

## AUTOMATIC QUALITATIVE POWDER DIFFRACTION PHASE ANALYSIS: SYSTEM RIFRAN 2.0

TOMÁŠ HAVLÍK, MILAN ŠKROBIAN, FRANTIŠEK PETRIČKO

*Department of Non-ferrous Metallurgy, Faculty of Metallurgy, Technical University, Letná 9/A, 043 85 Košice,  
Slovakia*

Received 20. 7. 1992

*Programme system RIFRAN is designed for automatic identification of polycrystalline substances by the qualitative X-ray powder diffraction phase analysis. For this purpose the database containing approximately 29 000 standards is used. This database can arbitrarily be completed and edited. The gist of identification consist in comparison of the peaks of a measured unknown substance with the peaks of standards. This identification is refined by using statistical criteria and knowledge of chemical (elemental) composition of the analysed substance. The results of identification are presented in alpha-numerical or graphic form on display, joined printer or are written in data field. The programme is written in Borland Turbo C++ computer language. The system is implemented with a personal computer of class IBM PC/AT working under operating system MS DOS. The authors are willing to give information about further development of the system and possibilities of its acquisition or advise how to gain an demoversion of the programme.*

### INTRODUCTION

The analytical identification methods is based on comparison of the measured spectra of unknown substance with the database of reference standards have obtained a new quality with the start of efficient computer technique of PC committee. That also bears upon the diffraction phase analysis for which there are at present more than 52 000 standard diffraction patterns stored in the greatest database and the number of these records increases by about 2 000 items every year [1]. Thus it results that the analysis itself essentially belongs in the region of bulk data processing and an efficient tool in this line is appropriate algorithmisation and computational processing of the results of analysis.

This region developed simultaneously with the development of computer technique. The capacity of operating memory, the rate of data transfer, the time of storage medium access, the capacity of this medium as well as convenient and flexible programming aids had influence on algorithmisation of the analysis itself. From this point of view, we can observe progress from the first works by Frevel [2], Johnson and Vand [3] or Frevel and Adams [4]. Later, the analytical programmes were directly implemented with powder diffractometer like Sandmann [5] and Diffrac [6]. The last communications were published by Marquart [7] and Nakhmanson [8]. A general review of the papers concerned with these problems was published by Vasiljev and Nakhmanson [9] or Smith and Gorter [10].

In 1990 Frevel [11] published a set of twenty selected and chronologically arranged algorithms for automatic powder diffraction phase analysis in such form as presented in Table I.

At present, the personal computers with IBM PC or DEC VAX are used for automatic phase analysis. Their use is based on their universality, compatibility, on the rate of data transmission and a great capacity of operating memory and storage medium. Recently, CD ROM [7, 28] was used as storage medium for database. A computer of class IBM PC is frequently used as an integrated part not only for evaluation

*Table I*

Twenty published programs for automatic diffraction phase analysis according to Frevel [10]

Autor	Year	Source
Hanawalt, Rinn, Frevel	1983	12
Nichols	1944	2
“Index”	1963	14
Smith	1963	15
Frevel	1965	16
Johnson, Vand	1967	3
Frevel et al.	1976	17
Young et al.	1977	18
Marquart et al.	1979	19
Edmonds	1980	20
Frevel	1982	21
Huang et al.	1983	22
Cherkuri, Snyder	1983	23
Goehner, Garbaskas	1983	24
Lin et al.	1983	25
Carr et al.	1986	26
Škrobian, Havlík	1986	27
Marquart	1986	7
Jenkins, Holomany	1987	28

Table II

Main menu of system RIFRAN and its individual offers

FILES	EDIT	COPY	SEARCH	RESULTS	DATABASE OPTIONS	END	HELP
<ul style="list-style-type: none"> <li>• Open existing file</li> <li>• Create new PDF file</li> <li>• Remove PDF file</li> <li>• Change directory</li> <li>• DOS command</li> </ul>	<ul style="list-style-type: none"> <li>• edit in rows</li> <li>• edit in columns</li> <li>• append new card</li> <li>• browse according card number</li> <li>• edit according card number</li> </ul>	<ul style="list-style-type: none"> <li>• copy according chemical elements</li> <li>• copy according chemical name</li> <li>• copy according mineralogical name</li> <li>• copy according subfiles</li> <li>• append to existing files</li> </ul>	<ul style="list-style-type: none"> <li>• input new pattern data</li> <li>• edit of existing pattern</li> <li>• searching</li> </ul>	<ul style="list-style-type: none"> <li>• alphanumeric output</li> <li>• graphic output</li> <li>• print to printer</li> <li>• storage to datafile</li> </ul>	<ul style="list-style-type: none"> <li>• input database in ASCII</li> <li>• export database in ASCII</li> <li>• sort of standards</li> <li>• transfer of database</li> <li>• imploding of database</li> <li>• exploding of database</li> </ul>	<ul style="list-style-type: none"> <li>• temporary DOS commands</li> <li>• end of programme</li> </ul>	<ul style="list-style-type: none"> <li>• contents</li> <li>• indexes</li> <li>• search</li> <li>• undo</li> <li>• help on help</li> <li>• about authors</li> </ul>

of the results of analysis but also for control of the diffractometer.

