JCPDS — International Centre for Diffraction Data

Course Schedules

1988

April 19-21
Rigaku/U.S.A. Danvers, Massachusetts

September 20-22
Atlanta, Georgia — location to be announced

November 15-17
San Diego, California — location to be announced

General Announcements

The 1987 J. D. Hanawalt Award for Contributions to Powder Diffraction Analysis

The 1987 Hanawalt Award for significant contributions to the field of powder diffraction analysis was presented to Dr. William Parrish at the IUCr Symposium on Powder Diffraction in Freemantle, Western Australia on the 21st of August 1987. Although this award is presented for recent work in diffractometry, it is fitting that the recipient has had a long career as one of the leaders in the field.

William Parrish first studied crystallography at the Massachusetts Institute of Technology and received his PhD in 1940. He was a Research Associate at MIT and an Instructor in Mineralogy and Crystallography at The Pennsylvania State University from 1939 to 1942. In 1942, he was appointed Chief Technologist in the War Department to take charge of the technical development of methods for manufacturing quartz oscillator plates for radio frequency control for the U. S. Armed Forces. It was necessary to control accurately the sawing angles for cutting the plates, and he developed unique X-ray diffraction methods for this alignment which became an integral part of the production process. The program could then produce large quantities of crystals, and Parrish was awarded a War Department Citation for his contribution.

In 1943, Parrish joined Philips Laboratories, and became Chief of the X-ray and Crystallography Section. He was responsible for developing many of the instruments and methods which were marketed by Philips Electronics Instruments and widely used in laboratories around the world. His most important achievement was the invention in 1947 of the X-ray diffractometer using Bragg-Brentano optical geometry which yielded high intensity and resolution with a good line shape. This design is basic to most diffractometers in use today, and it is estimated that there around 12,000 - 15,000 such instruments throughout the world making it the most widely used X-ray crystallographic instrument. An extensive systematic research program at Philips produced many important devices to enhance the utility of the diffractometer including the introduction of the scintillation and proportional counters with electronic filtering to improve the intensity response, linearity and peak-to-background ratio of the diffraction peaks. Other devices included the specimen rotator, alignment tools, transmission diffractometers and vacuum chambers. Parrish considers the powder diffractometer as his most important and satisfying achievement. The Freemantle meeting marked the 40th anniversary of this invention.

In the early 60's, Parrish became interested in the space program and proposed a program to the National Aeronautics and Space Administration to construct a low power, compact powder diffractometer to analyze the lunar surface by remote control. The tests were successful, but the rapid progress in the manned Apollo program relegated the X-ray studies of the lunar samples to the biological containment compartments at the Lunar Receiving Laboratory of the Johnson Space Center. In 1968, Parrish was appointed Chief of the Materials Characterization Branch, NASA Electronics Research Center, to develop structural methods for analyzing electronic materials.

Parrish joined the IBM Research Division in San Jose, California in 1970. As Manager of the Crystallography and Microstructure Department, he set up diffraction and fluorescence methods for characterizing new materials including thin films. Improvements in accuracy in structural and chemical characterization required new developments in instrumental methods, including the introduction of the computer in both data acquisition and data analysis. A large number of analytical programs were developed which were marketed by IBM and lead to recognition with an IBM Outstanding Contribution Award. Programs included a routine for profile fitting which could separate unresolved peaks in a complex profile. Other routines located peaks and simulated the Powder Diffraction File reference patterns for pattern matching.

In 1977, Parrish became interested in the new storage ring radiation sources and began studies at the Stanford Synchrotron Radiation Laboratory with Professor Michael Hart of Bristol, England. Diffraction topography was used to study garnet films grown on garnet substrates for magnetic bubble memory devices. Laue patterns were obtained which showed considerable detail, and double crystal topographs made it possible to separate the film and the substrate components of the sample to reveal their individual properties. In 1983, the Synchrotron studies were extended to powder diffraction. Parallel beam optics and silicon channel monochromators allowed high resolution, high peak-to-background and symmetric profiles which, coupled with the wavelength selectivity, produced remarkable diffraction patterns. Patterns could be obtained in either the conven-

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tional 2:1 scanning mode, in transmission mode, or with a fixed angle and Energy Dispersive Diffraction mode. This latter method allowed patterns to be obtained in very short times which would allow time resolved studies to be carried out. The new studies were applied to crystal structure refinements, anomalous scattering, texture analysis, precision lattice parameter determination, quantitative analysis, and depth profiling of thin films.

