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Powder Diffraction Program Information 1990 Program List*

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General comments and disclaimer

Over 280 programs for the analysis of powder diffraction data have been identified in this compilation. On the basis of information supplied by the program authors, the programs have been grouped into categories appropriate to the major type of calculation performed. The 21 categories which have been identified are:

Crystallographic databases
Analysis packages
Instrument control and data processing
d generation
Graphical *d*–*I* display
Phase identification
Automatic indexing
Refinement/indexing
Refinement/error analysis
Metric analysis
Pattern generation
Profile fitting – decomposition
Profile fitting – full pattern
Deconvolution
Crystallinity/strain/texture
Rietveld – structure refinement
Quantitative analysis
Structure determination (powder)
Structure display
Small-angle scattering
Miscellaneous programs.

For each program listed, information on the programming language, type of computer needed, conditions on the availability and support of the code and the program author or alternative source for the program is provided. Addresses of program authors and references are also given for all programs where available. Compiling this information has been a considerable undertaking and many programs may have been missed. As corrections and more programs are brought to the attention of the publication authors, they will be added to the master files and an update to this list will be prepared when the time is appropriate.

Many of the programs produce the same results as do other programs in the same category, so the diffractionist certainly does not need to acquire every program in the list to have a complete system of programs. However, because there are differences in programs for similar purposes, it is usually advisable to have more than one routine from a given group. Multiple programs are particularly valuable when the calculations involve different strategies on experimental data that are not free of errors. Selection of programs for one's own use depends on the types of experiments commonly performed and on the type of computer that is available.

The questionnaire which was used to collect the program information had several questions designed

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to obtain some statistical information on the computers in use and to determine if there might be a way to improve program distribution. There is no doubt that Fortran is still the most common programming language in use. Fortran77 was mentioned frequently, but other Fortran compilers were also indicated. Different compilers often have some subtle differences due to extensions above the Fortran77 standard which may mean that the codes may not compile the first time on a different compiler. The diagnostics produced usually flag the problems sufficiently for the typical programmer to work around the problem. Maybe 10% of the cases will involve more elaborate corrective measures.

Basic was the other language used frequently, mostly for PC programs. The problems of porting programs from one level of Basic to another is similar to Fortran, but the differences are greater. Many of the main-frame computers have Basic compilers which can intepret the PC languages, but it is usually easier to go from the main-frame to the PC than *vice versa*. Other languages such as C and Pascal were used in very few cases. It is evident that a universal language would be ideal, but it will never be developed.

The most common main-frame computers mentioned are the IBM and VAX series, but FACOM, Cray and others are used. Among the PC types, the IBM and compatibles were the most common, but the diversity of other manufacturers was significant. There was more variety in Europe and Japan than elsewhere. The Macintosh, which is a common system in the US for offices and manuscript preparation, was barely mentioned. The diversity of computers complicates the portability of programs, particularly when file manipulations are involved. Regardless, there has been considerable success in porting programs from one computer to another.

Program documentation also shows diversity both in the manner presented, some as text files and others as manuals, and in the detail that is in the instructions. Programs which are distributed free usually have very skimpy instructions. Some expensive commercial programs are well documented but not all. Preparing good manuals is difficult and time consuming. Freeware usually does not justify the necessary time as there are few benefits to the program author. For commercial programs, there is no excuse for poor instructions. For ease of distribution, the machine-readable file is ideal, but a good manual is easier to use and easier to illustrate with equations, plots and sketches. Examples of worked problems should always be provided to assist the user in implementing programs for the first time and as tests that the program has been installed properly.

A general problem the publication authors have found with most of the programs that have been tried is the difficulty of setting up the input files. Very few of the routines have an interactive front-end set-up program and those that do rarely test the interactive responses for reasonableness. Default values or reasonable responses should be offered for every question and any answer entered should be tested by the program and rejected if it falls outside a preset range. The rejection should return the respondent to the question rather than corrupt file preparation or accept the bad value for later disruption of the run. For example, if a wavelength of 200 Å is entered, it should not be accepted. Hopefully, future versions of popular programs will improve in this aspect.

One of the questionnaire inquiries was designed to test the interest and to evaluate the feasibility of establishing some means for assisting with program distribution. One option would be to set up a few centres willing to maintain the most current versions of programs supplied by program authors and to provide program copies on request for a copying charge. The advantage of the centre would be the currentness but the disadvantage would be the time and effort required to maintain the operation. In fact, the Dutch Association of Crystallographers have already founded such a centre.

The other problem with a central distribution centre is only a partial acceptance of the idea by the program authors. Many program authors would welcome the chance to supply only one centre with current versions but other program authors prefer to maintain more control over the program distribution. Commercial programs would have to be distributed by the producer. Obviously, full implementation of this option is not imminent.

The publication authors make no claim with respect to the completeness or accuracy in the coverage of the programs described in this list nor for their success in doing the calculations that are reported. It has been a formidable task to assemble this list, and we wish to thank the many contributors who have supplied information on programs with which we have had no direct experience. Some of the programs may have been misclassified and some may have codes misassigned, but without first-hand experience, it is difficult to be perfect. World-wide coverage has been the goal of this project, but some geographic regions are probably under reported. One hopes that the next list will be more nearly complete.

Although this list has been compiled under the auspices of the International Union of Crystallography and its Commission on Powder Diffraction, these bodies disclaim any responsibility for the effectiveness or availability of the programs listed. No endorsement of any program is implied by its inclusion in this list.

Table 1. *Codes used in the program lists*

Program language

A	Assembly	GWB	GW Basic
Alg	Algol	*P*	Pascal
B	Basic	QB	Quick Basic
C	C	TB	Turbo Basic
F	Fortran IV, 77, ANSI	TC	Turbo C
GFA	Atari	TP	Turbo Pascal

Computer type

MF	Main-frames	CDC, Cray, IBM, PDP, VAX
PC	Personal computer	IBM, MAC
TS	Time-sharing	
O	Other types	ENCORE, FACOM, PRIME

Distribution form of program codes

S	Source code
E	Execution codes only
EK	Key required to run
EP	Execution codes only with permission of Philips Netherlands

Costs and conditions for distribution of codes

C	Commercial product
F	Free
L	Lease and fee
$	Small fee < $100
$$	Large fee > $100
FL	Free for noncommercial users; lease and fee for commercial users

Type of documentation

DF	Machine-readable documentation
M	Manual
N	No documentation
R	Reference

Program support

A	Author support
N	No support
Blank	No indication

Program sources

PEB	Program is available from the Powder Diffraction Software Exchange Bank of the Dutch Association of Crystallographers.
*	Source address or reference not available
OLD	An old program available from many sources

Introduction

This list of computer programs for powder diffraction analysis of materials, prepared at the request of the International Union of Crystallography Commission on Powder Diffraction, is an update to the list prepared for the Mineralogical Society of America as part of their Short Course on Modern Powder Diffraction (Smith, 1989) augmented by contacting all the identified program authors with a standard form to increase the database of descriptive information and correct any misrepresentations. Many new programs have also been added. Most new programs were located by contacts made at meetings and through the literature. Each new program author was requested to supply the same information on the standard form to supplement the database. This list will never be complete because powder diffraction is a very dynamic field and new programs are being prepared all the time. Many of the listed programs continue to be revised and upgraded as new ideas occur to the program author and users supply suggestions. It is impossible to keep up with all these changes. This list may be revised and reprinted about every two years if there is sufficient interest and program authors continue to supply information to maintain the database.

The selection of programs for this listing has not been limited to software which is distributed free or with a small distribution charge. Commercial software has been included where the program is distributed independently of a package including hardware. This decision is based on several factors. First, the main purpose of this list is to disseminate information to potential users as to where they may acquire the necessary software to meet their specific needs. Second, although free software used to be the norm in the scientific society, times have changed. The cost of programming is rarely supported in modern research and analysis and computers have become so sophisticated that good programming requires time and effort of a specialist. Third, the commercial program is usually more refined and easier to use. The proportion of free programs is higher for main-frame computers than for personal computers also. Part of the reason for this situation is that many of the PC routines are conversions of programs which were first developed for main-frames. These conversions are usually done by entrepreneurs taking advantage of the change of our computing base from the main-frame to the PC. This trend will continue for the foreseeable future. The program list indicates the type of computer for which the program is intended.