System RIFRAN presented in this paper passed through many stages of development which were in the main dependent on availability of the computer technique and its applicability. The first versions of RIFRAN were written for a programmable desktop calculator EMG 666/B. This aid was equipped with 8 kB operating memory and a magnetic tape unit of the Compact Cassette type as storage medium. Thus the analysis was very limited as regards the possibility of criterial analysis and its overall speed. In spite of these limited possibilities, the results of analysis was so adapted that the judgement on probability of standard in the sample was based on chemical analysis as well as on statistical analysis [27]. Both versions of the programme were written in autocode EMG.

The version of system RIFRAN '89 represented an essential jump of development by the fact that it was adapted for the use of 8-bit home computer ATARI 130 XE equipped with 64 kB RAM memory, and floppy disk unit [30]. In this way, the overall speed of analysis significantly increased and the extent of database as well as the data access was ameliorated. The criterion analysis was improved and the output of results was refined by using the statistical analysis

on the basis of which the user determined the measure probability of a certain standard in sample. The graphic output in the form of stick-diffractograms was also an improvement. This output as well as the alpha-numerical output can be presented on a display or in an attached printer.

All programmes of this modification of system RIFRAN were written in Atari Turbo Basic computer language.

All the former versions of system RIFRAN were designed as analytical systems for specialised laboratories mainly because of the relatively narrow specialised database containing only hundreds of standard records. Such system afforded rather satisfactory results but it was implemented with poorly compatible technique owing to which the necessity always to form a new database appeared or it was necessary to complete the database according to specialisation of the new user. For this reason, a new generation of system RIFRAN was created. It is accessible for a great number users and is fully compactible. This version of system RIFRAN 1.0 [30] and the present modification RIFRAN 2.0 came into existence.

The basic idea of algorithm has remained, in principle, unchanged and confirmed its rightness by the good results obtained up to now. Moreover, it has

pat	chem
1-153	Iron Chloride Hydrate
1-229	Calcium Nitrate Hydrate
1-338	Calcium Chloride
1-386	Calcium Iodate
1-397	Sodium Aluminum Sulfate Hydrate
1-403	Nickel Sulfate Hydrate
1-744	Zinc Arsenate Hydrate
1-830	Antimony Tin
1-984	Tin Sulfide
1-1059	Iron Chloride
1-1092	Calcium Magnesium Chloride Hydr
1-1106	Iron Chloride
1-1129	Iron Aluminum Chromium Oxide
1-1130	Cobalt Manganese Oxide
1-1293	Vanadium Oxide
2-8	Iron Aluminum Silicate Hydroxid
2-27	Iron Aluminum Silicate Hydroxid

Tot: 3186 | E:\...IFRAN\RIP-DATAN\OWNBASE.RIP | 1

F1 - Help | Browse-View: \*F1\* PgUp PgDn Home End Enter, Esc | 22:10:58

Fig. 1. Menu for searching in opened database.

been raised to a higher power by all virtues of the systems implemented with a computer of class IBM PC/AT which work under operating system MS DOS. The basic idea of analysis consists in vectorial representation of diffractograms of an unknown sample and standards as described in [1, 30]

#### DATABASE OF STANDARS

The card of standard included in the database has been so designed that it is formally and functionally compatible with a standard card of the base Powder Diffraction File of the JCPDS-International Centre for Diffraction Data (further PDF). Besides description, chemical formula, name and mineralogical term, it contains the data on quality of data and registration in subfile as well as the possibility of stating (and using) the value of scale factor  $I/I_{cor}$  with respect to corundum  $\alpha\text{-Al}_2\text{O}_3$  for the purpose of quantitative phase analysis.

Further usable data are the values of positions of peaks "d" relative intensities " $I/I_1$ " and the values of Miller indexes [hkl] provided they are available. The card numbering according to PDF is preserved. If data integrated in the database are new or taken from other literary sources, they become a card file number beginning with 90-xxx and the annotation of the source of this standard is presented in comment.

The card edited in this manner is filled into the database. The editor and all other functions are not

independent programmes but a part of one integrated unit.

The database of standards (and every new or part of it) contains, in reality, five indexed sets including all data written in the card, i.e. PDF number, chemical formula, standard name, mineralogical term of the standard, data on structure of the standard, quality of data, Miller indexes [hkl], scale factor with respect to corundum and the values of interplanar spacing "d" and intensities " $I/I_1$ ".

All records are in binary form. In this way, a very fast access to the data of standard substances is ensured for the analysis itself and for further work with the database, such as editing, copying, addition of new records or deletion of useless records.

