

# General Announcements

## **NBS-ICDD Research Associateship Program — Goals Accomplished: A Tribute to 35 Years of Industry-Government Cooperation**

The JCPDS-International Centre for Diffraction Data (ICDD) and the National Bureau of Standards (NBS) are pleased to announce the successful conclusion of the X-ray powder diffraction Research Associate Program after 35 years of fruitful collaboration. Both the ICDD and NBS are looking forward to future cooperation between the two organizations as the ICDD moves into a new era of computerized data evaluation, new educational services, and new products for the X-ray diffraction community.

A Research Associate Program at NBS is one of the many ways that industry-government can cooperate to satisfy industrial needs. Typically, scientists from industries or associations work side by side with Bureau scientists on problems of mutual concern. The ICDD Research Associate in powder diffraction, established in 1951, had many significant accomplishments. There are two, however, which clearly stand above the rest: the large number of key standard reference powder patterns and the development of a prototype PDF computer data base and associated computer aided evaluation programs. Both have become recognized world-wide by the X-ray community.

In 1951 the first ICDD funded Research Associate joined NBS scientists to address the needs of industry for an improved PDF. The principal task was to produce experimental reference patterns by accurate and accepted methods on well characterized materials. The resulting patterns would replace earlier less accurate, often conflicting studies and provide a standard for X-ray powder diffraction to be followed world-wide. The results from this collaborative effort were published first in the series NBS Circular 539 (ten issues) then in NBS Monograph 25 (twenty-one issues), approximately one per year. Each of these reference patterns were abstracted and published in the Powder Diffraction File (PDF) shortly after NBS publication.

At first, attention was given primarily to the elimination of duplicate data in the PDF. Later, the materials studied were chosen pragmatically, based on the availability of materials and requests for the improvement of specific data. Most recently patterns for materials considered common have been evaluated and those not of today's standards have been redetermined. The program has upgraded many patterns published in the early sets of the PDF as well as added many new patterns from substances for which no data was available. The numbers alone, over 1500 experimental patterns and several hundred calculated patterns, do not fully reflect their importance to the value of the PDF.

The collaborative program also improved powder diffraction methods. The reference data are widely recognized as being measured with the best techniques and reported with exceptional accuracy. The procedures employed by the Associateship evolved along with the instrumentation and development of computer algorithms such as least-squares

lattice parameter refinement and digital pattern analysis. Indeed, the procedures adopted at NBS became the foundation of the publication guidelines of the International Union of Crystallography for X-ray powder diffraction patterns. The quality of the data has often resulted in NBS-ICDD Research Associateship patterns being singled out for reference when testing new methods of X-ray diffraction, new computer analysis algorithms, or alignment of instruments. The procedures currently used by the Associateship are reported in this issue of Powder Diffraction along with twenty of their most recent reference patterns.

The second major accomplishment of the collaborative program was the development of computer evaluation methods, computer data entry procedures and a prototype computer data base to replace the manual methods and paper files used by the ICDD for forty years. This data project began at NBS in 1978 with a pilot effort expanding on the evaluation procedures developed in NBS' Crystal Data Center. Success came rapidly and by 1979 the ICDD established a five year plan to ultimately bring the powerful computer entry procedures, evaluation methods, and data base design to ICDD headquarters in Swarthmore, Pennsylvania.

NBS scientists working on the data base project first concentrated on enhancing, testing, and debugging the evaluation program. Subsequently, with ICDD support, they concentrated on the creation of the computer data base and processing each PDF entry through the evaluation program. Once these critical first steps were completed, the ICDD established an intensive effort to review the computer evaluations for each pattern in PDF Sets 1 to 32 and to utilize the methods for data being entered for Sets 33 onward. By late 1984, the major numerical and consistency evaluations were completed and by October 1985 all the textual material was added. The ICDD now can produce any of their printed or computer media products directly from their data base. The dedication and commitment of NBS scientists to this project was crucial to its rapid success and full scale adoption.

The ICDD has now benefited by bringing in-house all production steps except for publication. This provides considerably improved control over the editorial evaluation, quality, timing and cost of ICDD publications. The benefits to the users of the Powder Diffraction File, the subject of an article in the next edition of Powder Diffraction, include consistent evaluation of all 45,000 patterns in the PDF; addition of revised quality marks, figures-of-merit and the Pearson symbol; and also important critical evaluations of name, formula, density, lattice parameters and d-spacings.