This program list is divided into general categories based on the type of calculation being performed and the nature of the data being analysed. The categories are generally recognized stages in powder diffraction analysis such as phase identification, indexing of a data set, phase quantification, structure refinement *etc.* All older programs used discrete *d* spacings and intensities, but many of the recent programs work directly on the digitized raw diffraction trace. Within each category, there is no effort to rank or evaluate programs. That decision is up to the user. The publication authors have not had experience with every program in the list so such an evaluation would be impossible. For a specific laboratory, only one program from a specific category, such as Rietveld analysis, might be sufficient, whereas from other categories, such as phase identification or indexing, several programs would be desirable where the results from each could be compared. There is a descriptive paragraph with each category listing which may assist the beginner in selecting programs but, in general, the discussions will not promote any specific program.

The information in the list accompanying each program entry indicates the programming language, the nature of the code which will be distributed, any costs involved, information on documentation and whether the program author will support the code. The meaning of the various symbols is listed in Table 1. The program author or other source for obtaining copies of the program are listed in the last column. This entry may refer to an address for requesting the program or to a reference which will have more information. The addresses are listed in the Appendix under the program author or company name. Every effort has been made to make this list accurate, but the publication authors disclaim any responsibility for errors that might exist. All errors should be brought to the attention of the publication authors for correction in subsequent lists.

Program descriptions

Crystallographic databases

	Computer						
Database	MF	PC	TS	CD-ROM	Distribution	Form	Source
CD	+	+	−	+	*L*	*S*	ICDD
CD	−	−	+	−	TS		NRCC
CSD	+	−	−	−	*L*	*S*	Cambridge
EDD	+	+	−	+	*L*	*S*	ICDD
ICSD	+	−	+	+	*L*	*S*	FIZ
MSD	+	−	+	−	*L*	*S*	NRCC
PDF	+	+	−	+	*L*	*S*	ICDD

CD	= Crystal Data	Mighell/Himes
CSD	= Cambridge Structural Database	Kennard/Watson
EDD	= Electron Diffraction Database	Carr
ICSD	= Inorganic Crystal Structure Database	Bergerhoff/Brown, I. D.
MSD	= Metals Structures Database	Rodgers/Wood
PDF	= Powder Diffraction File	Jenkins/Smith, D.

Although the Powder Diffraction File has been the primary source of powder-diffraction-pattern information for over 50 years, there are several other databases that are very important for modern analyses. The assembling, editing and maintenance of large databases is not a simple undertaking. The time required dictates that the operation is full-time, usually involving several individuals. Support for the operations varies with some being totally dependent on the sales of the database and others receiving some federal and industrial financial assistance. Even with the subsidies, the costs of operating databases require that the distribution of the data be controlled through legal agreements that restrict the copying of the data and use by third parties. Regardless of the costs, the value of the information in these databases makes them a necessity in the package of computer programs for data analysis in almost every laboratory.

The Powder Diffraction File, PDF, contains selected *d*-spacing and intensity patterns for over 50 000 inorganic and organic compounds along with supporting crystallographic and reference information. These data sets are the basis for phase identification and characterization. Crystal structure descriptions are the main information in the Inorganic Crystal Structure Database ICSD, the Metals Structure Database MSD and the Cambridge Structural Database CSD. For the powder diffractionist, these descriptions may be starting data sets for calculating powder diffraction patterns or for Rietveld refinements. Crystal Data, CD, is a compendium of unit-cell information with over 149 000 entries. If the cell parameters of a compound are known, the compound may be identified using this database. It is also an excellent resource for literature references by looking up specific compounds. The Electron Diffraction Database, EDD, is a derivative of the PDF and CD which uses the crystallographic data to calculate diffraction patterns appropriate to electron diffraction.

Among these databases, only the PDF is fully available in hard-copy form. Most of them have some derivative products in book form, but not the full database. All these databases are now available in computer-readable form. In fact, all the operations consider the computer-readable product as the primary goal and hard-copy forms may soon disappear completely. Some of the databases are available through on-line subscription services but the costs of connection usually limit the utility of this method of use. All the databases are distributed by lease on magnetic media and, with the increasing interest in CD-ROM, most of the databases are now available on this medium. Manufacturers of automated powder diffractometers, APD, usually incorporate the PDF in their software package and will probably start including the other databases as soon as software is developed around their use.

Analysis packages

Program	Language	Computer MF	Computer PC	Form	Cost	Support	Documentation	Source
ATARI	*B*	−	+	*E*	*F*	*A*	DF	Melzer
AUTO	*F*	+	−	*S*	*F*	*A*	DF	Snyder
CRYSTALS	*F*	+	−		$$	*A*		Watkin
CSD	*F*	+	+	*S*	*C*	*A*	*M*	Tsytsenko
DIFFRACTINEL	*F,A*	−	+	*E*	*C*	*A*	*M*	INEL
GSAS	*F*	+	−	*E*	*F*	*A*	DF	Larsen/Von Dreele
NRC/VAX	*F*	+	−	*S*	$	*A*	DF	Gabe
PATCOM	*C,F,P*	−	+	*S*	*C*	*A*	DF	Cherner
PC/NRC	*F*	−	+	*S*	$	*A*	DF	White
SHELXS-86	*F*	+	−	*S*	*F*	*A*	*M*	Sheldrick
SHELXTL-Plus	*F,A*	+	−	*E*	*C*	*A*	DF	Sheldrick
SHELXTL/PC	*F,A*	−	+	*E*	*C*	*A*	DF	Sheldrick
*SIR*88	*F*	+	−	*S*		*A*	DF	Burla
TEXSAN	*F*	+	−	*S*	*C*	*A*	DF	TEXSAN
XPAS	*B*	−	+	*S*	*F*	*A*	*M*	Singh/Gilkes
XTAL	*F*	+	−	*S*		*A*	*M*	Hall/Stewart
ZEOPAK	*F*	+	−	*S*	$$	*A*	DF	Johnson, G./Smith, D.

Although the main purpose of this list is to identify individual programs, there are several packages of programs which include many of the individual programs of interest to powder diffractionists. All APD manufacturers have a package of analytical programs which accompany their data-collection software, but they do not make the package available without the purchase of the hardware. *AUTO*, *DIFFRACTINEL* and *ZEOPAK* are packages specifically designed for powder applications which are independent of hardware and a new user would be advised to look into starting with such a package. All the other packages on this list are designed primarily for the single-crystal diffractionist, but they do contain some of the 'powder' programs. These packages vary considerably in cost to the user and in ease of implementation. It would be advisable to contact the program authors for more information.