At present the database contains about 29 000 standard records among which there are about 2 900 minerals, 7 000 organic substances and 19 000 inorganic substances. It goes without saying that the database continues to be completed according to need and availability of the published data. Now a days the attention is especially concentrated on new materials such as superconductors, ceramics, etc. These substances still occur in the standard PDF sets very sporadically. Thus for instance, there are 148 reference records concerning superconductive substances in the database. For comparison, there are only 17 standard diffraction patterns for superconductors in the 41st PDF series.

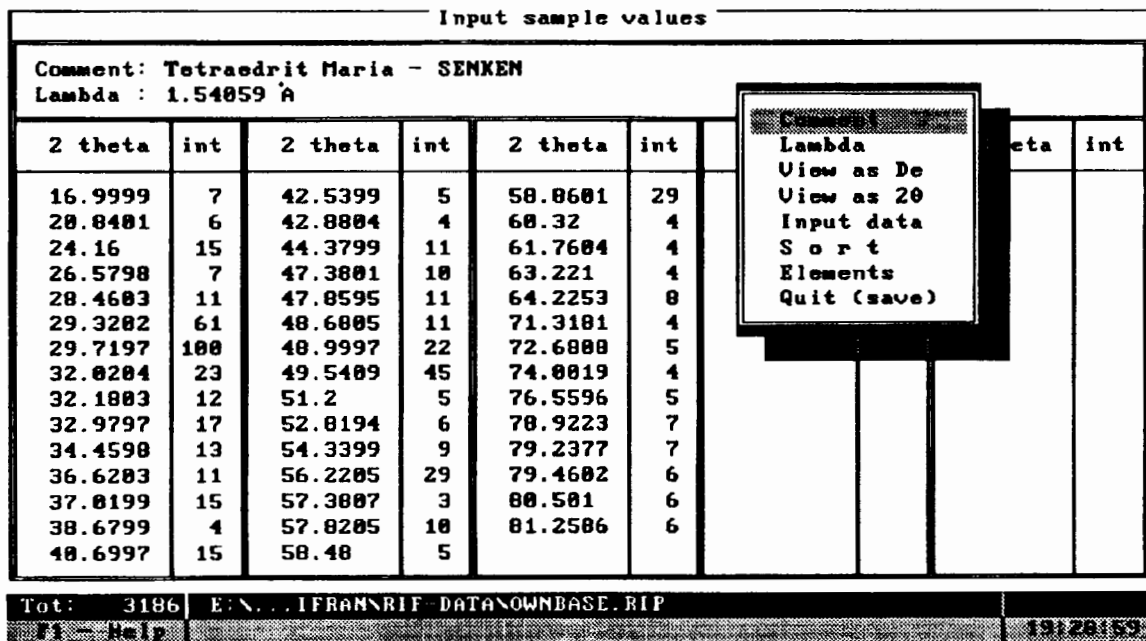


Fig. 2. Input data of measured sample.

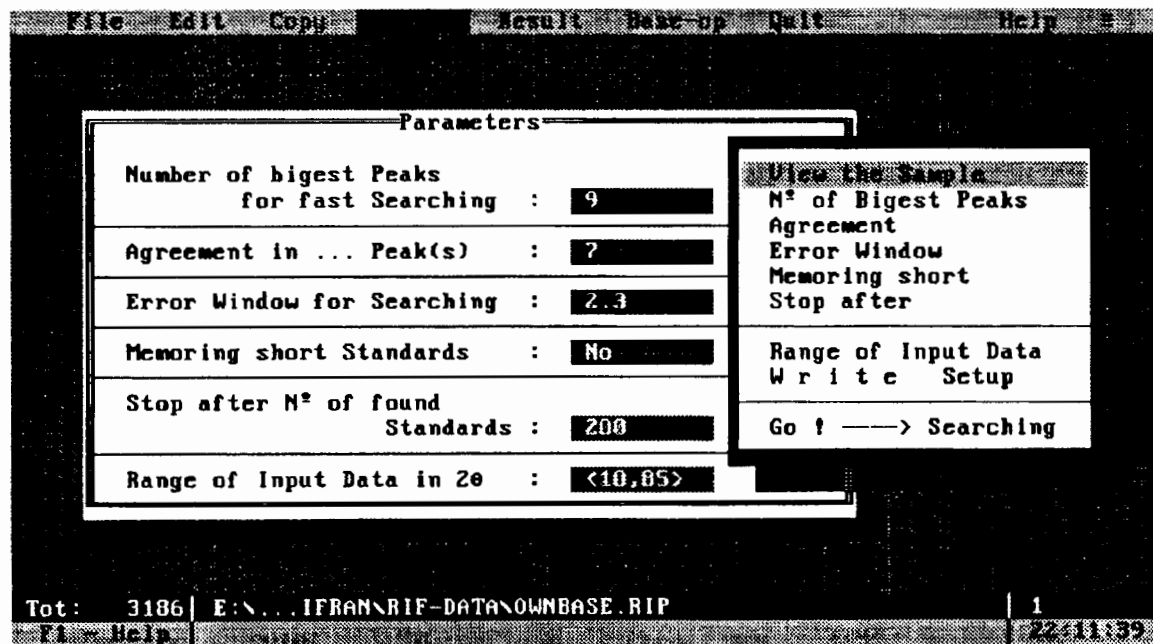


Fig. 3. Input data for criterion analysis.

