COMMISSION ON POWDER DIFFRACTION

INTERNATIONAL UNION OF CRYSTALLOGRAPHY

NEWSLETTER No. 9

November 1992

ACCURACY IN POWDER DIFFRACTION APD-II
Gaithersburg, Maryland, USA, May 26th-29th, 1992

The conference on **Accuracy in Powder Diffraction II** held at the National Institute of Standards and Technology (NIST), Gaithersburg, Maryland, from May 26-29th, 1992, was the most ambitious event yet undertaken by the Commission on Powder Diffraction (CPD) apart from the Satellite Meetings traditionally held in conjunction with the triennial IUCr Congresses. It was organized with the help of NIST and a local committee chaired by E. Prince who are to be congratulated for providing such a smoothly functioning operation and for taking such sensitive care of the individual needs of the participants. Generous financial support was provided by the JCPDS–International Center for Diffraction Data for invited speakers and by the IUCr for young scientists. The meeting was attended by a total of 175 registrants from 18 countries, of which the USA provided the largest number, 103. There were 26 invited lectures, and another 11 oral presentations selected from the 70 contributed abstracts. Written versions of the talks will appear as an NIST Special Publication similar to that published following the 1979 meeting now known as APD–I.

The program committee, chaired by R. J. Hill, attempted to provide a broad framework of topics which spanned the whole range of powder diffraction applications and fell into six categories: phase identification and quantification, accuracy and standards, new developments in software and data analysis, profile fitting, decomposition and microstructural effects, novel applications and structural science, and last but by no means least new developments in hardware, including detectors, and studies under non-ambient and time-resolved conditions. Other events included two JCPDS–ICDD workshops organized by C. M. Foris dealing with ***Powder Diffractometer Sensitivity*** (R. Jenkins) and ***Indexing Methods*** (D. K. Smith), and an Open Meeting of the CPD. The pro-

Participants at the APD-II meeting held at NIST, May 26th-29th, 1992

gram for the sixth session on the last day was designed to interface smoothly with a workshop on ***X-Ray and Neutron Diffraction at High Pressure*** organized by R. J. Nelmes and L. W. Finger for the High Pressure Group of the IUCr held immediately following APD-II and described in a separate report. The social program included a banquet at the conference hotel, and a very popular reception at the Natural History Museum of the Smithsonian Institution arranged by J. E. Post and colleagues. The meeting opened with a tribute to William Parrish delivered by T. C. Huang, his colleague for many years at IBM, who gave a very moving, enthralling and informative account of Bill's career of more than 50 years in powder diffraction with Norelco and IBM which included several fascinating insights into his many outstanding scientific accomplishments. Of particular interest were some photographs of Bill from the ***Norelco Reporter*** showing his diffraction equipment and some of his more illustrious colleagues. This talk provided a very clear picture of Bill's enthusiasm, drive and perseverance, and was much appreciated and enjoyed by everyone. It was a fitting tribute to one of Powder Diffraction's outstanding sons.

A brief account of the various sessions based mainly on reports submitted by the session chairmen follows below. We are grateful to L. Zevin, D. K. Smith, H. Toraya, J. B. Parise and D. Häusermann for their contributions.

Phase Identification and Quantification

The first session on this topic opened with a keynote talk by B. L. Davis on quantitative phase analysis with reference intensity ratios (RIR) which led the audience through the development of traditional RIR methods, their strengths and weaknesses, some tips on sample preparation, and included some examples of studies on mineralogical materials containing phases displaying solid solution. L. Zevin followed with a clear exposition of standardless methods of quantitative X-ray diffractometry pioneered by him in the 1970's and now sometimes modified to include chemical information. The method relies on the self-calibrating ability of a sample set with diverse compositions of the same group of phases.

