

Students at Madison, Wisconsin, U.S.A.

# Short Courses and Workshops

### JCPDS — International Centre for Diffraction Data Short Course on Search/Match Methods

The JCPDS-International Centre for Diffraction Data will continue to offer three-day short courses on Search/Match methods at the Swarthmore, PA, headquarters of the International Centre and elsewhere (see attached schedule).

The courses, which are now in their 5th year, are intended to build proficiency of the user in the interpretation of experimental data, especially in the application of the information provided in the *Power Diffraction File*. The courses should be useful to the novice as well as the experienced powder diffractionist, and all discussions start with the basic principles leading on to useful laboratory procedures. Workbooks are provided to all attendees and these contain a number of experimentally obtained X-ray diffraction data sets which are used as class exercises. During the workbook sessions, the classes are subdivided to match the needs and experience of the attendees.

The course will emphasize the nature and organization of the information in the *Powder Diffraction File* and retrieval and use of this information for interpreting experimentally collected diffraction data. The implications of the accuracy of measurement of d-spacings, and intensities of experimental data with respect to use of the powder file will be discussed, as well as common instrumentation and specimen-induced errors. The use of both manual and computer search/match methods for phase indentification will be practiced through the use of workbooks. Applications of File data for further characterizing phases will be illustrated using several mineralogical problems and a special X-ray diffraction minerals workbook. Other types of materials may be studied including organic and forensic materials, depending upon the needs of the participants.

#### **Course Schedule**

|                        | Optimization of data collection<br>Instrument alignment<br>Sample preparation<br>Evaluation of experimental diffraction<br>data<br>Instrument-induced errors<br>Sample-induced errors |
|------------------------|---|
| Afternoon              | Introduction to the <i>Powder Diffraction</i><br><i>File</i><br>Alphabetic search procedures<br>Hanawalt search procedures  |
|                        | Fink search procedures  |
| Morning                | Classical powder diffraction problems<br>Phase identification   |
| Morning                |   |
| Afternoon<br>Third day | Phase identification<br>Phase identification in polyphase<br>samples<br>Solid-solution analysis   |

For further information please contact:

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The cost of a course is \$550.00 which includes textual materials and lunches. Lodging, transportation and other costs are at the expense of the attendee.

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JCPDS — International Centre for Diffraction Data Course Schedules

## 1988

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

## **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,

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

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

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-tobackground and symmetric profiles which, coupled with the wavelength selectivity, produced remarkable diffraction patterns. Patterns could be obtained in either the conven-