

# COMMISSION ON POWDER DIFFRACTION INTERNATIONAL UNION OF CRYSTALLOGRAPHY NEWSLETTER NO. 7

NOVEMBER 1991

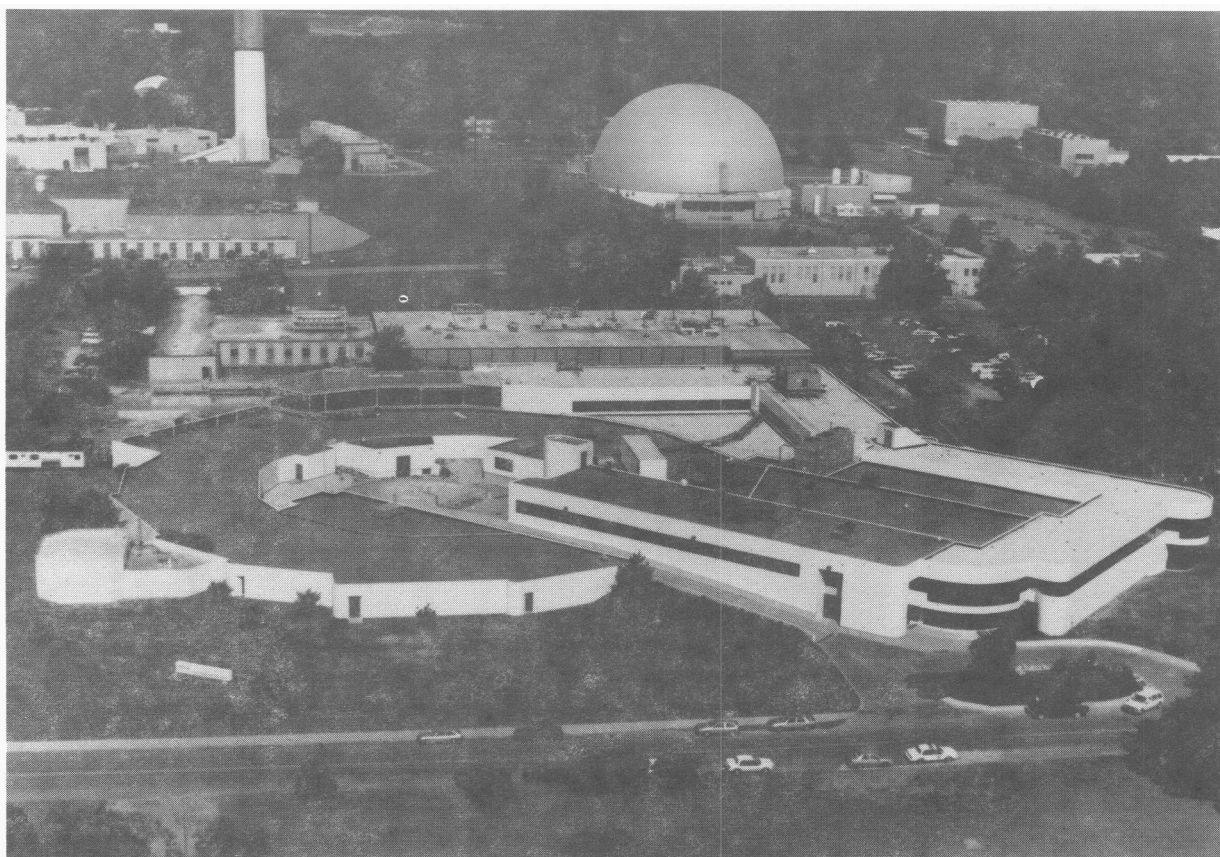
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## NEUTRON POWDER DIFFRACTION AT THE BROOKHAVEN HIGH FLUX BEAM REACTOR

The Brookhaven High Flux Beam Reactor (HFBR) uses highly-enriched  $^{235}\text{U}$  and a heavywater moderator to sustain a peak thermal flux of about  $10^{15}$  neutrons/cm<sup>2</sup>s at a power of 60 MW, similar to that achieved at the two other existing high flux facilities situated at Oak Ridge National Laboratory and the Institute Laue-Langevin in Grenoble. The HFBR achieved criticality in 1965 and functioned without serious interruptions until May, 1989, when it was shut down for an exhaustive safety review. After startup in July, 1991, operations were resumed at a reactor power level of 30 MW. At present the duty

cycle is approximately four weeks of operations followed by a one week shutdown period. A series of ex-situ thermal hydraulic tests designed to allow resumption of operations at a higher power level is under way.