The seven afternoon talks fell clearly into three categories: the full-pattern approach towards quantitative analysis, automatic search-match procedures, and the effects of sample-related phenomena on the precision of analysis. In the first talk R. L. Snyder discussed incorporation of the RIR in quantitative analysis by X-ray diffraction. Although RIR is not needed to scale calculated patterns, it is useful if a reference material is added in known proportion to the sample. In this case an undetected (amorphous) phase can be determined in any of the quantification techniques, including those based on calculated analytical standards. J. K. Stalick discussed the application of neutron diffraction data, a particularly interesting point being the analysis of major phases by phase scaling combined with Rietveld refinement and simultaneous analysis of minor phases without reference to their structures. Of course, calibration against pure phases is needed for the latter. One of the phases (CuO) was determined even when there were no apparent peaks of this phase. M. S. Nackmanson emphasized the importance of proper organization of the database in search-match procedures. The complete database can be divided into sub-databases consisting of clusters of isostructural compounds. Taking this into account in the program will shorten the search time and the list of probable candidates. R.G.Marquart described a user-assisted system for angular correction based on internal standards with well-established lattices. Three serious problems in quantitative diffractometry, i.e. microabsorption, preferred orientation and poor particle statistics, were discussed in the remaining three talks. The central point of the talk by D. K. Smith was that crystallite statistics can be a critical factor affecting the precision of analysis of minor phases. Beam divergence in the focusing plane has little effect on the number of reflecting crystallites, and broad-tube focus is more effective. He proposed a combination of a broad-focus tube and sample oscillation to improve particle statistics rather than sample spinning, perhaps a somewhat controversial conclusion requiring further investigation. H. Hermann described efforts to establish a reasonable statistical model for multiphase powder samples with rough surfaces, and presented some observations confirming the theory. At the present stage, however, it seems, that in many practical applications microstructural parameters such as grain-size distribution must be known before the theory is applied. H. Oettel treated preferred orientation in multiphase materials by application of the fibre texture model of Jarvinen. Texture parameters were used for intensity corrections in quantitative phase analysis.

Accuracy and Standards

The topic of this session was basic to the theme of the conference. In the opening address, P.-E. Werner discussed the relative merits of cameras and diffractometers for attaining accuracy in position and intensity measurements. Although the distinction between the instruments with respect to the measurement of intensities clearly favors the diffractometer with its digital output, the same is not true for position measurements. In fact, diffractometers do not have the potential resolution of a Guinier camera unless the instrument is equipped with a primary curved-crystal monochromator using essentially the same optics. The conclusion is that the instruments complement each other and both should be employed in modern research. Three other oral papers focussed on subtle effects and accuracy in experimental data. J. F. Bdrar showed where the details of peak shapes and their variations with angle and sample effects became important in the analysis of structures by Rietveld and other pattern fitting procedures. J. P. Cline described the NIST program on certifying Standard Reference Materials and the newly certified SRM's for powder diffraction. H. Toraya dis-

cussed the use of internal standards and the use of whole-pattern profile-fitting to achieve accuracy in determining accurate crystal data.

New Developments in Software and Data Analysis

There were six talks in this session centering around new techniques and software for structure analysis. L. McCusker reviewed the necessary steps for ***ab-initio*** structure solution from powder data, and emphasized the importance of minimizing the degree of peak overlap by improving sample crystallinity and instrumental resolution. Structure solution was also the theme of the next lecture by J. M. Newsam, who described how simulated annealing provides a new route to this end, and demonstrated its successful application to 90% of the known zeolite structures. M. Estermann gave details of a new method for unravelling the intensities of severely or completely overlapped peaks called Fast Iterative Patterson Synthesis, and illustrated this with an example of a molecular sieve structure where the application of the new technique allowed the determination of a previously unsolved structure. The general area of automatic indexing procedures and applications was reviewed by D. Louër, who stressed the fundamental importance of high precision in the measurement of peak positions, and the necessary experimental techniques and data collection strategies. Recent advances in the determination of atomic pair-distribution functions (PDF) obtained from direct Fourier transforms of powder data were described by B. H. Toby, who pointed out how this kind of analysis could reveal details of the local order not reflected in the crystallographic refinement, and also the fact that termination errors could be reduced to a minimal level with modern neutron time-of-flight and synchrotron X-ray instrumentation. In the final talk, J. Schneider discussed how short-range effects reflected in diffuse scattered intensity could be incorporated into a standard Rietveld program, as exemplified by a study of a sodium-thallium alloy.