Instrument control and data processing

Program	Language		Computer MF	Computer PC	Form	Cost	Support	Documentation	Source
ABSCYL	FM*	*F*	+	−	*S*	*F*	*A*	DF	Helmholdt/PEB
++ADM++			−	+	*S*	*L*	*A*	*M*	Wassermann/Lorenz
ADR	DC	*F*	+	−	*S*	*F*	*A*	DF	Mallory/Snyder
AUTOPEAK	PF	*F*	+	−	*S*	*F*	*A*	DF	RAL
BACKER	FM	*F*	+	−	*S*	*F*	*A*	DF	RAL
BKGRD	FM	*F*	+	−	*S*	$$	*A*	DF	Smith, D.
CALIBER/VAX	FM	*F*	+	−	*S*	*F*	*A*	DF	Hubbard
CALIBR/90	FM	*F*	−	+	*E*	$	*A*	DF	Hubbard
COMPOUND COR	FM	*F*	+	−	EP	FL	*A*	DF	Jansen/PEB
CONTAIN C	FM	*F*	+	−	EP	FL	*A*	DF	Jansen/PEB
DELREF	FM	*F*	+	−	EP	FL	*A*	DF	Jansen/PEB
DIFFRAC	PF	TP	−	+	*S*	*F*	*A*	DF	Allman/PEB
DIFFRACT-AT/BASIC	DC	*F,A*	−	+	*E*	*C*	*A*	*M*	Socabim
DRX	DC	QB	−	+	*E*	*F*	*N*	*M*	Vila (1)
ECN TO PHILIPS	FM	*F*	+	−	EP	FL	*A*	DF	Jansen/PEB
EXCHANGE	FM	*F*	+	−	*E*	*C*	*A*	DF	Socabim
GUFI	FR	*F*	+	+	*E*	$$	*A*	*M*	Dinnebier/Eysel
INTCAL	FM	*F*	+	−	*S*	*F*	*A*	DF	Snyder
I.S.I.P.	DC	TB	−	+	*E*	*F*	*A*	*R*	Rogers/Lane
JCAMP-DX	FM	*B*	+	+	*S*	*C*	*A*	*M*	McDonald/Wilks
JCAMP-PDF	FM	*F*	+	−	*S*	*F*	*A*	DF	Toby/PEB
LATCO	PF	TP,*F*	−	+	*S*	*F*	*A*	DF	Allman/PEB
MicroPEAK	PF	*F*	−	+	EK	*C*	*A*	*M*	Johnson, Q.
PDF2	DC	*B*	−	+	*S*	*F*	*A*	DF	Allman/PEB
PEAK	PF	*F*	+	−	*S*	*F*	*A*	DF	Sonneveld/Visser/PEB
QUASAR	FM	*F*	+	−	*S*	*F*	*A*	DF	Hall/PEB
REBIN RD	FM	*F*	+	−	EP	FL	*A*	DF	Jansen/PEB
RD TO ASCII	FM	*F*	+	−	EP	FL	*A*	DF	Jansen/PEB
SCALE RD	FM	*F*	+	−	EP	FL	*A*	DF	Jansen/PEB
SCAN	FR	TP,*F*	+	+	*S*	*C*	*A*	DF	Eriksson
SCANPI	FR	*F*	+	+	*S*	*C*	*A*	DF	Werner
SPECPLOT	PF	*F*	+	−	*S*	*F*	*N*	*M*	Goehner
VAXCON	FM	*F*	+	−	*S*	*F*	*A*	DF	Zhou/Snyder
ZERO SHIFT	FM	*F*	+	−	EP	FL	*A*	DF	Jansen/PEB

* DC = diffractometer control; FM = file manipulation; FR = film reading; PF = peak finding.

Before one can interpret data, one must collect it. All the APD manufacturers supply the data-collection software with their hardware, but there are many programs written for situations where the laboratory is automating their own hardware. The big trend in instrument control is towards the PC as the control computer both from the lower cost to the laboratory and the ease of using the PC as a stand-alone system. The capabilities of the PC have improved in capacity and speed so that it can eliminate the dependence of the laboratory on the central computer facilities for both instrument control and data analysis.

The programs which fall in the category of data collection and data processing may be subdivided into sections: diffractometer control, film reading, file manipulation and peak finding. These divisions are indicated by DC, FR, FM and PF respectively in the table. Film-reading programs are for processing Guinier films with a densitometer. They contain peak-locating algorithms as well as the densitometer interface. The file-management programs are designed to process digitized diffraction traces either transferring them from one format to another for interinstrument communication or to prepare the file for preliminary analysis such as background stripping and internal standard calibration. The peak-finding packages specifically convert the digitized data to *d* spacings and associated intensities. Several of these programs are hardware specific, especially the film-reading programs. On the other hand, programs like *JCAMP-DX* and *VAXCOM* are designed to allow the interpretation of files from many different types of hardware.

d generation

Program	Language	Computer MF	Computer PC	Form	Cost	Support	Documentation	Source
d-SPACE	*F*	−	+	*S*	*F*	*A*	DF	Nickel
GNHKL	*F*	−	+	*S*	*F*	*A*	*M*	Prewitt
Lines-2.0	*B*	−	+	*S*	*F*	*A*	DF	de Graff/PEB
XRD	*F*	+	+	*S*	*F*	*A*	DF	Kimmel

(Many others including indexing routines.)

Probably the single most common program in powder analysis is the generation of the *d* spacings given a specific crystallographic unit cell. There are so many versions that it would be fruitless to try and locate them all. What is included in the list are routines which were mentioned on the questionnaires supplied to obtain the other information in this report. Many of the other programs listed under other categories in this report contain *d*-spacing generators as part of the general calculation. All the indexing and cell-refinement programs generate *d* spacings and so do the intensity-calculating programs. Also, it is relatively easy to program the readily available pocket calculators to do this calculation.

Perhaps it is appropriate to mention here that there are also many programs which will prepare tables of angle-to-*d*-spacing conversions and perform other simple calculations. Although these tables are essentially made obsolete by the peak-finding procedures, there is still occasional need to check graphical plots for the corresponding *d* values. This calculation is easy to program on the pocket calculator or to add to any working package. However, the utility of having a package of these simple programs on the laboratory computer is not to be underestimated. The publication authors have often used a collection of small programs to calculate crystal densities, absorption coefficients, compound weight percents, equivalent Miller indices, angles between crystal directions *etc*.

Graphical *d–I* display

Program	Language	Computer MF	Computer PC	Form	Cost	Support	Documentation	Source
MicroDSPACE	*F*	−	+	EK	*C*	*A*	*M*	Johnson, Q.
μPDF	*F*	−	+	*E*	*C*	*A*	*M*	Marquart
PATCOM	*C,F,P*	−	+	*E*	*C*	*A*		Cherner
PLOT-RD	*F*	+	−	*S*	*F*	*A*	DF	Jansen/PEB
PPDP	*F,A*	+	+	*E*	$	*A*	DF	Okamoto/Kawahara
SIMUL/COMBIN	*F*	+	−	*S*	SS	*A*	DF	Smith, D.
SPECPLOT	*F*	+		*S*	*F*	*N*	*M*	Goehner
XRAYPLOT	*B*	−	+	*S*	*F*		*M*	Canfield

Graphical displays of powder patterns from databases or other *d–I* data sets are a necessity for the visualization of the agreement of experimental data and its interpretation. The diffractionist has most confidence in examining the raw diffraction trace against the diffraction traces of the phases which are most likely to comprise the sample under study. On-screen graphics allow the user to parallel or superimpose the traces for visual matching. Usually, the display used the simplest histogram form for display of the database information patterns, but some of the routines on the list use simulated peak shapes from triangles to analytical profiles. The closer the calculated peak shape is to the actual experimental shape, the easier it is to interpret the agreement. Programs involving graphics are often hard to transport because the graphics hardware is so varied, but the calculation routine would be essentially identical. Individuals familiar with PC graphics could adapt any of the free routines to almost any situation.

Phase identification

Program	Language	Computer MF	Computer PC	Form	Cost	Support	Documentation	Source
AFPY/AFPB	*F*	+	−	*S*	*F*	*A*	*R*	Fiala
DC26	*F*	−	+	*S*	*F*	*A*	*M*	Fiala
DIFFRAC-AT/SEARCH	*F,A*	−	+	*E*	*C*	*A*	*M*	Socabim
FAZAN	*F,P*	−	+	*S*	$$	*A*	DF	Burova
FSRCH	*F,A*	+	−	*S*	*F*	*A*	*M*	Carr
JOHNSON/VAND	*F*	+	−	*S*	*F*	*A*	DF	Johnson, G.
MicroID	*F*	−	+	EK	*C*	*A*	*M*	Johnson, Q.
μPDSM	*F,A*	−	+	*E*	*C*	*A*	*M*	Marquart
++PADS++		+	−	*E*	*C*	*A*	*M*	Wassermann
POWDER SUITE	*F,A*	+	−	*S*	*F*	*A*	DF	Toby/Harlow
PRIDENT	*F*	+	−	*S*	*F*	*N*	*R*	Garbauskas
SEARCH	*F*	−	+	*E*	*C*	*A*	*R*	Sietronics
SEARCH/MATCH	*F*	+		*S*		*A*	*R*	Lin
WAIT	*F*	−	+	*E*	$$	*A*	*M*	O'Connor
XRDQUAL	*F*	+	−	*S*	*F*	*N*	DF	Clayton/PEB
XRDCS/MS	*F*	+	+	*E*	$$	*A*	*M*	O'Connor
ZRD/SEARCH	*F*	+	−	*S*	$$	*N*	*R*	Siemens

Identification of phases by comparing the experimental set of d's and I's against the patterns in a database such as the PDF is probably the single most used application of powder diffraction. As soon as computers became well established in the early 1960's, programs were written to accomplish this goal. Numerical matching of extended data sets is tedious for individuals, so it is natural that computers be employed to perform the main task of searching the database. The problem increases in difficulty as the size of the databases continues to grow. The goal of search programs is to scan the full reference database selecting the phases with the highest probability of comprising the unknown phase. With simple problems or with luck, the complete answer can be located, but usually the problem is complex and the program can only rank the answers based on some algorithm and present the table of candidates to the user for the final decision. All of the programs available today use this philosophy.

