Powder Diffraction

JCPDS

Volume 1 Number 2 June 1986

Powder Diffraction An international journal of materials characterization

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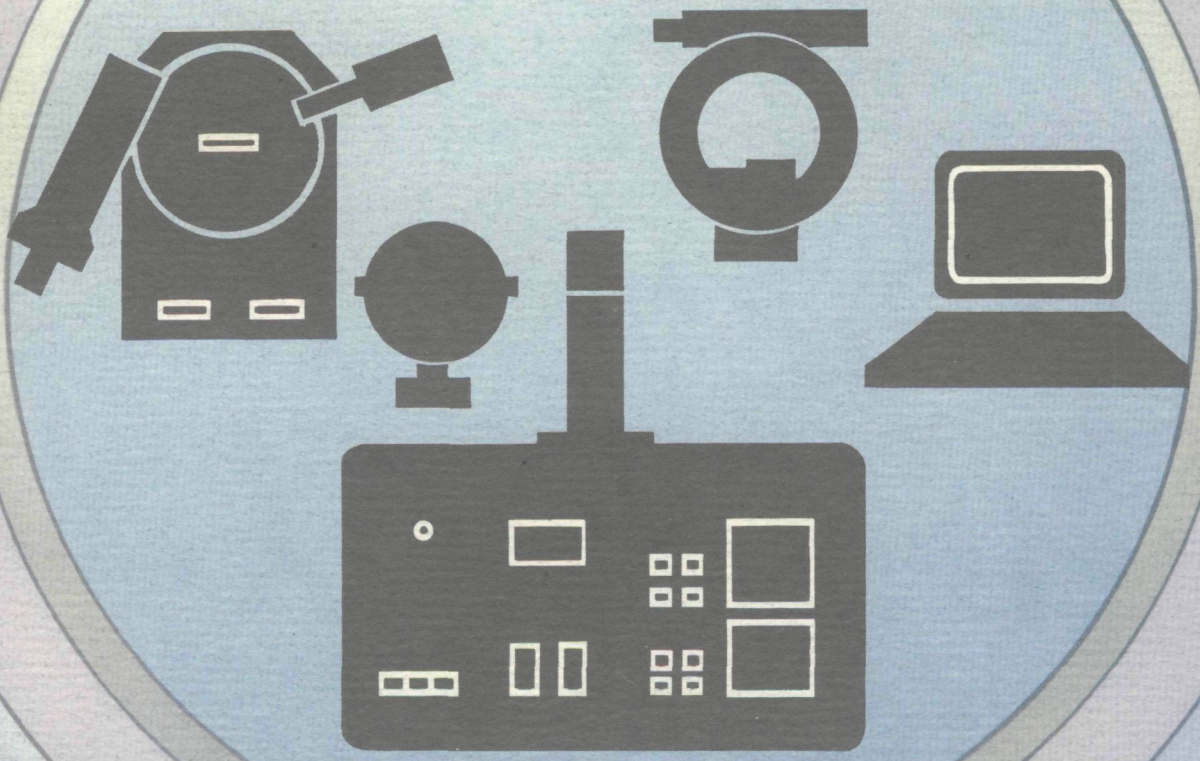

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PD2

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Powder Diffraction

An International Journal of Materials Characterization

Publisher
JCPDS International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, Pennsylvania 19081, U.S.A.

Powder Diffraction is a journal of practical technique, publishing articles relating to the widest range of application — from mineral analysis to epitactic growth of thin films and to the latest advances in software. Although practice will be emphasized, theory will not be neglected, especially as its discussion will relate to better understanding of technique.

Powder Diffraction is published four times annually by the JCPDS-International Centre for Diffraction Data.

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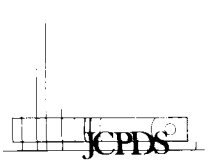

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The NBS Crystal Data Center builds and maintains a large scientific database of evaluated chemical and crystallographic data. Scientists have long used the published Crystal Data Determinative Tables to help solve problems in materials science. Now the Crystal Data information is available as a computer-readable tape. The NBS Crystal Data Distribution Package includes information on over 60,000 materials as well as accompanying search software.