Profile Fitting, Decomposition, and Microstructural Effects

The four talks in this session centered around microstructural effects and the application of profile fitting techniques to these topics. J.I. Langford emphasized how advances in pattern decomposition are providing a wealth of information about the microstructure of polycrystalline materials. He discussed the use of the Voigt function in the analysis and the need for high resolution and good counting statistics to obtain reliable and consistent information. V. Valvoda reviewed various methods of correcting for preferred orientation and experimental techniques for reducing such effects. The most reliable correction is provided by the use of a set of symmetrized spherical harmonics to describe the orientation distribution of the crystallites. T.M. Holden gave an informative overview of the application of neutron diffraction to the accurate measurement of residual stress, an increasingly important topic at many neutron facilities. Finally, A. Le Bail discussed the current status of methods to model anisotropic line-broadening effects, and emphasized the fact that these represent a great oversimplification of the problem. The development of more realistic methods will be a difficult challenge.

Novel Applications and Structural Science

This session consisted of six lectures covering examples of recent novel applications of powder diffraction techniques to structural problems. D.L. Bish described how the traditional Rietveld method could be applied to structure solution when used in conjunction with crystal-chemical principles and distance least-squares constraints, and illustrated this with examples of zeolite and clay mineral structures. The extension of the Rietveld method to the determination of anharmonic thermal parameters and the derivation of the probability density function was discussed by H. Boysen, including examples of diffusion paths in fast-ion conductors. J. B. Parise focussed on the application of molecular modelling techniques to the location of the aromatic hydrocarbon stilbene in the zeolite catalyst **ZSM-5** based on high-resolution synchrotron X-ray data. Recent advances in the use of anomalous dispersion in powder diffraction studies were reviewed by J.P. Attfield, who showed how synchrotron radiation close to an absorption edge could be used for the determination of cation distribution and oxidation states. R. W. Cheary discussed how line-broadening effects could be employed to study antiphase domains and intergrowths in barium hollandite structures, and in the final talk, R. Vargas described a simple physical model which could be used to interpret X-ray scattering data from a lamellar system of myelinated nerve sheaths.

New Developments in Hardware, including Detectors, and Studies under Non-ambient and Time-resolved Conditions

Most of the seven talks in this session focussed on new hardware developments in conjunction with synchrotron X-ray and neutron diffraction techniques. In the first lecture Y. Fujii reviewed the utility of the diamond-anvil cell for investigations of powders under high pressures, including the use of imaging plates to provide data suitable for Rietveld refinement, and described the high-pressure facilities available at the Photon Factory in Tsukuba, along with some recent studies of molecular crystals and metals. The distinction between single crystals and powders becomes less obvious on the basis of data presented by L. W. Finger, who described recent results obtained from synchrotron X-ray studies of sub-micron single crystals of bismuth, and outlined the problems associated with this kind of work, including sample mounting problems, potentially poor sample quality, and beam inhomogeneities. Some ***in-situ*** synchrotron X-ray studies of crystallization in metallic glasses were described by M. Sutton, with emphasis on phase identification and lattice parameter determination of transient phases not observable in quenched glasses. The problems of collecting X-ray data at high temperatures on large-grain alloys were

discussed by O. B. Cavin, who described a rocking curve method to overcome unwanted texture effects in these materials.