DESCRIPTION OF THE PROGRAMME

System RIFRAN 2.0 requires implementation with a personal computer of class IBM PC AT 286 or higher with a graphic card VGA or higher, 1 MB operating memory or more and with 20 MB harddisk

at least. In this case, the transfer time to the hard-disk is the slowest operation. Of course, the higher processor clock frequency of microprocessor is, the faster is the analysis. However, even at low processor clock frequencies the analysis last only seconds in

**HIT LIST - Results**

P * I 0.91862			12/13 [0.9231]						412/414 [0.9952]						
			P = Σokd / Σd						I = Σokl / Σl						
d	2θ	int													
5.2114	17.000	7	—	—	—	5	—	6	—	6	—	—	10	—	—
4.2590	20.840	6	—	—	—	—	—	4	—	70	—	—	—	50	90
3.6807	24.160	15	—	—	—	10	—	30	—	—	—	—	—	—	80
3.3509	26.500	7	—	—	—	—	—	—	—	—	—	60	—	100	—
3.1336	28.460	11	43	35	—	—	—	8	—	—	—	20	—	20	20
3.0436	29.320	61	—	—	100	—	100	—	65	—	—	—	—	10	—
3.0036	29.720	100	—	—	—	100	—	100	—	100	60	100	80	—	—
2.7929	32.020	23	—	—	—	5	—	15	—	80	—	—	—	—	—
2.7793	32.100	12	—	—	—	—	—	—	—	—	—	—	—	—	60
2.7130	32.900	17	100	85	—	—	—	—	55	—	40	—	—	40	—
2.6005	34.460	13	—	—	—	20	10	20	—	30	40	60	100	—	100
2.4519	36.620	11	—	—	—	10	—	10	—	15	60	—	10	30	—
2.4264	37.020	15	58	65	—	—	—	4	—	—	—	—	—	—	—
2.3260	38.600	4	—	—	—	5	—	6	10	4	—	—	30	—	—
2.2151	40.700	15	43	50	—	—	—	1	—	20	70	—	—	30	20
2.1234	42.540	5	—	—	—	10	—	10	—	—	—	—	—	10	40

Hit-List T: 3186 F: 29 CH: 7 POS: 1 S: chem <Ins> sort

Fig. 4. Output of analysis on display of computer.

the range of the first decimal order. At present the authors use a personal computer PC AT 386/40MHz and 4 MB RAM with mathematical co-processor 80 387/40 MHz and graphic card SVGA.

The programme is written in Borland Turbo C++ computer language.

The basic idea of analysis consist in comparison of individual peaks of the measured sample with positions of the peaks of standards stored in the database. The standards thus obtained in the first round ("Search") are subjected to criteria and chemical analysis ("Match"). The overall course of the programme can be described as follows:

After input of programme in memory of computer, the bids for further work are selected. All bids of main menu are given in Table II and system services are ensured by the "pull-down" menu.

At the start one of the data sets must be opened. It is not possible to open several sets at the same time. The opened set can be examined, searched and modified. Fig. 1 represents the bid for retrieving in the opened database. Of course, we can examine according to all possibilities (chemical formula, mineralogical term, chemical term, serial PDF number, etc.) or according to arbitrary character string. By depressing key "Enter" the complete topical PDF card appears. In this way, it is very easy to reproduce partial usable databases according to the mentioned possibilities for real analysis or to clear them. That is provided by the bid for copying.

There are two possibilities for the search itself. Either the data of new sample are submitted from the keyboard of computer or the data submitted before are used or they are modified in the bid EDIT. The submission of the data of new sample (Fig. 2) thus contains the prerequisite data: Comment, wavelength of the used radiation, input data in the values of  $2\theta$  or  $d$  which can be ordered downwards or upwards according to position or intensities of peaks as required by the user. The chemical composition in the form qualitative content of elements is an important part of input data. The system uses logical operands and for this reason gives more possibilities for analysis than the selection according to combination of some elements or necessary occurrence of each of the selected elements in the phase or some elements etc. It is very important to draw attention to the fact that chemically non-correct phases are not omitted from analysis though the chemical composition can be used for analysis. In this way a subjective error can be avoided and at the same time a phase that is chemically non-correct but exhibits equal structural type like the present phase can be selected though it is not included in the database. Thus the real present phase can be much easier find out in the subsequent stage of analysis.

