 3.52, 3.48, 3.39, 3.27, 3.22, 3.18, 3.11, 3.06, 2.95
1410 DATA 2.9, 2.92 2.92, 2.71, 2.68, 2.6, 2.53, 2.45, 2.4, 2.3
1420 DATA 2.16, 2.1, 2.07, 2.04, 2.02, 2.1, 88, 1.77, 1.63, 1.58, 1.54

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1430 DATA 1.46, 1.44, 1.41, 1.39
1440 PRINT "***** END OF FILE SEARCH *****"
1450 PRINT
1460 PRINT "Do you want to do another search) (Y/N";
1470 INPUT Y$
1480 Y$=MID$(Y$, 1, 1)
1490 IF Y$="y" OR Y$="Y" THEN 1530
1500 IF Y$="n" OR Y$="N" THEN 1570
1510 PRINT "Wrong entry!"
1520 GOTO 1460
1530 CLOSE Ğ1
1540 PRINT "Enter the file name:";
1550 INPUT F$
1560 GOTO 950
1570 PRINT "*****"
1580 CLOSE Ğ1: END

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To obtain a successful output, it is essential that the goniometer should scan $2\theta = 3$ to 70° and the input data must be carefully measured and entered into the program.

DISCUSSION AND AN APPLICATION

All the minerals that appear in the output list are not necessarily the minerals present in the sample diffractogram. Due to the reasons stated below at least some of these minerals must be discarded. Final selection is done by comparing the relative intensities of the sample pattern to those appearing in the mineral list (output). Since the d -values of the mineral appearing in the output is listed in a decreasing order of intensities it will be possible to discard many minerals from the output list when the major peaks are not matched.

The (LOW-INT.) minerals may immediately be discarded, if the name of the minerals which contains the first major eight peaks does not appear in the output list. Such minerals should be considered as "nonsense combinations". The (LOW-INT.) minerals together with their main mineral patterns are evidently more qualified to be in the final selection since in such a case the match is based on up to sixteen peaks.

The number of "nonsense combinations" is directly proportional to the size of the "window", to the total number of peaks entered into the program, and to the length of the data base. It is usually advisable to run the sample program twice (or more) with varying error percentages. The assignment of lower error percentages leads to a lesser number of minerals listed in the output.

Table 2. List of minerals identified (FUTPUT) as a result of run of the test data. Note that the finally selected minerals are ALBITE, EPIDOTE, THRUNGITE and TREMOLITE. The length of the data base is 256 minerals. Run time is four minutes.

LIST OF MINERALS IDENTIFIED										
Sample No: ABC										
MAX. error window: .015 MIN. error window: .005										
3.18	3.75	3.21	6.43	4.04	6.36	0	0	ALBITE-H		39
**** 1st Major line 3.18 agree with 3.18)										
4.03	3.22	3.66	6.37	3.77	3.68	0	2.44	ALBITE		184
3.19	4.03	3.21	3.66	0	0	3.68	2.93	ALBITE-L		55
**** 1st Major line 3.19 agree with 3.18)										
3.21	3.18	4.04	3.76	0	0	2.93	2.53	ANDESINE		76
*** 2nd Major line 3.18 agree with 3.18)										
3.19	3.18	3.21	3.26	4.04	0	0	0	ANORTHITE		20
**** 1st Major line 3.19 agree with 3.18)										
*** 2nd Major line 3.18 agree with 3.18)										
3.19	3.18	4.04	3.26	3.21	3.12	0	0	ANOTRHITE		20A
**** 1st Major line 3.19 agree with 3.18)										
*** 2nd Major line 3.18 agree with 3.18)										
3.18	3.76	3.21	4.04	0	0	0	0	LABRADORITE		120
**** 1st Major line 3.18 agree with 3.18)										
3.18	4.04	3.21	3.76	0	3.66	0	2.53	OLIGOCLASE		54
**** 1st Major line 3.18 agree with 3.18)										
2.44	2.29	2.1	2.06	0	1.63	4	1.63	CLINOZOISITE (LOW-INT.)		
2.44	2.29	2.1	2.06	0	1.63	4	1.63	CLINOZOISITE (LOW-INT.)		
2.82	2.26	4.01	2.11	2.05	0	0	0	ENSTATITE (LOW-INT.)		
2.9	2.68	2.69	8.04	4.02	2.6	2.46	3.4	EPIDOTE		17
3.22	2.52	2.29	2.15	2.06	1.63	0	0	GLAUCOPHANE (LOW-INT.)		
8.45	3.12	2.89	3.27	2.71	0	4.21	2.54	Mn-RIEBECKITE		65
2.7	2.52	3.38	8.36	0	3.11	0	0	Fe-RICHTERITE		15
8.38	3.12	2.71	3.27	3.38	0	2	0	TREMOLITE		43
3.12	8.43	3.27	2.93	2.7	2.81	2.15	0	AMPHIBOLE		23
7.05	3.52	2.6	14.1	0	0	2.45	2.39	THUNGITE		21
**** 1st Major line 7.05 agree with 7.05)										
*** 2nd Major line 3.52 agree with 3.52)										
7.05	3.52	2.52	14.1	4.71	2.15	0	0	THURNGITE		73
**** 1st Major line 7.05 agree with 7.05)										
*** 2nd Major line 3.53 agree with 3.52)										
2.54	7.11	14.1	1.54	0	0	2.44	2.59	SHERIDANITE		7
*** 2nd Major line 7.11 agree with 7.05)										