The afternoon session began with an exciting review by J.S. Loveday of two important new developments in the field of neutron diffraction at high pressure : a new large-volume (80-100 mm^3) cell based on the Soviet toroidal anvil design, which allows Rietveld refinement above pressures of 10 GPa and is steadily pushing the highest pressure limit past 20 GPa at the ISIS spallation source, and the development of a detector covering nearly 180° at a Russian reactor which can collect data of high enough quality for structure refinement at pressures up to 7 GPa from sample volumes as small. as 1 mm^3. The large-volume cell is not only much smaller than conventional large volume devices but it is also suitable for synchrotron X-ray work. J.A. Fernandez-Baca returned the proceedings to the USA with a description of the new multidetector powder diffractometer recently installed at the Oak Ridge reactor. This is currently equipped with a flat Ge(115) monochromator (later to be replaced by a vertically-focusing device) and 32 ^{3}He counters, and covers a 2θ range of 11-135° with a minimum resolution $\Delta d/d \approx 2 \times 10^{-3}$. This instrument has been successfully tested by refinements on several reference materials and complex oxides. Full-pattern fitting of synchrotron X-ray energy-dispersive diffraction data is a major challenge due to the numerous energy-dependent factors in the intensity expression, which becomes even more difficult in a diamond-anvil cell due to the very small sample volumes and correspondingly poor crystallite statistics. T. Yamanaka showed how these problems can he overcome by careful consideration of all these factors and the combination of cell rotation with oscillation, and presented results of structure refinements at high pressure and high temperature using data collected at the Photon Factory and the KEK Accumulator Ring.

In summary, APD-II made it quite clear that the renaissance in powder diffraction that was captured in the "snapshot" during the first meeting on Accuracy in Powder Diffraction held at the National Bureau of Standards in 1979 is continuing at an even greater pace today. In particular it is evident that Rietveld analysis is the powder diffraction technique of common choice and advantage for the study of materials of all kinds in many areas of solid-state science. The variety and quality of the information that can now be extracted from a powder diffraction pattern is literally staggering in its breadth and importance. Never before have so many previously neglected materials come under such close scrutiny, and never before has it been possible to study these materials under such a wide range of non-ambient conditions. Diffraction patterns previously collected only for phase identification or unit cell determination are now used to study such things as the subtleties of electron density distribution, the mechanism of phase transformations, and the distribution of cation oxidation states. We can look forward eagerly to APD-III, but perhaps we should recognize the pace of change is now so great that we should not wait another 13 years for this!

R. J. Hill and D. E. Cox

MEETING REPORTS

Czechoslovak Crystallographic Society Annual Meeting, Vojtekhov, Czechoslovakia, May l8th-22nd, 1992

About 95 participants, mostly from Czechoslovakia, attended the meeting, during which 27 lectures and 24 posters were presented. The main theme of the meeting was to address "real" structural phenomena such as paracrystallinity, crystallite interrelations in polycrystalline aggregates, lateral accommodation of di-octahedral and tri-octahedral layers in the structures of clay minerals, and molecular shape relaxation in the (para)crystalline phase. The wide variety of topics included epitaxy, paracrystallinity, textures of laser-deposited ceramic coatings, X-ray diffraction measurements of stresses in ceramics, structural variability of clay minerals, ore microscopy, structural databases and their statistical analysis, neutron and ion-beam diffraction, and small-angle scattering. A broad range of materials was covered, including steel, ceramics, minerals, coordination compounds, semiconductors, proteins, fullerenes, organic polymers, superconductors, molecular clusters and smdl molecules. The realm of powder diffraction was reflected in lectures by Z. Weiss on quantitative mineralogical analysis, R. Cernyf on joint refinement based on X-ray and neutron diffraction data, and M. S. Nakhmanson on the **COMPHUS** system of computer programs for powder diffractometry.

A romantic excursion to Karstic caverns hidden in beautiful woodland several miles from the conference hotel, and the ceremonial conference banquet completed this very successful meeting, for which the organization and program committees chaired by D. Olomouc, and A. Buchal, Brno, respectively, are to be complimented. The conference proceedings are available in the form of soft-bound volumes containing 260 pages which were distributed to participants at registration.