Parrish is the author of about 300 papers in virtually all aspects of X-ray powder diffraction. He organized the first World Directory of Crystallographers and was Chairman of the IUCr Committee to set up the Journal of Applied Crystallography. He was Secretary-Treasurer of the Crystallographic Society of America and a member of the USA National Committee on Crystallography. He has also served on committees of IUCr and the American Crystallographic Association on crystallographic apparatus.

Although the Hanawalt award is being presented to Parrish for his work employing synchrotron radiation in powder diffraction, it is difficult to separate this remarkable career from the most recent work. William Parrish is a young 73 and will surely remain active into the indefinite future. It was a pleasure for me as the Chairman of the JCPDS-International Centre for Diffraction Data to present the 1987 J. D. Hanawalt Award to this deserving recipient.

Deane K. Smith, Chairman
JCPDS-International Centre for
Diffraction Data

Deane Smith *William Parrish*

JCPDS-ICDD Bibliographic Search Procedures

This contribution describes the bibliographic procedures currently utilized at the JCPDS-International Centre for Diffraction Data. In the past, most of the data in the Powder Diffraction File have come from bibliographic searches of publications found in journals and other published sources. In recent years, however, increasing costs of journal publication have made editors more reluctant to publish actual powder patterns, thereby making location of new diffraction data more difficult. As a consequence, over the years, there have been increasing numbers of requests by the editor-in-chief to authors of articles that indicate the existence of desirable data. In addition to this, there have been voluntary contributions from persons who have such data. In order to better cover the vast literature in this field, the International Centre has recently supplemented the well established manual bibliographic process with computer searching. This article describes the processes which are currently in place at the JCPDS-ICDD.

Data for publication in the Powder Diffraction File are acquired in three ways: through survey of the literature, through grants-in-aid and through contributions from individuals and organizations. These data are critically reviewed by the editorial staff as described in Powder Diffraction, *1*, #3, p. 279. The first data sets were made up mainly of contributions from organizations such as the Dow Chemical Company (major contributor), New Jersey Zinc Company and the British Institute of Physics. By the early 1950's, a staff bibliographer had been appointed to search the literature for data, a grants-in-aid program had been established and editors had been selected to review the data entering the editorial system.

The major purpose of the bibliographic search has always been to locate powder diffraction data and references to the existence of such data from published sources and to supply these items for routing through the editorial system. In the process of bibliographic searching, most journals are looked at page by page, with particular attention given to the title, abstract, summary, experimental procedures, results and acknowledgments, and for particular reference to powder diffraction analysis. Pertinent information has been found in all parts of articles, even in footnotes and references. Data are found as tables which contain d, I/I_0, hkl and θ or $\sin^2\theta$, or only d and I, or only 2θ or $\sin^2 2\theta$, observed intensity and hkl; data may be in the text or in footnote or reference. Occasionally, d spacings are given without accompanying intensities; these articles are considered "writes" and are so designated. When data, or references to data, are found in an article, the procedure followed is to fill out a 3x5 card with reference to: 1) the journal by name abbreviation (as per Chemical Abstracts usage), volume number, issue number, pages involved and year; 2) the authors (surname and first initial of the first author and either surname of the second author, if there are only two authors, or et al if there are more than two authors); 3) the names or formulae of the substances whose diffraction patterns are given or referred to; 4) the editor to whom the article is to be sent; 5) a list of pages which contain powder difffraction patterns, and; 6) either the number of patterns in the article or a "write" if only references to data are found in the article.

A "write" is an article in which there is reference either to powder diffraction data or analysis or to instruments or methods involving powder diffraction methods. Any reference to powder diffractometry, Guinier-Simon, Guinier-Hagg, Gandolfi or Debye-Scherrer cameras, to powder diffraction analysis or examination, to isomorphism or non-isomorphism, or to data being held in a repository brings an article into the "write" category. Sometimes articles may show one (or more) diffraction pattern(s) and indicate that data from isomorphous or other substances are available; in such an instance, the 3x5 card is marked both with the number of patterns in the article *and* as a "write". Some journals rarely publish powder patterns, even when submitted, but call attention to the availability of such patterns from the editor's or publisher's office or from the author. The responsibility for writing for powder data rests with the Editor-in-Chief, as does judgment for other aspects of the data acquisition and publication. This is necessary because many "writes" are not worth writing for, either because the data are already in the file or the work obviously did not call for a full powder pattern. "Writes" have proved valuable as a source of new data.