END OF FILE SEARCH

Do you want to do another search? (Y/N)

If the user has some additional information about his sample—for instance sample chemistry, mineralogic association, metallogenic assemblage, etc., he may eliminate some of the minerals listed in the output.

The minerals whose first and second major peaks are in agreement with those of the reference patterns as indicated by “flags” should have a higher chance to appear in the final selection.

Minerals with a higher number of matching peaks, are logically more likely to be selected, however utmost care should be taken in such selection as in a multi-phase pattern the minerals of low amounts may show up only with their major peaks.

In many cases it will be seen that some of the peaks of the sample pattern may not have been accounted for in the output. The reason for such unaccounted peaks may be due to the restriction of the reference minerals in the data base to eight peaks (in most cases) instead of the complete spectrum. In such cases, a complete reference mineral pattern of the “found” minerals must be consulted. Errors made in recording, reading, entering the sample patterns and incomplete data files may be the other reasons for such unidentified peaks.

Illustration of the program is made on a test data from an actual pegmatite sample from southeastern Turkey. The d-values of the 5 most important peaks and 46 peaks of the diffractogram are given in statement numbers 1370 to 1430 at the end of the program (MATCH) in Appendix I.

The error “window” values are taken as 1.5 % for maximum and 0.5 % for minimum. The minerals in the output list after a complete search of the data base (DBASE) containing 256 reference minerals are shown in Table 2. The search/match and printing of the output takes 4 minutes with an IBM Personal Computer.

In the output list, the first eight minerals are various feldspars and the last eight minerals (GLAUCOPHANE LOW-INT. to SHERIDANITE) are mafic minerals. The crowded appearance of feldspar and mafic minerals strongly suggests the presence of at least one feldspar, chlorite and an amphibole in the sample. The identification of which feldspar and amphibole minerals are present is done by comparing the peak intensities of the sample diffractogram to the corresponding peak intensities of the reference mineral. It appears that ALBITE is the most likely feldspar. The match of major peaks 5.05, 3.59 and 14.1 suggests the presence of THURNGITE as a chlorite, and 8.37 peak suggests

the presence of an amphibole mineral TREMOLITE in the sample. While the major eight peaks of ENSTATITE and CLINOZOISITE are not in the printout, their (LOW-INT.) peaks appear in the list. This suggests that these two minerals are "nonsense combinations" and must be discarded. EPIDOTE is the other likely mineral present in the sample as all of its eight peaks match with the reference peaks. The presence of these four minerals in this sample is verified by thin section study under the microscope.

CONCLUSION

The computer program MATCH allows the identification of mineral components of rock and composite ores from x-ray diffraction films and charts. Input, in the form of interplanar spacings, 2- or 4- theta values are accepted. The program provides the user with the option of assigning error estimates to compensate for poor chart/film readings and peak shifts as an outcome of human and instrumental errors.

Although the number of possibilities are reduced to a minimum by means of several program parameters, the program output does not provide a final mineral list, but a list of possibilities from which the user has to make the final selection.

REFERENCES

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