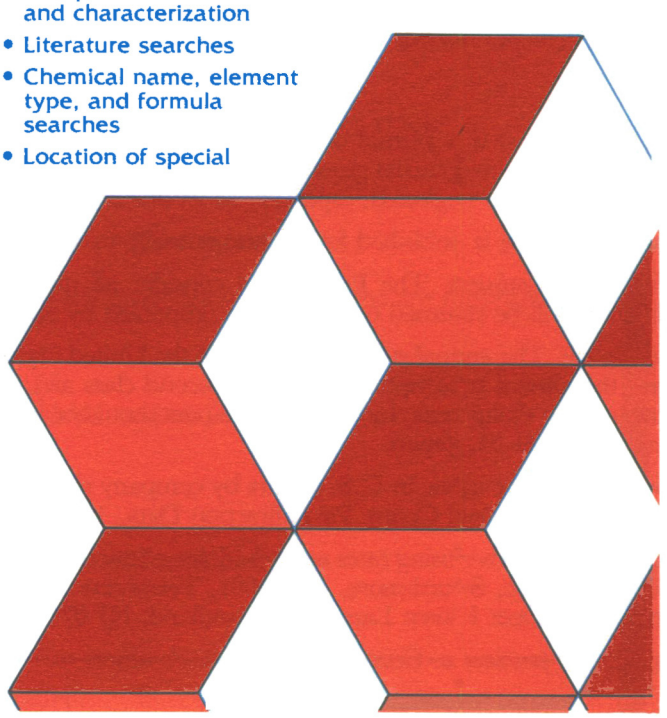
Research and Routine Applications

The database is of interest to scientists of many disciplines.

- **Analytical Chemistry:** Identify chemical compounds using one tiny crystal, non-destructive
- **Materials Science:** Find materials having desired physical and structural properties and design new materials
- **Crystallography:** Save time and money . . prevent redeterminations of crystal structures by checking to see if done previously
- **Mineralogy:** Study symmetry and pseudosymmetry of minerals with any given composition range
- **Ceramics and Metallurgy:** Identify phases even with incomplete diffraction data
- **Inorganic and Organic Chemistry:** Characterize reaction products and intermediates uniquely and quickly

The NBS Crystal Data Distribution Package is also of special interest to powder diffractionists, electron diffractionists, solid-state and structural chemists, and technical information specialists. Other typical uses include:

- Compound identification and characterization
- Literature searches
- Chemical name, element type, and formula searches
- Location of special chemical classes or types of materials
- Identification of compounds having specified properties
- Source of data for scientific and statistical research studies
- Searches on space groups, density ranges, crystal systems, and many other parameters



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Further information on the NBS Crystal Data Distribution Package is available from:

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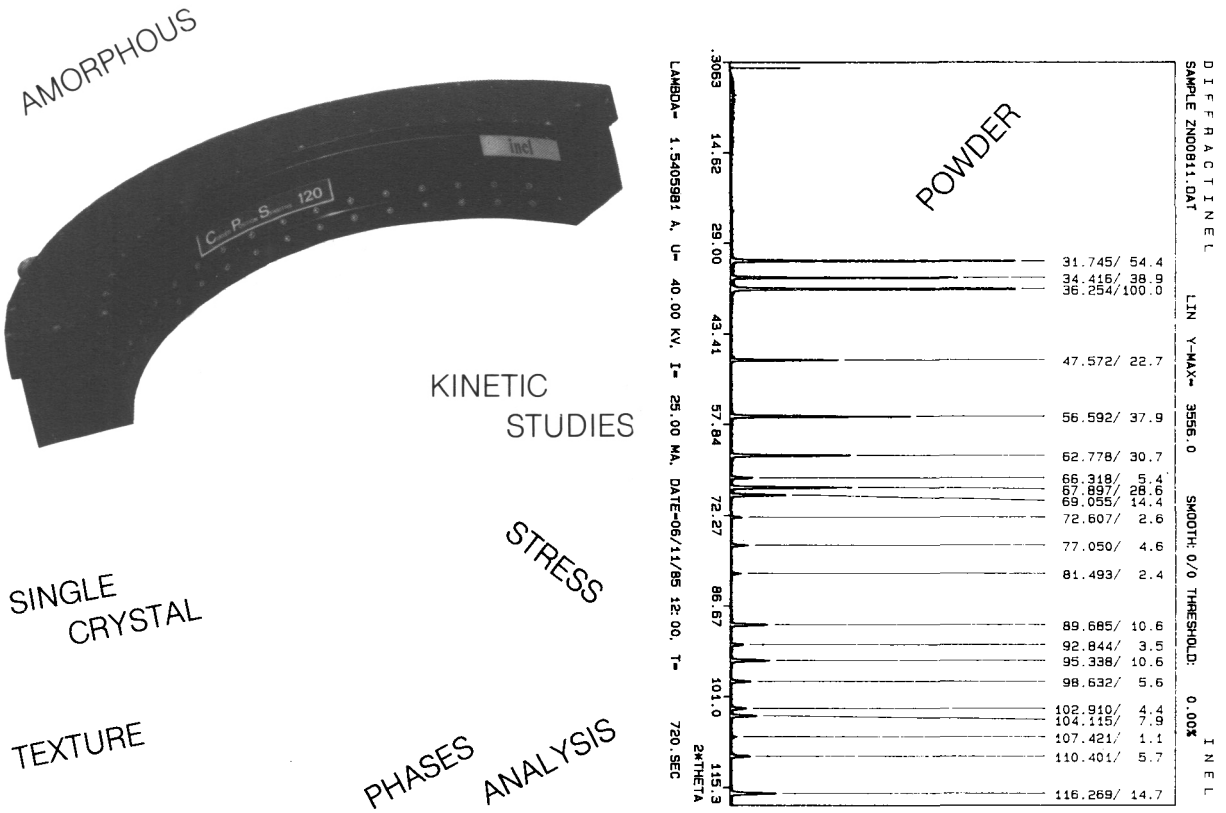