With the resumption of operations at the HFBR, neutron powder diffraction is once again an important part of the research activities. Construction of a dedicated high resolution machine for this purpose is nearing completion and, in the meantime, powder diffraction experiments can be



View of the HFBR containment building behind the National Synchrotron Light Source at BNL

## NPD at BNL (continued)

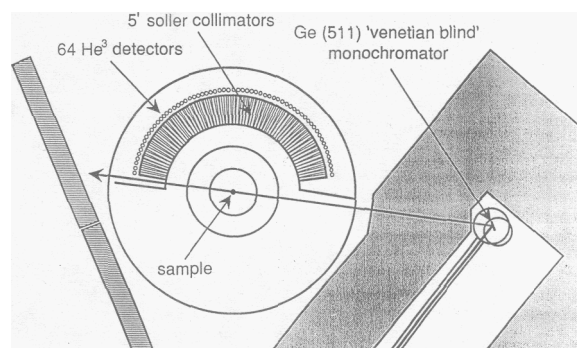
carried out on the triple-axis machines at H4S and H5. H4S is operated by a "Participating Research Team" similar in concept to those at the National Synchrotron Light Source (NSLS), consisting of a consortium involving the University of Pennsylvania, IBM, DuPont and Brookhaven. Although it has a relatively low monochromator take-off angle of 41 deg, it is nevertheless a very versatile powder diffractometer that offers a wide variety of options, including the choice of two vertically focusing monochromators, either pyrolytic graphite (002) at a wavelength of 2.37 Å (14.6 meV) or silicon (220) at 1.36 Å (44 meV). The latter is of a novel design developed by David Vaknin and colleagues [1], and consists of a stack of thin wafers clamped together in a simple bending device. If a pyrolytic graphite analyzer in the (004) setting is mounted in front of the detector (a 5 cm diameter  $^3\text{He}$  chamber with an active length of 10 cm), a minimum instrumental resolution  $\Delta d/d$  of about  $3 \times 10^{-3}$  can be achieved at 2.37 Å, and about  $5 \times 10^{-3}$  at 1.36 Å. A variety of Soller collimators with horizontal divergences ranging from 10- 40' allows considerable flexibility in choosing a compromise between intensity and resolution based on factors such as the amount of sample available and the nature of the experiment. The diffractometer can also be used in a high-intensity two-axis mode utilizing a multicounter bank consisting of 15  $^3\text{He}$  chambers spanning a range of 20 deg. In this mode, the instrumental resolution falls in the range  $1-2 \times 10^{-2}$  depending on wavelength.

H5 is operated by a PRT from IBM, Penn State University, Duke University, University of Missouri and Brookhaven. The wavelength can be varied continuously over a fairly wide range, typical choices being 1.65 or 2.45 Å (30 or 13.6 meV) with a pyrolytic graphite monochromator or 1.28 Å (50 meV) with a germanium (111) crystal. As in the case of H4S, a single detector can be used in conjunction with a pyrolytic graphite analyzer, or the diffractometer can be used in the two-axis mode with a multicounter bank comprised of 15  $^3\text{He}$  detectors covering a range of 90 deg. A variety of accessory equipment such as cryostats and furnaces is also available.

The scope of the neutron powder program will undergo a major change within the next few months with the commissioning of a new high resolution diffractometer (HRNPD), which is in the final stages of construction. This will be situated at beam-port H1A about 12 m from the source, and is generally very similar in design to the high resolution instrument D2B at the Institute Laue-Langevin [2] with the exception of the monochromator. A schematic view of the diffractometer is shown at the right [3].

It will utilize a multicounter bank containing 64  $^3\text{He}$  detectors 2.5 cm in diameter with an active length of 10 cm, each preceded by a Soller collimator with 5' horizontal divergence. There are two interchangeable in-pile collimators providing a choice of 5 or 11' for the incident beam divergence. In the higher resolution configuration, the minimum  $\Delta d/d$  is expected to be about  $6 \times 10^{-4}$ , comparable to that at D2B and the time-of-flight diffractometer HRPD at the Rutherford-Appleton Laboratory [5].