The submitted data of the measured sample are written and the search itself begins. The search is governed by criteria analysis the inputs of which are represented in Fig. 3. The number of peaks which the

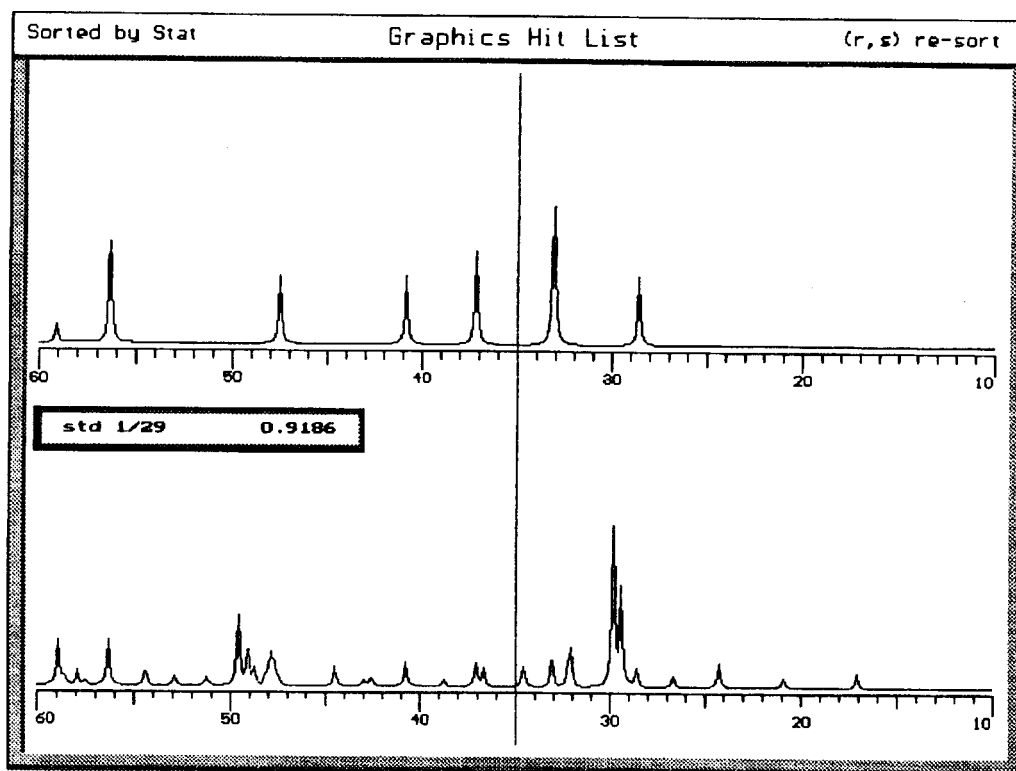


Fig. 5. Graphical output of analysis result.

standard must give for every sample and the minimum number of sample peaks which must be consistent with the given data are submitted.

The value of "error window" is given by the expression (1)

$$\Delta = d \pm EW \times 10^{-3} \times d^2 \quad (1)$$

and determines the tolerance interval in which the peak of a measured sample can be attributed to some of the standards. This indication is necessary not only because of objective and subjective errors but also because of real structure which has always influence on the position of peak. The value of error window is not constant. It depends on the position of peak.

Other function of searching makes possible to store the standards with low number of peaks, e.g. cubic substances in mixture with substances exhibiting small symmetry (Fig. 3). Otherwise these substances would automatically be excluded from the search because of the mentioned high values of criteria P and A.

Then we fix the number of standards after which the search stops and the experimental window in the range of measured angles  $2\theta$  where the search takes place. Both these functions accelerate the general course of analysis.

On the basis of criteria submitted beforehand the search proceeds and the real state of searching is so depicted that it can be decided according to preliminary results whether the analysis should continue. In opposite case, the procedure must be interrupted and the input data are to be modified.

If the continuation of analysis is approved, the search goes on and is subject to statistical and chemical criteria. The time of complete search depends on the type of applied computer, submitted criteria and, in particular, of the number of phases in the reference database. The searching of the whole database (circa 29 000 substances) with a computer IBM PC AT 286/16 takes approximately 4 min. For computer IBM PC AT 386/40 this time amounts to about 16 second. The use of the database for inorganic minerals (circa 2 900 substances) is the most frequent case and requires about 10 seconds. The time of analysis is also represented on display. The search finished, the results are presented in alpha-numerical or graphic form or are printed in the printer and if need be written in the data file according to wish of the user.

A typical representation of results in the form of table is given in Fig. 4. In the left part of output the diffractogram of measured substance is represented and in the right part the selected standards are arranged.