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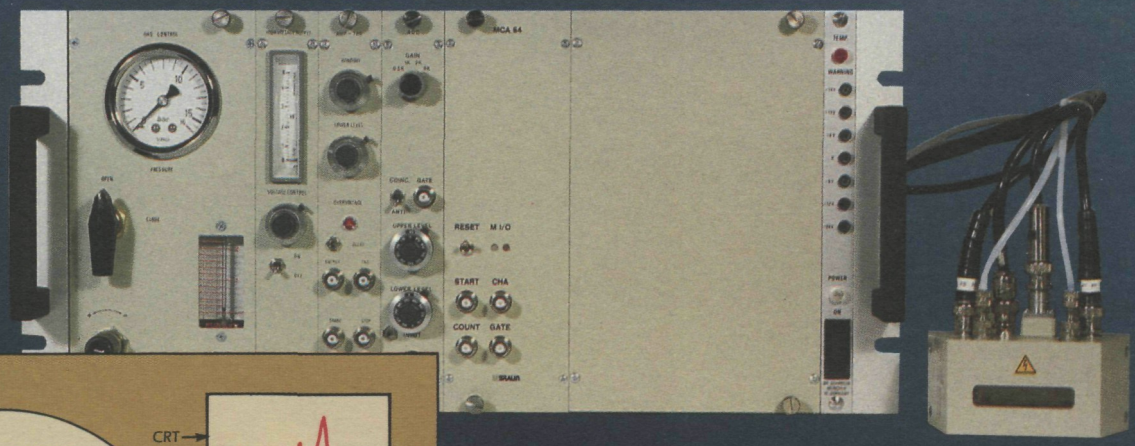
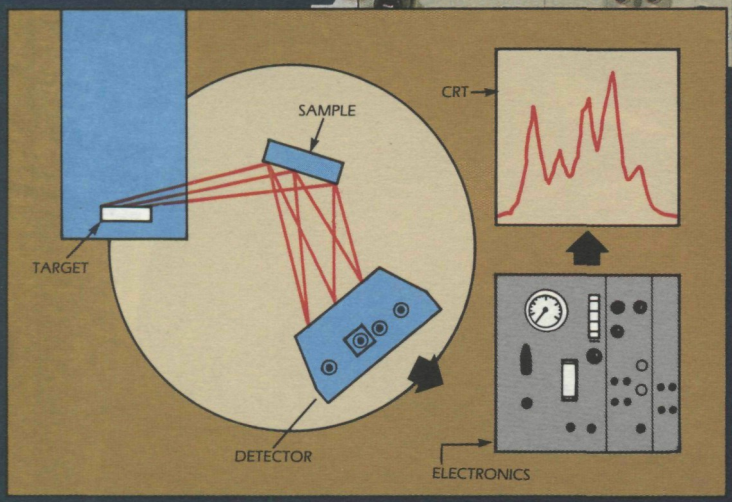
M BRAUN Position Sensitive Proportional Counter

for Simultaneous Detection of X-ray Diffraction Data





The M Braun Position Sensitive Proportional Counter is the most innovative product for rapid collection of X-ray diffraction data available. It enables the diffractionist to collect data at a rate 100 times faster than conventional scintillation counter/step scanning modes.

The detector has an inherent resolution of .01° FWHM, thereby providing data equivalent to standard counting techniques. However, since it acquires data over 10° 2-theta simultaneously, it dramatically increases throughput. Detectors can be utilized in a stationary mode or can scan rapidly to collect data over the entire 2-theta range.

Additionally, the detectors are gas proportional counters and exhibit excellent energy resolution. Choose between a straight or curved configuration to match the diffractometer radius.

Complete systems, with DEC-PDP-11 computers and software, can be provided including detector mounts, vertical divergence slits and filter holders. An 8K × 32 bit MCA is standard and includes a baud rate selectable RS232C interface. A 64K × 16 bit MCA is also available for time resolved diffraction studies. Software to interface the detector to your PDP-11 under RT-11, RSX11M or VMS may be selected to include peak search for D/I pairs.

Some typical applications include:

• Small angle X-ray scattering studies • Guinier diffractometer • Wide angle powder diffraction • Scattering experiments • High pressure • Time resolved diffraction.