J. Fida

X-Ray and Neutron Diffraction at High Pressure, Washington, DC, USA, May 30th-31st, 1992

This workshop was organized by L. W. Finger and R. J. Nelmes for the High Pressure Group of the IUCr and held at the Carnegie Institution. Advances in instrumentation and techniques for synchrotron X-ray powder diffraction studies at high pressures in diamond-anvil cells was a major theme. Energy-dispersive methods were reviewed by D. Hausermann, who emphasized the advantage of using conical diffraction geometry with an annular detector and the need to improve detector throughput for time-resolved studies at the next-generation

sources. Y. Fujii talked about recent advances using monochromatic radiation at the Photon Factory, Tsukuba, and gave details of several structural studies. L. W. Finger reviewed the development of monochromatic-beam techniques at the NSLS, Brookhaven, based upon the use of a horizontally-focussed beam end a Kr-filled position-sensitive detector operating in the escape-peak mode and capable of 0.03º angular resolution. M. I. McMahon described advances at the SRS, Daresbury, involving the use of an imaging plate to obtain data adequate for detailed structure analysis through Rietveld refinement. The development of high pressure cells for neutron diffraction was another important topic of the workshop. J. Loveday gave details of a novel cell capable of operating above 10 GPa at a pulsed-neutron source, I. N. Goncharenko described some experiments carried out with diamond and sapphire cells, and K. Futterer discussed a cell designed to operate at 1.5 GPa and 500ºC for use at a steady-state source. Diamond-anvil cells for X-ray diffraction up to 1500ºC with resistive-heating elements were discussed by P. D. Adams, while D. Schiferl described progress on the construction of a cell designed for operation up to 800°C, and some of the problems associated with precise pressure measurement at these temperatures.

Overall, the workshop provided ample evidence of the recent progress in the development and application of high pressure powder diffraction techniques. It also demonstrated that energy-dispersive X-ray methods, which have been the mainstay for structural studies at high pressures at many synchrotron sources over the past decade, are now being challenged by higher-resolution monochromatic-beam techniques that should allow the refinement of fairly complex structures if reasonably hydrostatic conditions can be maintained.

D. E. Cox

Second European Powder Diffraction Conference EPDIC-2, Enschede, The Netherlands, July 30th-August lst, 1992

The conference was held under the patronage of the Royal Dutch Chemical Society at the University of Twente as a satellite meeting of the 14th European Crystallographic Meeting. It attracted almost 400 participants including many scientists from Eastern Europe and the former Soviet Union as well as from the United States and other overseas countries. The charming atmosphere of the campus site together with the perfect work of the Organizing Committee chaired by T. W. Ryan of Philips, Amelo and H. Slaghuis of the University of Twente provided the basis for a very successful conference. The list of sponsors included the IUCr, the ICDD represented by L. Frevel and J. Visser, and all European companies currently active in the field of powder diffraction. Almost all of the European members of the IUCr CPD were present.

The scientific program was opened by Dr. L. K. Frevel of the ICDD with the presentation of the Hanawalt Award for excellence in the field of powder diffraction to Dr. Daniel Louer of the University of Rennes. His plenary lecture gave an overview of new diffraction applications in conventional X-ray instrumentation and their usefulness in materials science, especially in the ***ab-initio*** determination of crystal structures.

More than 200 contributions covering all aspects of the analysis of polycrystalline materials by diffraction methods were presented in three parallel oral sessions each morning and in the accompanying poster session. These sessions were preceded by six invited lectures which provided a good insight into both forthcoming trends (D. L. Price on the analysis of disordered materials by X-ray and neutron diffraction, M. Marezio on powder diffraction using synchrotron radiation, and P. F. Fewster on thin polycrystalline films) and also the state of the art of powder diffraction (L. B. McCusker on structure determination from powder diffraction data, P. van Houtte on stress measurement in textured materials, and B. B. Zvyagin on electron diffraction in powder crystallography).