Among the many search programs that are available, no two use exactly the same search strategy. Because the computer is tireless, a trial-and-error approach is feasible. Essentially every pattern in the database is tested during each run using prescreening or specifically ordered data files to minimize the number of steps involved. The basic question asked of each pattern is what is the probability of the reference pattern being contained in the pattern of the unknown. Some figure of merit is assigned the pattern and in the final presentation a list of candidate phases is presented ranked on the figure of merit. The most successful programs are not always the ones that run the fastest.

All the search programs contain routines that allow the user to evaluate the candidate phases by matching the d–I data sets with the experimental data. This step is known as the match step and is always necessary to evaluate the search candidates. This comparison may be numerical or it may be graphical involving some of the displays described in the previous section. Numerical matching is often less convincing because the small d-spacing errors require numerical windows for proper alignment.

Because search programs are so different in their procedures of manipulating experimental data, their success also varies considerably. There are often many tricks to getting the best results which come from long experience with a specific program. Program authors always have more success than casual users. Typically, users find one program to their liking, often based on some early successes, and then never try any of the other routines. Probably the best procedure is to employ two or three of these routines on complex problems and compare the different results to determine the best answer. Comparison of programs is made easier by set-up programs that take the standard d–I data set from the peak-finding routine and prepare the input files in the proper formats for the specific search programs. Such set-up routines are only available in packages where several search programs are used. Users can write their own set-up programs, and the time will usually be well spent.

Automatic indexing

Program	Language	Computer MF	PC	Form	Cost	Support	Documentation	Source
AIDED	*F*	+	–				*R*	Setten
DELAUNAY	*F*	+	–	*S*	*F*	*A*	DF	Gorter/PEB
DICVOL	*F*	+	–	*S*	*F*	*A*	DF	Louër/PEB
*DICVOL*90	*F*	+	–	*S*	*F*	*A*	DF	Louër
GOEBEL/WILSON	*F*	+	–	*S*	*F*		*R*	OLD/PEB
ITO	*F*	+	+	*S*	*F*	*A*	DF	Visser/PEB
KOHL	*F*	+	+	*S*	$	*A*	*R*	Kohlbeck/PEB
LINES 2.0	GFA	–	+	*S*	$	*A*	*M*	de Graaff/PEB
MicroINDEX	*F*	–	+	EK	*C*	*A*	*M*	Johnson, Q.
POWDMULT	*F*	+	+	*S*	$	*A*	DF	Wu
PWDCDS (*POWDER*)	*F*,*A*	+	+	*S*	*F*	*A*	*R*	Taupin/PEB
SCANIX 2.0	*F*	–	+	*E*	$	*S*	DF	Paszkowicz
TRANSFOR	*F*	+	–	*S*	*F*	*A*	DF	Gorter/PEB
TREOR-5	*F*	+	+	*S*	*F*	*A*	DF	Werner
TREOR-90	*F*	+	–	*S*	*F*	*A*	DF	Werner/PEB

With the increased accuracy of the data obtainable from the APD, indexing procedures are becoming more successful. Although indexing procedures date back to the 1960's, the more sophisticated routines were started in the 1970's, and there has been a recent rejuvenation of interest and improvement in these programs. All of the early programs were written for main-frame computers, but the current programs are being directed towards the PC. Most of the major routines are now available in PC form. The main-frame programs are all free, but the PC versions are not.

The programs fall into two broad classes depending on whether they use trial-and-error methods or analytical methods as the basis of the calculations. Trial-and-error methods assume a specific crystal system and attempt to fit the data to the indexing equation for that crystal system. Large d spacings are used as guides to initial cell-parameter selections. Analytical methods assume the crystal is triclinic, then examine the lattice for higher symmetry. The more successful routines use limitations such as cell size or cell volume to keep the calculations in bounds. Some of the programs are, by design, more successful with specific crystal systems; no single program is truly universal in its application. It is best for the user to have at least three indexing routines available and perhaps as many as five.

The single most important factor which controls the success of indexing regardless which routine is employed is the accuracy of the data. Accuracy means that the data are measured to angle errors of less than $0{\cdot}03°\,2\theta$ and that the data have been corrected for systematic diffractometer errors. With this accuracy, the success rate is around 90%. Optimal indexing usually uses 20 to 30 low-angle peaks, but some high-symmetry cells can be solved with fewer peaks. Some users give up when indexing does not solve all their problems, but this result is not a good criterion as some unit cells are unusual with extremely long axes in one direction or pseudosymmetric which makes a solution difficult even with perfect data. The best success is often achieved by comparing the results of several indexing trials with different programs. Where the same answer is reached by several programs, success is usually assured. However, sometimes derivative cells are located and further tests are needed. That is where cell reduction routines to be described below under metric analysis are useful.

Refinement/indexing

Program	Language	Computer MF	PC	Form	Cost	Support	Documentation	Source
APPLEMAN	*F*	+	–	*S*	*F*	*N*	DF	Appleman/PEB
INDEXING	*B*	–	+	*S*	*F*		*R*	Novak/Colville
LAPOD	*F*	+	–	*S*	*F*	*A*	*R*	Langford
LSCURI/PC	TP	–	+	*S*	*F*	*A*	DF	Garvey
*LSQ*85	*F*	+	–	*S*	*F*	*A*	DF	Hubbard/PEB
*LSQ*90/*PC*	*F*	–	+	*E*	$	*A*	DF	Hubbard
*LSQ*90/*VAX*	*F*	–	+	*S*	*F*	*A*	DF	Hubbard
*NBS***LSQ*85	*F*	+	–	*S*	*F*	*A*	*M*	Mighell
PC/APPLEVANS	*F*	–	+	*S*	*F*	*N*	*M*	Benoit
PCPIRUMF	+	+	*S*	*F*	*A*	*R*	Werner/Eriksson	
POWD/MULT	*F*	+	+	*S*	$	*A*	DF	Wu
PPLP	*F*	+	–	*S*	$	*A*	DF	Gabe

Where a cell is already known, it can be used as the starting point for indexing the pattern. For high-symmetry compounds, such indexing is usually trivial, but for low-symmetry compounds, this is not often the case. One can usually assign Miller indices to the low-angle peaks with confidence but not the high-angle peaks. Refinement/indexing programs use the philosophy that the low-angle peaks can be used to improve the cell parameters which can then be used to index the higher-angle lines. This procedure can be iterative to index all the peaks in the pattern. The *APPLEMAN* program, written in the late 1950's is the best known of these programs, and all the other programs in this category are derivatives of this routine.

Refinement/error analysis

Program	Language	Computer MF	PC	Form	Cost	Support	Documentation	Source
ARGONNE/B-106	*F*	+	−	*S*	*F*	*N*	*R*	Mueller/PEB
EXDIF	*F*	+	+	*S*	*F*	*A*	DF	Kimmel
FINAX	*F*	−	+	*S*	$$	*A*	DF	Hovestreydt
LCLSQ-8·2	*F*	+	+	*S*	$	*A*	*M*	Burnham/PEB
LUPIN/LOOPY	*F*	+	−	*S*	*F*	*A*	DF	Brown, A.
Micro-CELLREF	*F*	−	+	EK	C	*A*	*M*	Johnson, Q.
PC/CELRF	*B*	−	+	*S*	*F*	*A*	*M*	Prewitt
PODEX	*F*	+	−	*S*	*F*		DF	Foris
POWDRFIT	*F*	−	+	*S*	*F*	*N*	DF	Caillat/Bartell

The problem with refinement coupled with indexing is that there is no way to include error analysis because drift would occur in the data matching as the indexing proceeds to higher angles. To include error analysis, all the Miller indices must be assigned prior to the calculation. Then, an error function can be included with the calculation. Actually, it is not necessary to know the error *a priori* because several errors can be tried, and the best-fit data results can indicate the most probable error. The oldest of these programs is *ARGONNE/B*-106 and the other programs essentially follow this routine.