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ThetaPlus+ gives you precise two-theta drive plus qualitative **and** quantitative analysis—all in one easy-to-use, highly versatile package.

We have developed stepping motor assemblies for a wide variety of diffractometers. These specially designed mechanical interfaces provide smooth, reproducible drive motions, allowing precise computer control of the two-theta angle.

For **qualitative analysis,** ThetaPlus+ offers you four different methods of peak extraction:

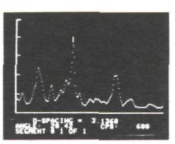
The first is fully **automatic:** you simply specify peak width and peak-to-background ratio, and the computer does the rest. This is most useful with large, non-overlapping peaks.

Automatic Peak Search

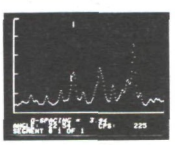
SUMMARY OF PEAKS FOUND

TWO-THETA ANGLE	D-SPACING	NET INTENS.	RELATIVE HT.
51.63	1.7683	514.12	100
26.55	3.3536	411.3	80
65.71	1.4193	318.75	62
37.86	2.3736	272.48	53
28.3	3.1493	154.23	30
41.7	1.5815	87.4	17
43.82	2.8637	82.26	16
24.99	3.5592	82.26	16
78.4	1.2183	66.83	13

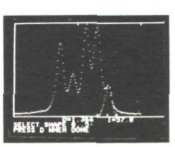
The second is **manual:** just position the cursor at the top of a peak and press "P".



The third method does a **parabolic fit:** all you do is position the cursor anywhere within a peak and press "F".



And the fourth performs **deconvolution,** by allowing you to subtract the background and then fit the peak with any of six stored profiles. This method is especially useful in low two-theta regions, where abnormal background and abnormally shaped peaks can otherwise make analysis difficult.



ThetaPlus+ also offers you two different methods of identifying unknowns:

1. Time saving search/match of most likely standards

Just set a few parameters, and ThetaPlus+ gives you a printout of the most likely phases, the number of lines uniquely matched for each, and three different figures of merit.

SEARCH MATCH RESULTS

ANALYSIS OF FILE SYNROC-E

SEARCH PARAMETERS:

MINIMUM LINES FOR POSITIVE MATCH/TOTAL LINES SCANNED: 7/20
ERROR-WINDOW MULTIPLIER: .15 OFFSET ANGLE: 0 DEGREES.

PHASES FOUND:	LINES FOUND	FIGURES - OF - MERIT /UNIQUENESS:/ INTEN-SITY:	POSI-TION:	OFF-SET:	LINES FOUND	INT. RATIO
HOLLANDITE	19	.97	.76	.00	12	.77
CAZRT1207	18	.94	.72	.00	14	.20
CAT103	17	.89	.61	.00	12	.28
AL203	10	.75	.32	.02	6	.06
TIO2 (R)	7	.38	.18	.00	4	.05

A high value (close to 1.0) indicates that *most major lines* matched.

A low figure may indicate too wide a search window.

A high value warns you of a systematic error *in measurement.*

2. Visual comparison of diffraction patterns

ThetaPlus+ lets you compare the unknown with up to 5 standards at a time (Figure 1), subtract any one of the standards (Figure 2), then compare the residual with a second standard (Figure 3), and so forth. In this way, you can interactively "take apart" a pattern to determine the compounds present in the unknown.

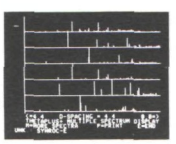


FIGURE 1

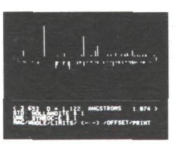


FIGURE 2

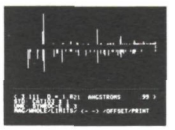
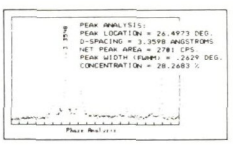
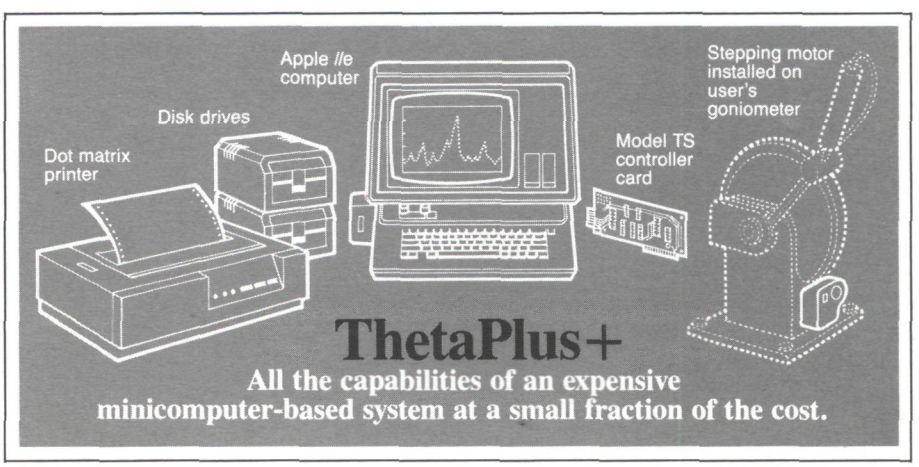