The poster session was held in combination with the commercial exhibition in the university sportshall, an arrangement which was well-accepted by all participants. Prizes for the three best posters judged on scientific content as well as style and presentation were awarded during the closing ceremony. Also announced was the European Powder Diffraction Conference Award sponsored by the X-ray division of Philips Analytical. This award honors outstanding scientific achievements by young scientists in the areas covered within the EPDIC program. The first presentation is planned to take place at EPDIC-3, and the powder diffraction community is invited to submit names of suitable candidates to the chairman of the Program Committee of EPDIC-3, Ekkehart Tillmanns of the University of Vienna.

In keeping with tradition, a workshop on the JCPDS-ICDD Powder Data File was given by J. Visser, Delft, and W. Eysel, Heidelberg, and a second workshop presenting the non-commercial PC program system GUFI for powder diffraction measurements and evaluation was held by R. E. Dinnebier from Heidelberg.

Apart from the scientific success of the meeting, all participants also greatly enjoyed the social program, the highlight being the conference dinner at the University Student Center, the Bastilla, an unusual place with unusual architecture. Not so usual either was the after-dinner belly-dancer performance which was greatly appreciated and received a standing ovation from the audience!

EPDIC-3 is planned to be held September 25-28th, 1993, in Vienna with the local organization chaired by A. Preisinger of the Technical University of Vienna. Future EPDIC meetings will then take place every two years rather than annually.

E. Tillmanns

Summer School on the Rietveld Method, Cieszyn, Poland, August 13th-l5th, 1992

Two years after the first PC-based Summer School on the Rietveld Method was held in 1990 (see the report in CPD Newsletter No. 5), a second was held on August 13th-15th at the same place, the Department of Arts of the Silesian University in the town of Cieszyn at the Polish-Czechoslovakian border. The School followed the XVth Conference on Applied Crystallography held on August 9th-12th1 1992, at the same location.

Sponsored by the IUCr, the School was organized by the CPD, the Silesian University in Katowice and the Institute of Ferrous Metallurgy in Gliwice. The organizational tasks were shared mainly by Professor Z. Bojarski, the local chairman, Dr. D. Stróz, the secretary, Dr. K. Stróz, chief of the computer laboratory, and Professor R. A. Young, director of the School and one of the lecturers. The other principal lecturers were Professor A. K. Cheetham, University of California at Santa Barbara, and Dr. R. B. Von Dreele, Los Alamos National Laboratory. Dr. H. M. Rietveld attended as an honored guest of the School and delivered the opening lecture, a retrospective account of the Rietveld method.

The multi-task program of the School included general lectures each morning, starting from a brief overview of important successes of Rietveld refinement and continuing with lectures on how the method works, how to use it and how to deal with various problems in its use, such as difficulties with peak shapes, non-structural contributions and problems with data collection. In the afternoons, the participants were split into two groups alternating between practical training sessions on computers of the IBM PC/AT type running the DBWS-9006 program with diffraction data and examples provided, and special tutorial sessions dealing with such topics as comparison between X-ray and neutron studies, the role of synchrotron X-ray diffraction and anomalous dispersion, refinement strategies and advanced refinement techniques. In the evenings the computer laboratory was open for students to use on their own.

A total of 42 students from several European countries attended the School, which provided an excellent opportunity for the participants to learn the method and discuss their refinement problems with experts. For a great many of the participants, this was their first practical contact with the Rietveld refinement technique, and it was observed during the practical sessions that beginners had trouble editing the input-output files in Fortran format. However, most of the students were ultimately able to work through several examples and to leave with some results of refinements. Each participant was encouraged to take home a source code version of the DBWS-9006PC program, the files for the sample problems, an executable copy of the PLOT program and two descriptive booklets; "Using the Rietveld method at RSS-92"and ((User's guide to DBWS' 9006PC ", which contain all the necessary information for carrying out self-supervised Rietveld refinements on one's own PC. With these items and the instruction provided at the School, the participants should be able to proceed to more advanced problems.