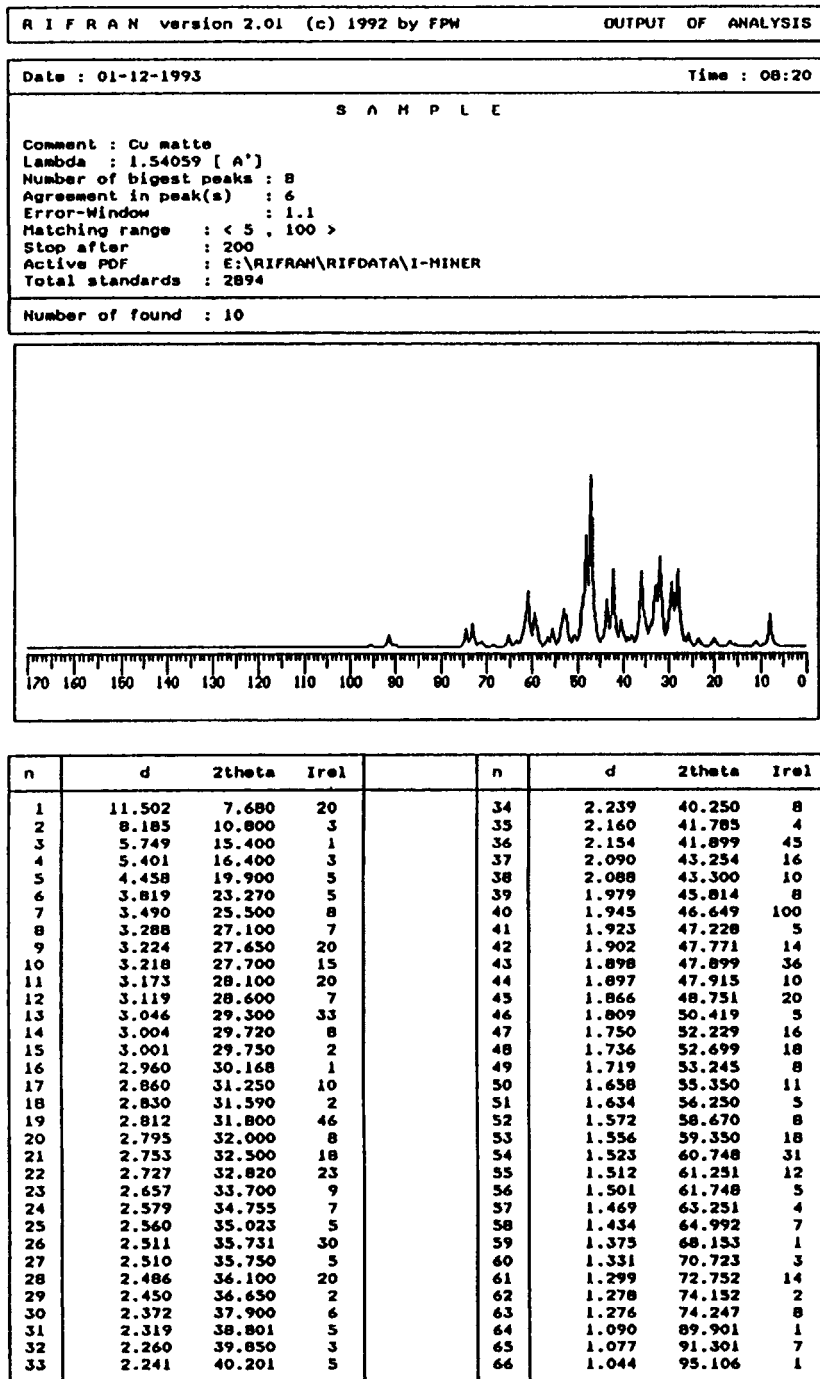


Fig. 6. Alpha-numerical output of analysis result.

They are ordered either according to chemical composition and the chemically non-correct standards are marked by an asterisk or according to statistical analysis. Normal classification of standards is governed by statistical criteria. These criteria are based on the ratio of the number of the diffraction attributed to

standard to the total possible number which is expressed by criterion P (Fig. 3). As there are many substances which have one or little intensive peaks (e.g. cristobalite  $\text{SiO}_2$ , PDF index equal 11-695), it could happen that such a substance would not satisfy the criterion in the case of its presence in mixture

Positive standards		
● 4-836	Copper Cu	Copper Syn 1.0000
● 25-1182	Iron Sulfide Fe <sub>9</sub> S <sub>11</sub>	Smythite 0.4754
● 6-464	Copper Sulfide Cu S	Covellite Syn 0.3905
● 9-324	Copper Iron Sulfide Cu Fe <sub>2</sub> S <sub>3</sub>	Cubanite 0.2716
● 11-151	Iron Sulfide Fe S	Troilite 0.2163
4-865	Potassium Sodium Aluminum Sulfate Hydr ( K, Na ) Al <sub>3</sub> ( O H ) <sub>6</sub> ( S O <sub>4</sub> ) <sub>2</sub>	Alunite 0.3395
11-253	Iron Aluminum Silicate Hydroxide Fe <sub>5</sub> Al <sub>4</sub> Si <sub>6</sub> O <sub>22</sub> ( O H ) <sub>2</sub>	Ferrogodrite 0.2545
11-61	Silver Iron Sulfide Ag Fe <sub>2</sub> S <sub>3</sub>	Sternbergite 0.2273
18-723	Lithium Beryllium Calcium Fluoride Sil Li <sub>2</sub> Ca <sub>3</sub> Be <sub>3</sub> ( Si O <sub>4</sub> ) <sub>3</sub> F <sub>2</sub>	Hsianghualite 0.2260
10-319	Manganese Iron Oxide Mn Fe <sub>2</sub> O <sub>4</sub>	Jacobsite Syn 0.2119

Fig. 6. Cont.

with other substances irrespective of this presence in large volume. In order to eliminate this risk, we use criterion I which quantities the ratio of the sum of all found integral intensities to the total possible sum of intensities. Then the product  $P \times I$  is a synthetic criterion and the found standards are ordered according to decreasing value of this product. We can also switch over and obtain the ordering according to chemical composition. In this case the chemically suitable standards are preferentially ordered in the same way.