FIGURE 3

For rapid **quantitative analysis,** ThetaPlus+ will compare a single peak intensity against stored calibration curves to yield percent concentrations. Alternatively, you can compare the sum of the intensity integrals from up to 10 regions in the unknown with the sum of the corresponding integrals in the reference pattern. This increases precision and minimizes errors due to inhomogeneities and preferred-orientation effects.



All these capabilities—and more—explain why ThetaPlus+ is used by major corporations, universities, and research laboratories throughout the world. To learn more about the best way to automate your x-ray diffractometer, call or write today.



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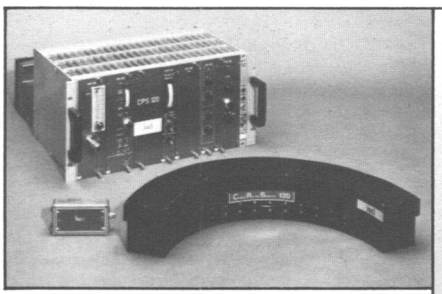

DETECTOR SYSTEM

Curved Position Sensitive Detector
American Instruments/
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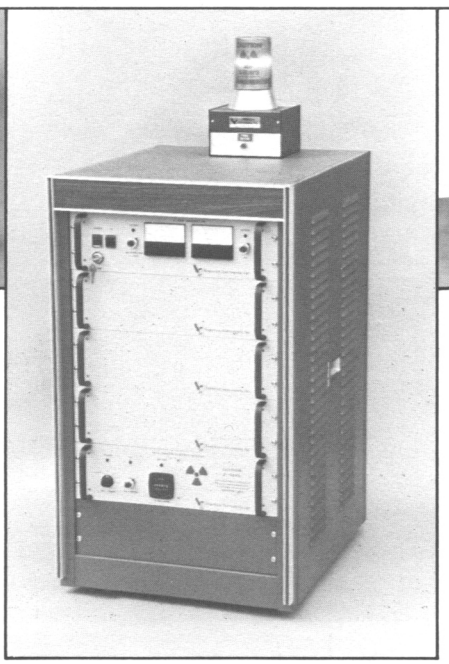
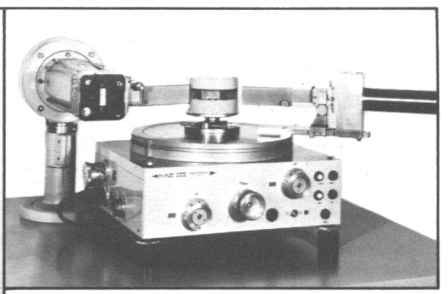
The CPS 120 is a curved position sensitive detector system with angular range of 120° two theta. It has the capability of giving a live display of the entire two theta diffractogram on a multi channel analyzer. The output from the multi channel analyzer can then be directed to a plotter or computer for data reduction. No movement of the sample or the detector is required. This detector system can be retrofitted to an existing diffractometer or purchased as a complete x-ray diffraction system. With a spacial resolution of better than .02° and high quantum efficiency, this detector system can be used for all phases of diffraction investigations, powder, texture, kinetic study, single crystal and stress.



X-RAY GENERATOR SYSTEM

State-of-the-Art Switching Power Supply Technology
American Instruments MAX 3000

Because it is based on the latest, most sophisticated, off-the-line switching, RF high voltage power supply technology, the MAX-3000 weighs less than 220 lbs. and in its basic configuration measures only 22″ x 37″ x 27″ overall. It operates at an efficiency of better than 75% at full load, minimizing heat build-up for long component life and high reliability, even when used continuously at high outputs. Inherent in the off-the-line design is protection against all common hazards to equipment, including overloads, shorts and transient input spikes. In addition, since the power supply operates with extremely low stored energy, it is far less likely to produce a destructive HV pulse that could be harmful to X-ray tubes or personnel. Required maintenance is minimal, but because of the modular design, free of oil and potting compound, it is quickly and easily accomplished when needed. In short, with the MAX 3000 you get a far more sophisticated, more reliable X-ray generator at far less cost. At last, X-ray generators have caught up with today's technology.