Because this calculation is mathematical rather than trial and error in nature, it is not necessary to have more than one routine in one's analysis package. All of the listed routines are essentially equivalent.

Metric analysis

Program	Language	Computer MF	PC	Form	Cost	Support	Documentation	Source
BOOLEAN/LATTICE	*F*	+	−	*S*	*F*	*A*	DF	Johnson, G.
CREDUC	*F*	+	−	*S*	*F*		DF	Gabe
EDD/UNITCELL	*F*	+	−	*S*	*F*	*A*	DF	Himes/Mighell
GEOMSTDV	*F*	+	−	*S*	*F*	*A*	DF	Rutten/PEB
GEORING	*F*	+	−	*S*	*F*	*A*	DF	Gorter/PEB
LEPAGE	TB	−	+	*E*	*F*	*N*	DF	Spek/PEB
MISSYM	*F*	+	−	*S*	*F*		DF	Gabe
*NBS*AIDS*83	*F*	+	+	*S*	*F*	*A*	*M*	ICDD/PEB
NEWLAT	*F*	+	−	*S*	*F*	*A*	DF	Mugnoli
*NIST*SEARCH*	*F*	+	−	*S*	*F*	*A*	*M*	Himes/Mighell
*NIST*LATTICE*-90	*F*	+	−	*S*	*F*	*A*	*M*	Himes/Mighell
POWABS	*F*	+	−				*R*	Byrom/Lucas
PC/R/TRUEBLOOD	*F*	−	+	*S*	*F*	*A*	*M*	Blanchard
REDUCT	*F*	+	+	*S*	*F*	*A*	DF	Westdahl/Werner
SGROUP	*F*	+	−	*S*	*F*	*A*		Yerkess/PEB
TABLES	*F*	+	−	*S*	*F*	*N*	M	Abad-Zapatero/O'Donnell
TRACER-II	*F*	+	−	*S*	*F*	*A*	DF	Lawton
VOLUM	*F*	+	−	*S*	*F*	*A*	DF	Bosman/PEB

One of the problems of powder diffraction determinations of the unit cell is that the symmetry is not observed directly. The symmetry is implied by the lattice geometry determined by the indexing procedure. All lattices have alternative ways of describing the same periodicity, and the true symmetry must be determined by further tests such as optical properties. There are mathematical tests that check lattices for higher symmetries and centred lattice types. These calculations involve reducing the lattice to a cell following specific rules then examining that cell for parameter relations. Most of the programs listed under metric analysis do this cell reduction.

Once the reduced cell and probable highest-symmetry lattice is identified, the cell information may be used to identify the material. Crystal data are a compendium of unit-cell data, and they can be used for numerical cell comparisons to locate all compounds that have similar cells. Because of the many ways possible to describe the same lattice even in the same crystal system, rules must be followed both for the database and for the cell to be matched. Also, because of the chance that the true cell is a multiple of the observed cell, super- and subcells must also be considered. The program *NIST** *SEARCH* is used to interrogate the CD database while testing all the possibilities. With a database the size of CD, metric searching is a powerful technique for identification where other identification procedures have failed.

MISSYM is a metric- and symmetry-analysis routine for interrogating single-crystal structure information for missing symmetry. Many times single-crystal structures are solved using direct computer methods with no lattice-symmetry information determined by film studies. Consequently the structure may be solved in the wrong space. *MISSYM* examines the atom coordinates as well as the lattice for missed symmetry elements and suggests alternative space groups and lattice descriptions.

Pattern generation

Program	Language	Computer MF	PC	Form	Cost	Support	Documentation	Source
DISPOW	F	+	−	S	F	A	DF	Gabe
EDDA (EDX)*	F	+	−	S	F	N	DF	Gerward
EDDA/PC (EDX)	F	−	+	S	F	N	DF	Gerward
ENDIX	F	−	+	S	$$	A	DF	Hovestreydt
INT	F	+	+	S	F	A	DF	Kaplan/Kimmel
INTER (2D)†	QB	−	+	E	$	A	M	Vila (1)
LAZY PULVERIX	F	+	−	S	F	A	DF	Yvon/PEB
LAZY PULVERIX/BROWN	F	+	−	S	F	A	DF	Brown, A.
LAZY PULVERIX/PC	F	−	+	S	F	A	DF	Yvon
MicroPOWD	F	−	+	EK	C	A	M	Johnson, Q./Smith, K.
*MOD*2 (2D)	TB,F	+	+	S	F	A	M	OLD
*MOD*88 (2D)	TB	−	+	E	$$	A	M	Reynolds
PC/POWIN	B	−	+	S	F	A	M	Prewitt
PC/XDPG	B	−	+	E	$	A		Russ
*POWD*12	F	+	−	S	F	A	DF	Smith, D./PEB
*POWD*12+	F	+	−	S	$$	A	DF	Smith, D.
PRECRAY/SIMVAX	F	+	−	S	F	A	R	Espinat
PROF DET	F	+	−	S	F	A	DF	PEB
SIMULATE (TOF)‡	F	+	−	S	F	A	DF	RAL
TOFSIMU	F	+	−	S	F	A	DF	IPNS
XPOW	F	+	−	S	F	A	M	Sheldrick
XPSI	F	+	+	S	F	A	DF	Kimmel

* EDX = energy dispersive X-ray diffraction intensities.
† 2D = calculations for 00*l* intensities from two-dimensional layer structures.
‡ TOF = time-of-flight intensity calculations.

The best way to interpret the information in a powder diffraction pattern is to calculate the theoretical pattern from the structure model including the diffraction effects. There are many programs which do this calculation, although they have all been derived from either *POWD* or *LAZY PULVERIX* which first were written in the 1960's. The calculation of integrated intensities is fairly straightforward starting from the crystal structure description. The *POWD* family of programs takes the integrated intensities and creates a diffraction trace by calculating profiles for every peak and adding them to simulate the actual trace. The *POWD* program is responsible for most of the calculated powder patterns in the PDF. The peak intensities are reported which are determined from the calculated trace.

One advantage of intensity calculations is the ease of testing possible models of the compounds under study. It is a simple matter to calculate the substitutional effects of replacing one element for another in a structure. Lattice distortions and crystallite size effects may be included. The 00*l* peaks from two-dimensional structures such as clay minerals can be modelled using *MOD*2 and *MOD*88. These patterns can be compared to experimental data obtained on deliberately oriented samples.