With considerable contributions from the 35 years of cooperation with the National Bureau of Standards, the ICDD has become a stronger organization ready today to serve the powder diffraction community in new and exciting ways. The ICDD looks forward to new educational services, focussed pattern production from grants, and improved product delivery. NBS will continue to develop XRD measurement methods, Standard Reference Materials, and reference patterns for selected materials. Both NBS and the ICDD anticipate continued cooperation and look to the future knowing that a strong and enduring foundation for phase identification has been laid.

## The J. D. Hanawalt Powder Diffraction Award

The award is sponsored by the JCPDS-International Centre for Diffraction Data. It is to be presented every three years for an important, recent contribution to the field of powder diffraction. The award will consist of a certificate and \$1000. The awardee is expected to submit an abstract and present a paper on the work being recognized at the IUCr Satellite Meeting on X-Ray Powder Diffractometry, Perth, Western Australia, August 20-22, 1987. Travel expenses to the meeting will be provided.

The award was first presented in 1983 to Dr. Ludo Frevel at the Denver X-ray Conference. Work that is eligible for consideration for the second presentation of the award must have been published between 1 January 1980 and 31 August 1985. There are no restrictions as to age, experience, or nationality of the recipient.

The 1986 selection committee members are Walter Eysel (Universitat Heidelberg), Ben Post (Polytechnic Institute, NY), Brian O'Connor (Western Australian Institute of Technology), Catherine Foris (DuPont) and Camden Hubbard (U.S. National Bureau of Standards). The selection committee will welcome suggestions, nominations, and documentation of accomplishments for possible recipients through 30 April 1986 from any interested persons. These can be sent to any committee member or directly to the chairman C. R. Hubbard, A257 MATL, National Bureau of Standards, Gaithersburg, Maryland 20899, U.S.A., (telex 894493).

## Grants-In-Aid from the JCPDS-Joint Committee on Powder Diffraction Standards

Each year the JCPDS-International Centre for Diffraction Data extends financial support in the form of Grants-in-Aid to a limited number of scientists for the provision of X-ray powder data. These grants are intended to supplement existing funded projects involving the preparation and recording of data from new materials. First time grants are usually of the order of \$2,000 to \$5,000 for projects resulting in 10-25 new patterns. Proposals addressing the immediate needs of the powder diffraction community will be given highest priority, especially projects involving organic compounds and materials used in forensic investigations. Materials involved with any new and evolving technologies are also of specific interest.

Grants-in-Aid proposals will be considered from any qualified investigator who can demonstrate expertise in the preparation of high quality powder diffraction patterns, or in the synthesis of high purity materials, provided that such materials are of interest to the Grants-in-Aid Committee. All Grant-in-Aid recipients are required to prepare bi-annual reports on progress and extension of a Grant beyond a given year is contingent on satisfactory performance. Proposals should be submitted in accordance with specified

guidelines and new proposals are reviewed in January of each year. A final decision is generally reached in March. All Grants become effective the beginning of the JCPDS fiscal year, currently 1st April.

Guidelines for the preparation of Grant proposals can be obtained from the JCPDS and proposals for grants should be addressed to:

Secretary, JCPDS-International Centre for  
Diffraction Data  
1601 Park Lane  
Swarthmore, PA 19081, U.S.A.

## Smithsonian Institution Department of Mineral Sciences Seeks to Extend Collection of Studied Minerals or Other Inorganic Substances

The Department of Mineral Sciences at the National Museum of Natural History is very interested in increasing the number and availability of well-characterized standards for powder diffraction analysis and mineralogical research. Material from our extensive collection of over two hundred thousand specimens is available to qualified investigators for legitimate scientific purposes. We would like to receive additional samples of *studied* minerals or other inorganic substances which would increase the usefulness of our collection as a resource for the scientific community. We also welcome help in characterizing the unstudied material in our collection. With our new automated powder X-ray diffractometer and excellent analytical facilities, we are eager to collaborate and cooperate with scientists to develop high quality powder diffraction data for as wide a variety of minerals as possible. Anyone interested in obtaining or contributing samples should send a short letter outlining the nature and purpose of the request or a description of the material to be contributed to Jeffrey Post or Daniel Appleman at the Dept. of Mineral Sciences, NHB 119, Smithsonian Institution; Washington, D.C. 20560.

## Back issues of Standard X-ray Diffraction Powder Patterns

The JCPDS Associateship at the National Bureau of Standards has on hand a limited supply of back issues of NBS Circular 539, Sections 1-10, as well as NBS Monograph 25, Sections 1-19. Individual copies may be obtained at no charge as long as supplies last.

Please contact: Mrs. Marlene Morris  
National Bureau of Standards  
Building 223, Room A209  
Washington D.C. 20899

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