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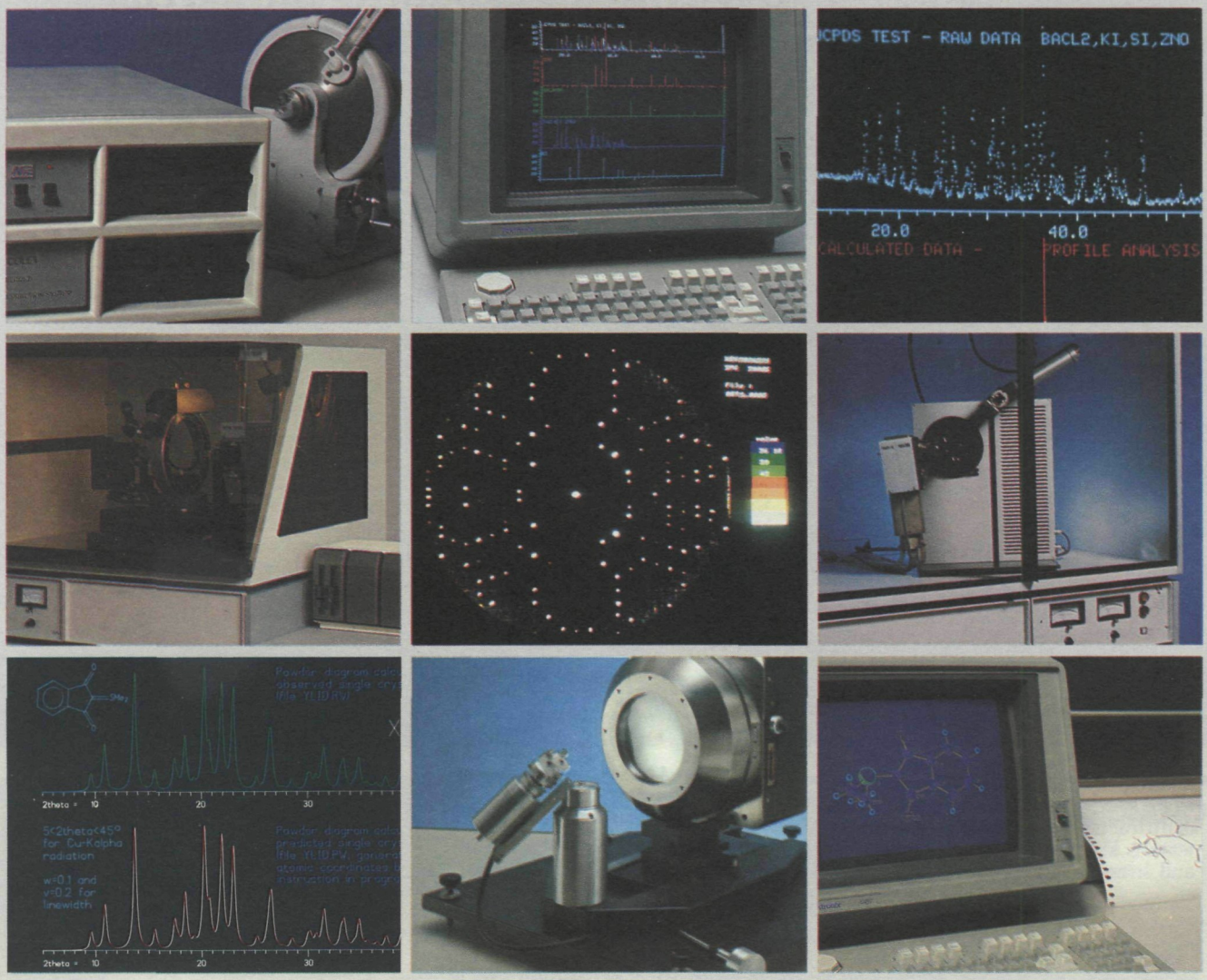

Nicolet X-ray Instruments brings together state-of-the-art instrumentation to meet your x-ray diffraction needs: in large and small molecule x-ray crystallography, in x-ray analysis of polycrystalline materials, as well as general materials analysis applications. Our commitment to advanced instrumentation provides higher productivity and performance whether you are upgrading existing instrumentation or adding new fully automated systems to the laboratory.

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Editorial

The Status of Powder Diffraction Data

One of the incentives for initiating *Powder Diffraction* was to encourage the continuing collection and archiving of new and revised reference powder diffraction patterns. The reader may ask the question "Is the state of our powder diffraction data really a problem?" The answer is both yes and no. There are large amounts of good data available, and considerably more of moderate quality which are very useful for the identification of compounds. However, most of the latter group are relatively inaccurate and need upgrading, and there are still large numbers of known compounds whose powder data have not yet been recorded.

The Powder Diffraction File (PDF) is the largest database of powder diffraction patterns. Including set 35, the PDF contains 42299 data sets of which 30376 (72%) are classified as inorganic and 11923 (28%) are classified as organic. The inorganic number is impressive but still represents only a fraction of the known inorganic compounds. The organic coverage is an even smaller proportion of the known compounds.