Profile fitting – decomposition

Program	Language	Computer MF	Computer PC	Form	Cost	Support	Documentation	Source
ABFfit	*F,P*	+	+	*E*	$$	*A*	*M*	Antoniadis
AUTOPEAK	*F*	+	−	*S*	*F*	*A*	DF	RAL
CUVFIT		+	−					Wang
DIFFRACT-AT/FIT	*F,A*	−	+	*E*	*C*	*A*	*M*	Socabim
DOREES	*F,P*	+	−	*E*	$$	*A*	DF	Jansen
FIT	TC	−	+	*E*	*F*	*A*	*R*	Petkov/Bakaltchev/PEB
KET,KETA	*F*	−	+	*E*	$$	*A*	*M*	Kogan
LAT1	*F*	+	−	*S*	*F*	*A*	*R*	Tran
LSQPROF	*F,P*	+	−	*E*	$$	*A*	DF	Jansen
MicroSHADOW	*F*	−	+	EK	*C*	*A*	*M*	Johnson, Q.
PEAK	*F*	+	+	*E*	$$	*A*	*M*	Dinnebier/Eysel
Pi'oPiliPa'a	*F*	+	−	*S*	*F*	*A*	*M*	Jones
POWDER								Rossel/Scott
POWDERPATTERN	*F*	+	−	*S*	*F*		*R*	Hubbard/Pyrros
PROFAN	*F*	+	−	*S*	$	*A*	*R*	Will
PROFAN/PC	TP	−	+	*S*	*F*	*A*	*R*	Merz
PROFIT	*F*	+	+	*S*	$$	*A*	*M*	Sonneveld/Langford
PRO-FIT	*F*	+	−	*S*	*F*	*A*	*R*	Toraya/PEB
REGION	*F*	+	−	*S*				Hubbard/Pyrros
SCRAP	*F*	+	−					Cooper
SHADOW	*F*	+	−	*S*	*F*	*A*	DF	Howard, S./PEB
TOFMANY	*F*	+	−	*S*	*F*	*A*	DF	IPNS
TXTPVGT	TP	−	+	*S*	$	*A*	DF	Bourniquel
XRAYL	*F*	+	−	*S*	*F*	*A*		Zhang/Hubbard

Profile fitting – full pattern

Program	Language	Computer MF	Computer PC	Form	Cost	Support	Documentation	Source
ALLHKL	*F*	+	−	*S*	*F*	*A*	DF	Pawley
EDINP	*F*	+	−	*E*	$	*A*	*R*	Pawley
FINAX	*F*	+	−	*S*	$	*A*	*R*	Hovestreydt
FULLPROF	*F*	+	+	*E*	*F*	*A*	DF	Rodriguez-Carvajal
POWLS	*F*	+	+	*S*	$$	*A*	*M*	Will
PROFIT	*F*	−	+	*S*	*F*	*N*	*M*	Scott
WPPF	*F*	+	−	*S*	*F*	*A*	DF	Toraya

With the availability of accurate digitized diffraction traces, peak analysis is becoming a very popular option for locating peaks and for determining the profile parameters. The terminology of profile analysis is confusing for diffractionists who are starting this type of analysis. The programs in this section are correctly classified as decomposition programs. Each of these programs uses a predetermined profile either defined analytically or learned from an isolated peak to fit all the other peaks in the pattern including the α_2 component. This procedure is to be distinguished from deconvolution which is a Fourier analysis of the peak shape. There are several ways to approach the problem of decomposition.

First, the peaks can all be considered as independent, and each profile can be fit using free parameters. Usually, the profile shape is fixed and the parameters of peak intensity, profile half-width and peak position are varied. The relative positions of the α_1 and α_2 components are known, and their intensity ratios are fixed at 0·5. Where there is a mixture of phases, the peak shape may vary among the phases. If crystallite size is a factor and the crystallite shape is non-spherical, the half-width may vary within the peaks of the same phase. It should be apparent from this discussion that no single program can be optimized for all these options.

The programs listed under the heading *Profile fitting – decomposition* differ from the ones listed under *Profile fitting – full pattern* in the way the peaks are treated. In the former category, each peak is generally considered as independent of the other peaks even in a cluster, and usually only a limited range of the pattern is considered during each application of the program. In the latter category, all the peaks (or a large number) in the pattern are considered at one time. If the sample is single phase, all the peak positions are related, and the program should constrain the peak locations to those compatible with a unit cell. Usually, the profile shape is also constrained. The purpose of this approach is to resolve individual peaks, so that the intensities can be determined. The single goal of this approach is to obtain intensities for crystal structure analysis. These intensities can then be used with the usual single-crystal analysis programs which employ direct methods and Patterson analysis. All the programs in this section operate on the full pattern to provide individual intensities.

Deconvolution

Program	Language	Computer MF	Computer PC	Form	Cost	Support	Documentation	Source
CALIB/FITCONV/WAXS	*B*	−	+	*S*	*F*	*A*	*M*	Enzo/Polizzi
CRYSIZE	*F*	+	−	*S*	*F*	*A*	DF	Zhang/Hubbard
DECON	*B*	+	+	*S*	*F*	*N*	*R*	Wiedemann
LWL	*F*	+	−	*S*	$	*A*	*R*	Louër
UNFOLD	*F*	+	-	*S*	*F*	*A*	DF	Roof
WARREN/AVERBACH	*F*	+	−	*S*	$$	*A*	*M*	Cohen

The diffraction profile contains considerable information on the perfection of the crystallites in the sample. The necessary profile for this information is the sample profile, *i.e.* the component of the diffraction profile which is due to the sample only. In order to measure this profile it is necessary to remove the instrument and source components. These components must be removed mathematically as there is no way to eliminate them experimentally. The mathematical procedure is called deconvolution.

There are several numerical techniques that have been devised to accomplish the deconvolution mostly based on Fourier transform theory. The numerical methods are necessary because the profiles cannot be expressed analytically. The methods lead to values of the effective half-width of the sample profile, profile shapes and skewness parameters. If these parameters can be determined as a function of diffraction order, then the strain component can be separated from the size component. In 1950, Warren & Averbach developed the theory for using multiple orders of peaks to deconvolute the profile into Fourier coefficients. These coefficients are then plotted as a function of the square of the order to obtain the size and strain components.

Crystallinity/strain/texture

Program	Language	Computer MF	Computer PC	Form	Cost	Support	Documentation	Source
CRYSTALLINITY	*F*	+	−	*S*	*F*	*A*	DF	Jansen/PEB
POLYMER	*F*	+	−	*S*	*F*	*A*	DF	Wims
POP		−	+					Wenk
RAD	*F*	-	+	*E*	*F*	*A*	DF	Petkov
SIZEDIST	*F*	+	-	*S*	$	*A*	*R*	Louër/Le Bail
STRESS-AT	*F,A*	−	+	*E*	*C*	*A*	*M*	Socabim
TEXCAM	TB	−	+	*E*	*F*	*A*	DF	Rogers/PEB
WIMV1		+	+					Kallend
XTL-SIZE	*F*	-	+	*S*	*F*	*A*	*R*	Bonetto/PEB

There are methods other than Fourier techniques for determining effective crystallite size and size distributions. Most commonly employed is the Scherrer method, which can give a picture of the crystallite shape by analysing the breadths of all the peaks in the pattern. Macrostrain can be measured by detecting peak shifts relative to an unstrained sample. Percent crystallinity can be indicated by the ratio of the crystalline pattern to the amorphous pattern. Texture can be analysed by following the intensity of specific peaks as a function of the position of the sample with respect to the beam. It was not the plan of this project to locate all the programs that make these measurements, but several were collected during the project which are listed in the table.

Rietveld – structure refinement

Program	Language	Computer MF	PC	Form	Cost	Support	Documentation	Source
ATALANTA	*F*	+	–	*S*	*F*	*A*	*R*	Benham/Ross
CCSL	*F*	+	–	*S*		*A*	DF	RAL
*DBWS*9006	*F*	+	–	*S*	$	*A*	*M*	Young
*DBWS*9006*PC*	*F*	–	+	*S*	$	*A*	*M*	Young
EDINP	*F*	+	–	*E*	$	*A*	*R*	Pawley
GSAS	*F*	+	–	*E*	*F*	*A*	*M*	Larson–Von Dreele/PEB
FULLPROF	*F*	+	+	*E*	*F*	*A*	DF	Rodriguez-Carvajal
HILL/Version.90.06	*F*	–	+	SE	$	*A*	*M*	Lengauer
LHPM-7	*F*	+	–	*S*	*F*	*A*	*M*	Hill/Howard, C.
LOOPVELD	*F*	+	–	*S*	*F*	*A*	DF	Pawley/PEB
MicroRIETVELD	*F*	–	+	EK	*C*	*A*	*M*	Johnson, Q.
MINREF		+	–	*S*				Elsenhans/PEB
MORGUE	*F*	+	–	*S*	$	*N*	*M*	Byrom/PEB
PC/WYRIET	*F*	–	+	*E*	$$	*A*	*M*	Schneider
RIETAN	*F*	+	–	*S*	*F*	*A*	*R*	Izumi/PEB
RIETVELD	*F*	+	–	*S*	*F*	*A*	DF	IPNS
RIETVELD	*F*	+	–	*S*	*F*	*A*	DF	ILL
RIETVELD	*F*	+	–	*S*	*F*	*A*	DF	DL
RIETVELD	*F*	+	–	*S*	*F*	*A*	DF	RAL
RIETVELD	*F*	+	–	*S*	*F*	*A*	DF	Prince
RIETVELD	*F*	+	–	*S*	*F*			Nurmela
RIETVELD	*F*	+	–	*S*	*F*	*A*	DF	Hewat/Cox
*T*53	Alg	+	–	*S*	*F*	*A*	DF	Rietveld/PEB
XRS-82	*F*	+	–	*S*	*F*	*A*	*M*	Bärlocher
XRS-82 (*VAX*)	*F*	+	–	*S*	*F*	*A*	DF	Rudolph/Clearfield