By using a cursor passing the relevant standard substances the attained values of criteria are obtained. By depressing key Enter the complete PDF card of a given standard appears on the spot.

The results of analysis can also be expressed in the summary alpha-numerical form. In this case, the complete output is presented in descriptive form, i.e. PDF number, chemical formula, name and mineralogical term arranged according to the results of criterial analysis.

The results of analysis can also be represented in graphic form if the user demands. This mode allows to adjust the extent of results displayed in the angle range between  $2\theta_{\min}$  and  $2\theta_{\max}$  from left to right or vice versa. Fig. 5 represents a graphic output of the results of analysis. The diffraction pattern of measured sample is represented in the lower part whereas the diffraction pattern of relevant standard is in the upper part. By using the keyboard other standards can be shown according to the results of analysis. By depressing key Pause the complete PDF card of the pertinent standard appears.

The system enables us to depict a line cursor with fast or slow shift in graphic output and exactly to control the overlap of the investigated peaks of measured sample and standard.

The results of analysis in alpha-numerical or graphic forms can immediately be printed in a joined printer or written in data field for further use (Fig. 6).

The input data of every measured sample are automatically written in storage medium of the computer and provided they have not been cleared, they can be used together with the results of analysis any time in the future.

## CONCLUSION

The computer system RIFRAN represents a very useful and efficient aid for identification of polycrystalline substances by the X-ray diffraction method. It is fully compatible with the personal computers of class IBM AT working under operating system MS DOS. The joined database of standards containing almost 30 000 substances will entirely satisfy even the most exacting users. Moreover, the system permits all operations with the database, i.e. padding, copying, division, etc. All results obtained until now confirm the comparability of this system with contemporary modern systems [7, 8] which has been ascertained by direct comparison of these systems. The system significantly facilitates the analysis. However, the role of human is irreplaceable in this case like in the others.

The price of system RIFRAN is fixed by agreement. All demands for installation version of the system on 5.25" or 3.5" diskettes is to be addressed to : Tomas



Havlik, Department of Non-ferrous Metallurgy, Faculty of Metallurgy, Technical University, Letna 9/A, 043 85 Kosice, Slovakia.

## References

- [1] Fiala J.: *Silikáty*, 31, 173 (1978).
- [2] Nichols M. C.: UCRL - 70078, Lawrence Livermore Laboratory, 1966, Paper No. B-3, 1966.
- [3] Johnson G.G., Jr., Vand V.: *Ind. and Eng. Chem.*, 59, 19 (1967).
- [4] Frevel L.K., Adams C.E.: *Anal. Chemistry*, 30, 1335 (1968).
- [5] Schreiner W.N., Surdukowski C.: *J. Appl. Cryst.*, 15, 513 (1982).
- [6] Gobel H.E.: *Adv. X-Ray Analysis*, 24, 123 (1981).
- [7] Marquart R.G.: *Powder Diffraction*, 1, [1], 34 (1986).
- [8] Nakhmanson M.S., Fekhlincev M.S.: *Diagnostika sostava materialov rentgenodifrakcionnymi spektralnymi metodami*, Mashinostrojenie, Leningrad 1990.
- [9] Vasilijev E.K., Nakhmanson M.S.: *Kacestvennyj rentgenofazovyy analiz*, Nauka, Novosibirsk 1986.
- [10] Smith D.K., Gorter S.: *J. Appl. Cryst.*, 24, 369 (1991).
- [11] Frevel L.K.: *Newsletter No. 4, CPD*, January 1990, 2-3.
- [12] Hanawalt J.D., Rinn H.W., Frevel L.K.: *Ind. Eng. Chem. Anal.*, 10, 457 (1938).
- [13] Frevel L.K.: *Ind. Chem. Anal. Ed.*, 16, 209 (1944).
- [14] "Index", ASTM Special Technical Publication 48-M2, Philadelphia, PA, 1963.
- [15] Smith D.K.: *Am. Cryst. Assoc. Annual Meeting*, March 28-30, paper E11, 1963.
- [16] Frevel L.K.: *Anal. Chemistry*, 37, 471 (1965).
- [17] Frevel L.K., Adams C.E., Ruhberg L.: *J. Appl. Cryst.*, 9, 199 (1976).
- [18] Young R.A., Macie P.E., Von Dreele R.B.: *J. Appl. Cryst.*, 10, 262 (1977).
- [19] Marquart R.G., Katsnelson I., Milne G. W. A, Heller S.R., Johnson G.G. Jr., Jenkins R.: *J. Appl. Cryst.*, 12, 629 (1979).
- [20] Edmonds J. W.: *J. Appl. Cryst.*, 13, 191 (1980).
- [21] Frevel L.K.: *Anal. Chemistry*, 54, 691 (1982).
- [21] Huang T.G., Parrish W., Post B.: *Adv. in X-ray Analysis*, 26, 93 (1983).
- [23] Cherkuri S.C., Snyder R.L.: *Adv. in X-ray Analysis*, 26, 99 (1983).
- [24] Goehner R.P., Garbauskas M.F.: *Adv. X-ray Analysis*, 26, 81 (1983).
- [25] Lin T.H., Zhang S.Z., Chen L.J., Cai X.X.: *J. Appl. Cryst.*, 16, 150 (1983).
- [26] Carr M.J., Chambers W.F., Melgard D.: *Powder Diffraction*, 1, 226 (1986).
- [27] Škrobia M., Havlik T., Havlik M.: *Powder Diffraction*, 1, 235 (1986).
- [28] Jenkins R., Holomany M.: *Powder Diffraction*, 2, 215 (1987).
- [29] Škrobian M., Havlik T., Havlik M.: *Hutnícke listy*, 5, 341 (1985).
- [30] Havlík T., Škrobian M., Havlík M., Petričko F.: *Silikáty*, 34, 38 (1990).