Examining the patterns in the PDF on the basis of quality reveals a more accurate picture of the status of the data. Since 1945, PDF Editors have assigned quality categories for each experimental data set which are identified as *, i, b, and o in order of decreasing quality. Initially, these assignments were subjective; but since 1980, the assignments have been made objectively for patterns which are indexed. The quality evaluation is based on the deviations of the experimental diffraction angles compared with the best fit values based on the refined cell coupled with an evaluation of the intensity measurements. For the inorganic portion of the PDF, 75% are indexed and can be evaluated objectively. Around 35% are classified as * or i which is the level of accuracy generally needed for good search results using computer assisted methods. The other 65% may lead to good identifications but are harder to recognize and confirm, due to poorer figures-of-merit in the computer evaluations. For organic compounds only 16% meet the * or i quality requirements.

The statistics for the most recent PDF set (35) are also enlightening. For the inorganic patterns, 79% are indexed and 52% meet the * and i criteria. For the organic patterns 17% meet these requirements. These figures indicate an improvement over the earlier sets, but there is still considerable room for increasing these numbers even higher.

There are many ways to improve the status of powder data, but it will require the efforts of all diffractionists. The PDF relies mostly on data which appear in the open literature supplemented by patterns submitted directly to the International Centre of Diffraction Data. Some data collecting efforts are supported by Grants-in-Aid from the ICDD. With the incorporation of more and more automated powder diffractometers in analytical and research laboratories, it is now feasible for these laboratories to collect and process very representative data sets for new compounds and to improve the data for old compounds. Unfortunately, many of these patterns do not find their way into open reports or publications which reach the public domain and ultimately the PDF. Diffractionists need to obtain the support of their employers to complete the descriptions of these data, and then need to submit them for publication. *Powder Diffraction* can help by acting as a publication medium. This is an appeal to all diffractionists to clean out your closets and old files and write up the data for a short note or add the documentation and prepare a paper on a group of related materials.

Guidelines for documentation and presentation of data were prepared by a subcommittee of the American Crystallographic Association and were accepted by the International Union of Crystallography for use in their Journals. These guidelines are included in the Notes for Authors *(Powder Diffraction 1*[i], 64, 1986). These guidelines indicate the data required to fully document the material and experimental conditions and the manner of presentation of the data. Where the materials allow this documentation, the information should be provided; but not all materials are so cooperative. For compounds such as corrosion products, precipitates in alloys, rare minerals and compounds which do not crystallize well, patterns which meet the * or i quality may not be obtainable. We have to use lower quality data for these materials. Remember that the many patterns in the PDF which do not meet the high quality standards are still the best available for those compounds. Thus, the quality should not be a deterrant to submission of the data if it is the best obtainable. Of course, the documentation should indicate the difficulties encountered.

Perhaps the proportion of good data has stabilized at around 50%, but this proportion may be an artifact of our complacency in accepting the status quo. Authors, pick up your pens and start sending in those hidden data sets.

Deane K. Smith
Editor and Chairman ICDD

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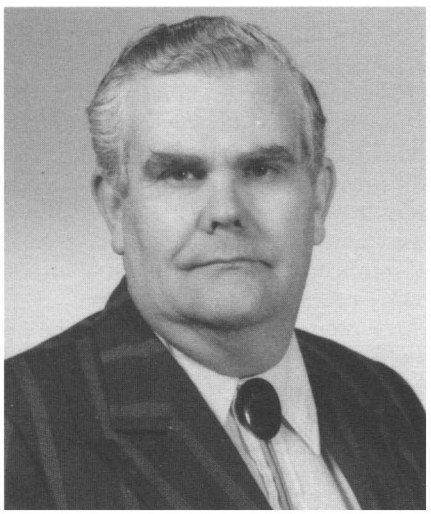
Deane K. Smith
Editor in Chief

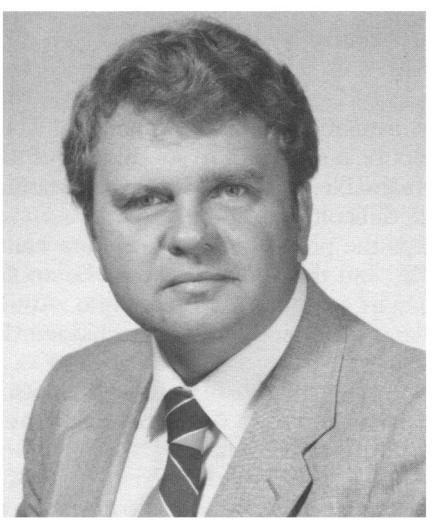


Deane Smith is Professor of Mineralogy, Department of Geosciences, at The Pennsylvania State University. He has over 30 years experience in X-ray powder diffraction of minerals, ceramics and related materials. He has published over 80 papers in fields related to X-ray diffraction. His fields of research include studies at high temperature, modeling crystal structures for powder diffraction studies and the organization of mineral X-ray data.