The Rietveld method was first introduced in the late 1960's and has become the most versatile technique in powder diffraction analysis. Its primary function is to fit a structure model to the experimental data by calculating the diffraction pattern and using the differences between the calculated and experimental traces to improve the parameters in the model. The refinement procedure is essentially the least-squares method, and the refinement must be approached with caution. There are several levels of sensitivity of the parameters to the experimental data, and the beginner may easily lock into false results. The four main groups of parameters are the scale factors and background, the pattern parameters, the structure-position parameters and secondary parameters such as the temperature factors and orientation effects. The technique has been somewhat more convenient for neutron diffraction where the pattern profile function is more nearly Gaussian, but modern neutron diffractometers with high resolution require the more-complex functions. For the X-ray situation, the choice of profiles has always been a problem, and there are now several options usually employed including Cauchy (Lorentzian), Cauchy-like functions and mixed Cauchy–Gaussian combinations.

The list contains a large number of Rietveld programs which include programs for neutron diffraction as well as X-ray diffraction. It is not possible to single any one program out for general use, but the *DBWS*9006 and *GSAS* programs probably are the most widely used. At the present time, the Rietveld programs are undergoing extensive revision in most laboratories where the method is used extensively. Almost all the major neutron and synchrotron facilities in the world are developing their own version of the program. Part of the driving force for these program revisions is the expansion of the method to more than structure refinement. Considerable use is now being made of the pattern parameters for such measurements as crystallite size, strain and phase quantification.

Quantitative analysis

Program	Language	Computer MF	Computer PC	Form	Cost	Support	Documentation	Source
ARCOQUANT	*F*	+	−	*S*	$$	*A*	DF	Smith, D.
DBW-4.1	*F*	+	−	*S*	*F*	*A*	*M*	Bish/Howard, S.
*DBW*3.2*S*	*F*	+	−	*S*	*F*	*A*	*M*	Young
*DBW*3.2 (Modified PEB)	*F*	+	−	*S*	*F*	*A*	*M*	Wiles/Young/PEB
FAZAN	*F,P*	−	+	*S*	$$	*A*	DF	Burova
GMQUANT	*F*	+	−	*S*	*F*	*A*	DF	Smith, D./PEB
HOWARD-2.0	*F*	+	−	*S*	*F*	*A*	*M*	Howard, S.
LSQX	*F*	+	+		*C*	*A*	*N*	Vonk
MicroQUANT	*F*	−	+	*EK*	*C*	*A*	*M*	Johnson, Q.
++PADS++	*F*	−	+	*E*	*C*	*A*		Wassermann
PC/PEAKS	*C*	−	+	*S*	*C*	*A*	*M*	Hill/Foxworthy
PC/QXRD	*F*	−	+	*S*	$$	*A*	*M*	Hill
PFLS	*F*	+	−	*S*	*F*	*A*	*R*	Toraya
PLUVA	*F*	+	−		$$	*A*	DF	Schenk
QPDA	*F*	+	−	*E*	*F*	*A*	*M*	Hill/Madsen
*QUANT*85	*F*	+	−	*S*	*F*	*A*	*M*	Hubbard/Snyder
RIMPAC	GWB	−	+	E	$$	A	M	Davis
SIROQUANT	*F*	+	+	*E*	*C*	*A*	*M*	Taylor

Quantitative phase analysis by X-ray powder diffraction is one of the few techniques which is truly phase sensitive rather than element sensitive. The first applications followed the development of the theory by Alexander & Klug (1948). Although the technique was applied effectively to some special problems, the data collection was laborious and limited the general application of the method. When the APD became the data collector, the data were easier to analyse and the technique saw enhanced use in the 1980's which has continued to the present time.

There are basically three ways of doing quantitative analysis at the present time. One technique uses integrated intensities (areas) of individual peaks for each of the phases in the mixture if peaks are resolvable and clusters of peaks when they are not. With the raw data in digitized form, it is easy to integrate the desired diffraction ranges for the calculation. *QUANT*85, *PC/PEAKS*, *microQUANT* and *RIMPAC* use this approach. *GMQUANT* and *ARCOQUANT* use the full diffraction trace with a reference database of digitized traces of reference patterns. The other programs are Rietveld programs modified to emphasize the quantification of phases in a mixture by adjusting the pattern scale factors for absorption effects. All these approaches are effective if the sample-preparation problems can be overcome.

Structure determination (powder)

Program	Language	Computer MF	Computer PC	Form	Cost	Support	Documentation	Source
*SIRPOW*90	*F*	+	+					Cascarano
STRUMO	*F*	+	−	*F*	*F*	*A*	DF	Brown, I. D.

There has long been a reluctance to claim that structures can be solved based on powder data alone, but recent successes have proved that the time to exploit the technique is now. Several programs, mentioned under full-pattern fitting, have been designed to resolve intensities so that they can be used in single-crystal calculations, but recent efforts have been to design programs that work directly on the powder information as a package. Two such programs have been identified so far, and they are listed separately under a different heading.

Structure display

Program	Language	Computer MF	PC	Form	Cost	Support	Documentation	Source
ATOMS	*B*	−	+	*E*	*C*	*A*	*M*	SHAPE/PEB
B&S	*B*	−	+	*E*	*C*	*A*	*M*	SHAPE
CENG. ORTEP	*F*	+	−	*S*	$	*A*	DF	ILL
CRYES	GWB	−	+	*E*	*C*	*A*	*M*	Vila(2)/Vegas
CRYST	*F*	FACOM		*S*	$	*N*	*M*	Sakurai
FIGATO	*F*	+	−	*S*	*F*		DF	Langlet/PEB
INORGEGA		−	+	*S*	*F*	*A*	DF	Jansen/PEB
MODEL/NAMOD	*F*	+	−	*S*	$$	*A*	DF	Smith, D.
MOLDRAW	QB	−	+	*E*	$	*A*	DF	Ugliengo
MOLPLOT	*F*	−	+	*S*	*F*	*A*	*R*	Radhakrishnan
NAMOD	*F*	+	+	*S*	*F*	*N*	*R*	Beppu (PDB)/PEB
ORTEP (Updated PEB)	*F*	+	−	*S*	*F*	*N*	*M*	Johnson, C./PEB
PLOTMOL	*F*	+	+	*S*	$	*A*	DF	Gabe
PLOTMD	*F*	+	−	*S*	*F*	*A*	DF	Luo
PLORTEP	*F*	+	−				*R*	Bandel/Sussman
PLATON	*F*	+	+	*S*	$$	*A*	*M*	Spek/PEB
PLUTO (Updated PEB)	*F*	+	−		$$	*A*	*M*	Motherwell/PEB
PLUVA	*F*	+	−	*S*	$$	*A*	DF	Schenk
PRETEP	*F*	+	+	*S*	*F*	*A*	DF	Izumi/PEB
QSHAPE	*B*	−	+	*E*	*C*	*A*	*M*	SHAPE
SCHAKAL-88B	*F*	+	+	*S*	*L*	*A*	DF	Keller
SCHAKAL-88B/*V*16	*F*	−	+	*E*	*L*	*A*	*M*	Keller
SDP	*F,C*	+	+	*E*	*C*	*A*	DF	Frenz
SHAPE	*B*	−	+	*E*	*C*	*A*	*M*	SHAPE
STRUPLO	*F*	+	−	*S*	*F*	*A*	*M*	Fischer
STRUPLO/PC	*F*	−	+	*S*	$	*A*	*M*	le Lirzin

Powder diffractionists may feel that structure graphics are not in the realm of powder diffraction, but with the increased activity in solving crystal structures from powder data that is not true. Also, there is considerable research on the effects of atom substitutions in structures and the ability to display easily the structure image on a screen often helps one to see what is happening. With the availability of the several structure databases which contain structure descriptions, a coupled display program results in a very powerful tool in the laboratory.