Ewa Sobczak

ENCOMIUMS

Dr. **Daniel Louër,** Université de Rennes, France, was presented with the J. D. Hanawalt Award of the International Center for Diffraction Data for excellence in the field of powder diffraction during the opening ceremoney at the European Powder Diffraction Conference EPDIC-2 recently held in Enschede, The Netherlands. Dr. Louer also serves on the Commission on Powder Diffraction, and his colleagues on this join in offering their congratulations for this well-deserved honor.

Dr. **James Jorgensen,** Argonne National Laboratory, USA, has won the 1992 Annual Award of the Division of Materials Sciences, U.S. Department of Energy, for sustained outstanding research in solid-state physics based on his extensive work in the field of powder diffraction with pulsed neutrons.

NEWS FROM ITALY

The Associazone Italiana di Crystallografia has announced the first of a series of annual meetings addressed to young crystallographers to be held in Pisa, Italy, December 14th-16th, 1992. At this meeting, emphasis will be given to the basic aspects of powder diffraction in the angle-dispersive mode, especially phase identification and quantitative analysis. The program will cover topics such as the instrument function, interpretation of the diffraction pattern, methods for qualitative and quantitative phase analysis, and a demonstration of related computer packages. For further details, contact Professor G. Berti, Dip. Scienze della Terra, Via S. Maria 53, 56126 Pisa, Italy (Phone 39-50-568254; Fax 39-50-500932; e-mail berti@mai1box.dst.unipi.it).

STATUS OF CPD PROJECTS

The report on the first phase of the **Round Robin on Rietveld Refinement** project has now appeared in *J. Appl.* Cryst. 25 , 589-610 (1992).

This phase dealt only with the sets of X-ray and neutron data sent to all participants for in-house Rietveld analysis. Dr. R. J. Hill is the coordinator for this project and carried out all of the analyses of the results, and then wrote and rewrote the paper until all the CPD members were satisfied with it as a Commission report. Dr. Hill is now analyzing the results from the second phase, in which participants collected their own data on a sample of monoclinic zirconia provided by him. In both cases, the results show that the worker-to-worker disparities were greater than most would have imagined, and efforts are being made to pinpoint some of the causes of these disparities. It is clear that this Round Robin was sorely needed.

The CPD has undertaken a leading role in the further development of the **CIF/STAR** format system for

use with powder diffraction data and in promoting it to become a universal standard for the archiving and exchange of such data. In addition to being very flexible in accommodating different types of data, the CIF/STAR system has the outstanding advantage that it communicates the experiment. It thus offers, for example, a solution to the problem of how to retain the possibility of working back to the original raw data from the "processed" data with which one actually works obtained from various national and international facilities, each with its own protocol. The ICDD has now adopted the system for its future databases and is cooperating with the CPD in the further development needed. The lead person for the CPD involvement is Dr. J. I. Langford and for the ICDD is Dr. B. H. Toby.

The CPD-engendered multi-author book on **"The Rietveld Method"** is now in the final stages of the publication process and should be available in early **1993.**

The **Program Information Exchange Bank** is accumulating information about updates of computer programs for the analysis of powder diffraction data and programs not previously listed with the intent to publish an updated version of the compendium by Smith and Gorter which appeared in ***J. Appl.* Cryst.** ***24*** **,** ***369-402 (1991).*** Please send any relevant information you may have to Professor D. K. Smith at the address listed on the last page of this Newsletter.

The CPD has under consideration **a Round Robin on Crystallite Size and Microstrain** to be carried out jointly with the ICDD. Questions about the feasibility of such a project are now being addressed. Professor R. L. Snyder at the New York State College of Ceramics, Alfred University, is taking the lead role for the ICDD in this project.

The CPD has been active in the area of **Meetings, Workshops and Schools.** Reports of two recent CPD-engendered and co-organized events, the meeting on **Accuracy in Powder Diffraction I1** held in May, **1992,** in the USA, and the **Summer School on the Rietveld Method** held in August, **1992,** in Poland, are presented elsewhere in this Newsletter. Forthcoming events are the **Rietveld Summer Schools** scheduled for December, **1992,** in Argentina and Brazil, and **a** workshop on **Computational Methods in X-ray Powder Diffraction Analysis** scheduled for January, **1993,** in Egypt. In addition, the CPD is also co-organizing **a Satellite Meeting on Powder Diffraction** in Hangzhou, China, immediately following the XVIth Congress of the IUCr scheduled for August, **1993,** in Beijing.