- [31] Havlík T., Škrobian M., Petričko F., Havlík M.: *Zborník "Aplikácia difrakčných metód v materiálovom výskume a praxi"*, Herlany máj 1991, 141-145.
- [32] Moravcova H., Fiala J.: *Vestník ustr. ustavu geologickeho*, 55, [4], 237 (1980).

Submitted in English by the authors

## AUTOMATICKÁ KVALITÁTVNA PRÁŠKOVÁ DIFRAKČNÁ FÁZOVÁ ANALÝZA: SYSTÉM RIFRAN 2.0

TOMÁŠ HAVLÍK, MILAN ŠKROBIAN, FRANTIŠEK  
PETRIČKO

*Katedra kovohutníctva, Hutnícka fakulta, Technická  
Univerzita, Letná 9/A, 043 85 Košice*

Systém RIFRAN (Rýchla Identifikácia Fáz Rentgenovou Analýzou) predstavuje novú generáciu vo svojom vývojom rade, prístupný pre široký okruh užívateľov a plne kompaktilný s počítačmi IBM PC/AT pracujúcim pod operačným systémom MS DOS, alebo DR DOS. Program je napísaný v jazyku Borland Turbo C++.

Základná myšlienka analýzy spočíva vo vektorovom vyjadrení difraktogramov neznámej vzorky a štandardov. Analýza spočíva v porovnaní polôh jednotlivých difrakcií meranej vzorky s polohami difrakcií štandardov uložených v databáze. Takto získané štandardy sa v prvom kole („search“) podľa predom zadaných obmedzení podrobia kritériálnej a chemickej analýze („match“).

Karta štandardu, zaradeného do databázy bola konštruovaná tak, aby bola formálne i funkčne kompaktilná so štandardnou kartou bázy Powder Diffraction File of the JCPDS - International Centre for Diffraction Data. Číslovanie kariet je zachované podľa PDF.

Všetky zápisy sú v binárnej forme. Takýmto spôsobom je zabezpečený veľmi rýchly prístup k údajom štandardných látok ako pre samotnú analýzu, tak aj pre ďalšiu prácu s databázou.

V súčasnosti obsahuje databáza asi 29 000 štandardných záznamov a databáza je podľa potreby a dostupnosti publikovaných údajov priebežne doplňovaná. V súčasnosti je pozornosť zameraná najmä na nové materiály, ako supravodiče, keramiku a podobne.

Výsledky analýzy môžu byť zobrazené podľa želania užívateľa v alfanumerickej podobe, v grafickom móde, alebo zapísať ich do datového súboru na pamäťové médium. Všetky výsledky možno tlačiť na pripojenej tlačiarni.

Všetky ďalšie informácie o ďalšom vývoji systému Rifran, prípadne možnosti jeho používania ochotne poskytnú jeho autori, vrátane domonštračnej verzie programu na 5.25" alebo 3.5" diskete.

*Obr. 1. Ponuku vyhládavania v otvorenej databáze.*

*Obr. 2. Zadavanie údajov o meranej vzorke.*

*Obr. 3. Vstupné údaje pre kritériálnu analýzu.*

*Obr. 4. Výstup analýzy na obrazovke počítača.*

*Obr. 5. Grafický výstup výsledkov analýzy.*

*Obr. 6. Tabulkový výstup výsledkov analýzy.*