Ron Jenkins
Managing Editor

Ron Jenkins is the Principal Scientist at the JCPDS-International Centre for Diffraction Data. He has worked in the fields of X-ray diffraction and X-ray spectrometry for more than 25 years and has published over 120 papers and seven books related to these fields. He has served as Editor-in-Chief of the X-Ray Spectrometry Journal since its inception in 1972. His research and development interests have centered mainly around the development of instrumentation for X-ray analysis and he holds many patents in this area.

Ron Anderson
Departments Editor



Ron Anderson is an Advisory Physicist with IBM with over 25 years experience as a practising electron microscopist and X-ray diffractionist. His primary research interests include analysis of ceramics, thin metals films and semiconductor devices. Beside authoring numerous scientific papers, primarily in the field of electron microscopy, he recently completed a four year term as Editor-in-Chief of the EMSA Bulletin.

Editor's Note and Introduction to Chemical Analysis by X-Ray Diffraction

The selection of the historical article to reprint in this issue of *Powder Diffraction* is a natural sequel to the one selected for the first issue. This paper is probably the better known of the two articles as it marked the beginning of what is now the *Powder Diffraction File.* It is also a tribute to *Industrial and Engineering Chemistry* and the Dow Chemical Company who had the foresight to financially support the publication so the 1000 recorded diffraction patterns could be distributed to other laboratories and the scientific community. Up to 1938, diffraction films were retained as the permanent record of the pattern characteristic of the compound, but this paper introduced the presentation of the data in table form (a form which is still used today.) Reprints were quickly exhausted, and the General Electric Company sponsored a second reprinting of 500 copies. Even this reprinting was insufficient to meet the demand, and in 1941 the American Society for Testing and Materials reissued the data sets on 3" × 5" cards. This reissue became Set 1 of the PDF.

The 1938 publication also provided the nucleus for the formation of a Joint Committee on Chemical Analysis by Powder Diffraction Methods. This "Joint Committee" was initially formed in 1939 under the auspices of ASTM Committee E-4 and the National Research Council. The British Institute of Physics soon joined these two organizations, and the American Society for X-ray and Electron Diffraction (now the American Crystallographic Association) replaced the National Research Council. Subsequently, many other scientific and industrial organizations have affiliated with this "Joint Committee".

The initial role of the Joint Committee was to approach industrial and scientific organizations for support to continue the publication of diffraction data and to initiate a structure for overseeing this activity. W. P. Davey established the first editorial office at the Pennsylvania State University in 1940. This operation subsequently moved to downtown State College, Pennsylvania, then to ASTM headquarters in Philadelphia. In 1969, the operation incorporated as the Joint Committee on Powder Diffraction Standards which was located first in Philadelphia and presently in Swarthmore, Pennsylvania. This non-profit corporation is presently known as the JCPDS-International Centre for Diffraction Data.

The authors of this paper have all been very important in Joint Committee activities. J. D. Hanawalt was always analyzing and improving the search methods and remains to this day one of the best at using the PDF for compound identification. He was a member of the Board of Directors of JCPDS for many years and was its Chairman from 1975 to 1978. Even today he maintains his interest in the search procedures, and it was only in 1982 that he stepped down as chairman of the Search Procedures Subcommittee. His continued interest is illustrated by his paper in the first issue of *Powder Diffraction.* H. W. "Sid" Rinn was JCPDS Chairman from 1956 to 1961 and retained an active interest until his death in *1967.* L. K. Frevel is currently a Member-at-large on the JCPDS Board of Directors. He received the first J. D. Hanwalt Award in 1983 for his outstanding contribution to powder diffraction analysis.

The significance of the 1938 paper and the quality of the data is indicated by the status of the present PDF. The *Hanawalt Search Manual* still uses the basic concepts described in the 1936 and 1938 papers, employing the three strongest diffraction lines for the search procedure. Many suggestions have been offered over the years to improve the efficiency of searching, but they are minor compared to the initial concept of grouping the data to minimize the number of steps of finding the appropriate data set. The data were also quite good especially considering that they were all obtained using film techniques. Almost one half of the 1000-Set 1 patterns are still active patterns in 1986. Their average figure-of-merit is essentially the same as for the later sets. One has only to read the paper to realize the care that was used in obtaining these data.

Powder Diffraction has reprinted only the text and the table of substances from the original document. For those diffractionists who are familiar with this paper, its significance is already acknowledged. Those who have never read this article before will quickly recognize its role as one of the really important contributions to the field of powder diffraction analysis.

Deane K. Smith
Editor-in-Chief

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