Several other events are actively under consideration by the CPD, as follows (titles and dates are tentative at this stage); a **Workshop on Powder Diffraction Software: Methods and Applications** to be held in Russia in June, **1994, a** meeting on **Structure Determination using Powder Diffraction Techniques** in the first half of **1994, a** meeting emphasizing **Powder Diffraction with Neutrons and Synchrotron X-Rays** possibly in June **1994** at either the Institut Laue-Langevin or Brookhaven National Laboratory, a meeting on **X-Ray Powder Diffraction** in September, **1995** in Czechoslovakia, and a **Satellite Meeting on Powder Diffraction** to be held in conjunction with the **1996** IUCr Congress in the USA.

Readers are encouraged to send suggestions for meetings, schools, workshops and any other types of project which the CPD might undertake or be associated with.

R. A. Young

FUTURE MEETINGS

Jan **1993: Fourth International School of Crystallography: Computational Methods in X-Ray Powder Diffraction Analysis,** Aswan, Egypt. (Prof. Karimat El. Sayed, P.O.Box **8014,** Masaken Nassr City, Cairo **11371,** Egypt; tel: **02-2601742,** telex: Hecor **4054,** e-mail: **karima@egfrcuvx.bitnet).**

Mar **10–12, 1993: Deutsche Gesellschaft für Kristallographie,** Bochum, Germany. (Frau Schwerte, Ruhr-Universitat Bochum, Institut fur Mineralogie, Postfach **102148, 4630** Bochum **1,** Germany).

Mar **29–Apr 2, 1993: British Crystallographic Association Spring Meeting,** Manchester, UK. (Dr. B. Beagley, Dept. of Chemistry, UMIST, PO Box 88, Manchester **M601QD, UK).**

May **23–28, 1993: American Crystallographic Association Meeting,** Albuquerque, New Mexico, USA. (Dr. A. Larson, LANSCE **H805,** Los Alamos National Laboratory, Los Alamos, NM **87455,** USA; tel: **505-667-2942).**

July **18–26, 1993: 10th International Clay Conference,** Adelaide, Australia. (l0th ICC Secretariat, Elliservice Convention Management, PO Box **753,** Norwood, South Australia, Australia **5067).**

Aug **21–29, 1993: XVIth IUCr General Assembly and International Congress of Crystallography,** Beijing, China. (Prof. M.-C. Shao, Institute of Physical Chemistry, Dept. of Chemistry, Peking University, Beijing **100871,** China).

Aug **31–Sep 3,1993: Satellite Meeting on Powder Diffraction,** Hangzhou, China. (Prof. R.-G. Ling, Central Laboratory, Hangzhou University, Hangzhou, China **310028;** fax: **86-571-870107).**

Sep **25–28, 1993: Third European Powder Diffraction Conference EPDIC-3,** Vienna, Austria. (Prof. E. Tillmanns, Institut fur Mineralogie und Kristallographie der Universitat Wien, Dr. Karl Lueger-Ring **1, A-1010** Wien, Austria; tel: **431-40103-2333,** fax: **431-4037622).**

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Name: LUCA LUTTEROTTI

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CALL FOR CONTRIBUTIONS TO THE CPD NEWSLETTERS

The next issue of the CPD Newsletter will be edited by Dr. J. Fiala is to appear in the spring of 1993. He would greatly appreciate contributions from readers on matters of interest to the powder diffraction community, such as meeting reports, notices of future meetings, developments in instrumentation, techniques and computer programs, and news of general interest. Please send articles and suggestions directly to him at his address given below.

Many thanks,
D. E. Cox, Editor for this Newsletter

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