The problem with structure graphics is the dependence of the programs on the hardware. There are many sophisticated graphics systems available today and some of the programs have taken advantage of them. Most of the programs in the list were initially designed for the pen-driven plotter, some of which have been upgraded to newer plotters. When one of the programs is requested, it is necessary that the requestor obtain information on the graphics requirements.

Small-angle scattering

Program	Language	Computer MF	PC	Form	Cost	Support	Documentation	Source
FFSAXS	*F*	+	−	*S*	*F*	*A*	DF	Vonk/PEB
ITP-81	*F*	+	−	*S*	*F*	*A*	DF	Glatter/PEB
LIPFIT	*F*	+	−	*S*	*F*	*A*	DF	Gooris/PEB
RAD	*F*	−	+	*S*	*F*	*A*	DF	Petkov
SAXSFIT	*F*	+	−	*S*	*F*	*A*	DF	Gooris/PEB
SIMUL/SCAT	*F*	+	−	*S*	*F*	*A*	DF	Hansen/PEB
STACKS	*F*	+	−	*S*	*F*	*A*	DF	Gooris/PEB
TRACON	*F*	+	−	*S*	*F*	*A*	DF	Gooris/PEB

Although small-angle scattering is not technically powder diffraction, powder samples may be analysed and powder diffractometers may be modified to obtain the experimental data. There was no effort made in this project specifically to cover the field of small-angle scattering. The list presented here has been obtained through the courtesy of Drs Ing. S. Gorter of the Dutch Association of Crystallographers, and it is included here for those who may be interested. No comments will be made on these programs because the publication authors lack experience in their use.

Miscellaneous programs

Program	Language	Computer MF	Computer PC	Form	Cost	Support	Documentation	Source
CAMMAG	*F*	+	–	*S*	*F*	*A*	DF	Gerloch/PEB
DIMFIT	*F*	+	–	*S*	*F*	*A*	DF	Gorter/PEB
ELMIC	*F*	+	–	*S*	*F*	*A*	DF	van Dijck/PEB
ESR	*F*	+	–	*S*	*F*	*A*	DF	Ammeter/PEB
FPLOT	*F*	+	–	*S*	*F*	*A*	DF	Rutten/PEB
HKL-XTAL	*F*	+	–	EP	FL	*A*	DF	Jansen/PEB
HOLE	*F*	+	–	*S*	*F*	*A*	DF	de Kok/PEB
LABSCO	*F*	+	–	*S*	*F*	*A*	DF	Driessen/PEB
MADELUNG	*F*	+	–	*S*	*F*	*A*	DF	Gorter/PEB
MTH-RD	*F,P*	+	–	*S*	*F*	*A*	DF	Jansen/PEB
MU	GFA	+	–	S	F	A	DF	de Graaf/PEB
ONE-TO-POWDER	*F*	+	–	EP	FL	*A*	DF	Jansen/PEB

Other programs

There are other programs which are implied in the texts of papers that are undescribed or provided with inadequate information to classify properly. Certainly, there are even more programs which have not come to the attention of the publication authors. To be as complete as possible, these papers have been included in the reference list. One example is macros for commercial PC programs such as the spreadsheet and database packages. Whether code for these programs would be available and at what cost must be determined. Some of the codes involve local graphics hardware and they may not be easily portable. One major advantage of PC systems is the public bulletin boards which can be a source for distributing and acquiring codes and meetings where PC stations are set up for code demonstrations and dissemination.

Obtaining programs

Most of the programs listed in this compilation are available from the program author(s) or as part of one of the analytical packages of programs. The program tables indicate the probable level of costs involved and the program author or program source. More detail on the program source is provided in the following address list or in the references. The program-author list is indexed by the name of the program author or company responsible for the program. If there is no entry in the source list, there will be an entry in the references. When asking for copies of programs, requestors should expect to supply media especially for free programs.

When requesting programs, the requestor should recognize the tremendous amount of time and talent required to prepare good programs. This effort must be recognized. If the program is delivered at no cost or for minimal copying and media fees, the program must be referenced in any publication that results from calculations made using the program. Usually, without the program, the research would not have been accomplished. If the program was commercial and purchased outright, then the requirement for referencing the work becomes unnecessary, but it would still be a service to readers in the same way that equipment and samples are recognized.

Another problem with programs that is appearing often is the second-author modification of routines which are then distributed independently of the primary program. Sometimes the second program is being marketed for financial gain without any agreement with or remuneration to the primary-program author. This practice is most common with, but not limited to, PC programs patterned after main-frame versions. The basic problem lies in the interpretation of copyrights but there are ethical aspects as well. If the requestor remembers there is a requirement to recognize the previous work that has lead to the new advances, whether they are new results or a modified program, this problem will be minimized.

Future revisions of this list

The maintenance of this list of programs will depend on its value to the powder diffraction community which will be measured by the comments, criticisms, suggestions and new program information it generates. Users should direct all remarks to the publication authors, not to the IUCr office or to the Commission on Powder Diffraction. Corrections are welcome and all new program information will be filed for the next update.

Program authors desiring to have a program listed should follow the format in the questionnaire in the Appendix. All of the questions are essential and the more information supplied the better. When this list was first conceived, one plan was to have a short abstract on each program. Unfortunately, the response to requests for information was too variable to retain this goal. About 25% of the program authors did not return the form. Before the next list is compiled, each program author will be asked once again to bring the data up to date and to prepare a program abstract.

There are certainly many laboratories that have collections of programs for powder diffraction applications that have not been identified in this project. Some researchers do not think they have any programs of outside interest. Some prefer not to have to polish for distribution a program they wrote for personal use and they do not want to have to take the time to prepare instructions on its use. Others do not want to have to answer questions on how to use their programs. Still others consider their version too similar to distributed programs to be of interest to others. Whatever the reason, the result is unfortunate in that the program does not achieve its full potential through input from other users. All these programs should be included in this list.

Another problem is geographic in nature. Researchers in countries other than the industrial nations consider their programs of little interest to others. Commonly, the programs are written for computers of limited availability. Actually, these programs are of considerable value in this list because they allow users who have similar computers to locate colleagues with whom they can exchange routines. Program authors in this category are encouraged to submit program information.

The publication authors thank the many program authors who responded to the requests for information. Special thanks are extended to Professor Gerald G. Johnson Jr and Dr Susan Q. Hoyle who read the manuscript several times and to Professor R. A. Young and the other members of the Commission on Powder Diffraction who have supplied considerable information for this report, reviewed the manuscript and continue to encourage us to continue the project.

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Powder Diffraction Program Information Centre Program Questionnaire

PLEASE PRINT ALL ANSWERS

1. Program name:

2. Program function:

3. Author(s):

4. Address for primary author (including Email address):

5. Program language (machine, operating system, compiler vendor and version):

6. Will source code be supplied (Y/N):

7. Would current and updated code be supplied to a central distribution site if one were to be established (Y/N):

8. Computers on which the program has been used successfully (indicate hardware requirements, memory size, math coprocessor (if any), graphics software and hardware, *etc.*):

9. Appropriate keywords (database, indexing, data reduction, identification, cell matching, intensity calculations, profile matching, profile deconvolution, crystallinity, structure refinement, structure solution, stress analysis, display, other):

10. Full literature references to program and its uses (if any):

11. Instructions for obtaining a copy of the program including any costs involved and the type of medium for the copy:

12. Sources for versions of the program which have been modified to run on computers other than the author's:

13. Documentation – machine readable or hard-copy:

14. Support will be provided by the author (Y/N):

15. Program abstract:

Additional comments (note item number):

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