With some journals that occasionally or rarely contain powder data or references, the table of contents is examined carefully, looking for names of materials or for words like polymorphs or crystal structure. These papers are looked at because, occasionally, powder patterns are used to determine cell parameters, isomorphous or non-isomorphous substances or existence of a single phase. It is necessary to be conscious of trends and of materials of current or great interest, e.g. physics journals that rarely carried powder data in the past are currently likely to contain articles that refer to or contain diffraction data of superconducting materials. In addition, editors of journals occasionally change directions and new journals appear.

Over the years, the number of journals scanned has increased to more than 350 journals in the fields of physics, chemistry, crystallography, polymers, pharmaceuticals, ceramics, mineralogy, metallurgy, etc. A rule of thumb used to determine the value of a journal was that a journal would be dropped if no useful data had been found therein for a period of five years. Within the last year, as the number of journals continued to increase, surveys were made of the number of "hits" from the journals and of the value of two computer searches of data bases for powder diffraction data. As a result, the decision was made to separate the literature search into two parts, one to continue the use of manual search of about 150 journals that have, in the past, provided about 97% of the data from the literature and the other to use the other data bases and to see some journals, at National Bureau of Standards and United States Geological Survey libraries, that are not available in the Philadelphia area or at Pennsylvania State University.

The advent of computer searchable databases has enabled the International Centre for Diffraction Data to have more complete bibliographic coverage. There are more than 1000 journals publishing crystallographic information, and the number of new journals or newly reviewed journals continues to grow. Although a large percentage of the published data is single crystal information, it may be noted that the phase has also been characterized by powder diffraction methods. In an effort to reduce publication cost, powder data are frequently placed in data banks, retained in storage by the journal, or merely retained unpublished by the author. Thus, making use of searchable databases may allow us accessibility to more of this information. As is true of any database, the correct selection of key words can put an unlimited number of journals at our disposal. Therefore, in conjunction with the manual bibliographic effort described above, the computer effort has been started. Under this scheme, two computer abstracting services, NERAC, Inc., Storrs, Connecticut and Data Abstracting Search Services, Clarksburg, Maryland, are currently being utilized.

In the NERAC scheme, about 12 different databases are searched. Three different strategies; X-ray diffraction, X-ray cameras, and X-ray powder diffraction are used with the selected key words. Citations are provided weekly, based on title, abstract or scan of the article. Under this service, in addition to the regular groups of journals covered, many less accessible government reports and university reports are cited. There is also very complete coverage of the patent literature. Under the Data Abstracting Search Service, three sections of Chemical Abstracts: Physical, Inorganic and Analytical Chemistry; Applied Chemistry and Chemical Engineering; and Organic Chemistry are regularly searched and articles are retrieved. This service provides citation for a large number of new or newly reviewed journals. Although at least 12 libraries are on regular bibliographic visits, many journals in the new category are in obscure libraries and can only be obtained via the interlibrary loan service. Before the combined bibliographic effort, approximately 350 journals were accessed. During the early stages of the new system, potential data has been obtained from about 100 new or newly reviewed journals. The dual systems, manual and computer searching, in use at this time, complement each other and provide more complete bibliographic coverage.

The diffraction community is encouraged to send powder data to the International Centre for inclusion in the Powder Data File. This is particularly important for cases where the data would be put into storage, held by the author, or published in a journal for which access is difficult. Some data published in dissertations are not easily obtained and could be sent directly to headquarters. Data can be sent to the Editor-in-Chief or the Bibliographer who will acknowledge its receipt.

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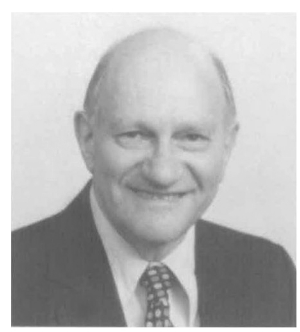

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