The monochromator will consist of a large vertically-focusing "venetian-blind" array of rectangular Ge segments in the (511) setting with an overall height of 33 cm. The take-off angle is 120deg, corresponding to a wavelength of 1.89 Å. The fabrication of such a monochromator, which ideally should have a uniform mosaic spread between 10-15' with reasonably high peak reflectivity, is a formidable and challenging task. The process normally used for this purpose involves plastic deformation of large crystal blocks by hot-pressing, preferably with in-situ gamma-ray diffraction to monitor the rocking curves in different regions [6], a very specialized and expensive procedure. However, a different approach is being used for HRNPD, namely a modification of the process used for the bent-wafer monochromator in use at H4S [1]. This involves the production of composite crystals with a controlled mosaic spread from stacks of Ge (511) wafers which have been individually plastically deformed and then bonded together. These wafers are 7.5 cm in diameter and about 0.3 mm thick, cut from a small number of cylindrical boules with their original sequence and orientation carefully noted. A number of preliminary experiments carried out by Larry Passell and coworkers have shown that uniform Gaussian mosaic spreads of about  $10^\circ$  can be obtained in this way. Absolute peak reflectivities approaching 25% at 1.36 Å have been measured for stacks consisting of 20 wafers [3]. After deformation, the individual wafers are bonded together by separating them with thin



Schematic view of the new high resolution powder diffractometer HRNPD. Reproduced from [4] by permission of the authors.

## NPD at BNL (continued)

sheets of Sn and heating to 400 C. They are then cut into rectangular segments with a diamond saw. The first such composite was successfully fabricated and tested in October, 1991, and production of the remainder is currently under way prior to final assembly in the holder.

HRNPD will be operated by a PRT with external funding provided by government agencies and the industrial members. At present the participating institutions include IBM, DuPont, NIST, Biosym, SUNY at Stony Brook, Oregon State U., Alfred U., Iowa State U., U. California at Santa Barbara, U. Missouri, Georgia Tech. and Brookhaven. The principal spokesperson is Professor Ray Young. Of the available beam time, 50% will be allocated to members of the PRT and their collaborators, and 50% to general users on a proposal basis. Proposal forms for experiments at HRNPD, H4S and other instruments can be obtained from the HFBR User Administration, c/o Mrs Rae Greenberg, Physics Bldg. 510A, Brookhaven National Laboratory, Upton, N.Y. 11973 (Phone: 516-282-5564, Fax: 516-282-5888).

D. E. Cox,  
Physics Dept., Brookhaven National Laboratory

### References

- [1] D. Vaknin, D. S. Coburn and A. S. Arrott, Nucl. Instrum. Methods A273,447(1988).
- [2] A. W. Hewat, Mater. Science Forum 9,69 (1986).
- [3] L. Passell, S. Bar-Ziv, D. W. Gardner, D. E. Cox and J. D. Axe, Proc. First European Powder Diffraction Conf., Munich, March 1991 (in press).
- [4] J. D. Jorgensen and J. M. Newsam, Mater. Res. Soc. Bull.15,49 (1990).
- [5] W. I. F. David, W. T. A. Harrison and M. W. Johnson, Mater. Science Forum 9,89 (1986).
- [6] A. Freund and J. B. Forsyth, Treatise Mater. Technol. 15,461(1979).

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## ENCOMIUMS

Professor A. J. C. Willson received the honorary degree of L.I.D. from Dalhousie University in Halifax, Nova Scotia. The degree was awarded in a special ceremony on 19 October 1991. Prof. Wilson took his Master's degree in physics at Dalhousie before going on to M.I.T. for his Ph.D. and then to Cambridge for another doctorate and permanent residence in the U.K.

Dr. H. Toraya has been appointed Asian Region Editor of the journal Powder Diffraction.

## NEW SPECTROMETERS AT CHALK RIVER AND POWDER DIFFRACTION WORKSHOP

Construction of DUALSPEC (Dual Beam Neutron Spectrometer) at the NRU reactor, Chalk River, was completed in January, 1991. The project was jointly funded by the Natural Sciences and Engineering Research Council (NSERC) through McMaster University and AECL Research. DUALSPEC will be run as a National Facility, in a "user mode" with the Canadian Institute for Neutron Scattering overseeing the operation.

DUALSPEC consists of two spectrometers utilizing beam holes at the reactor that are closely spaced vertically. The unique design of the facility allows independent operation of the two component spectrometers. The instrument on the lower beam hole is a polarized beam triple-axis spectrometer, while that on the upper beam hole is a high resolution powder diffractometer. Both instruments move on air pads over a dance floor. Both have interchangeable collimators (collimations of  $0.2^\circ$ ,  $0.4^\circ$  or  $0.6^\circ$  and a three position cold filter (open, sapphire or Be) before the monochromator. The monochromator take-off angle ( $2\theta$ ) is continuously variable from  $0^\circ$  to  $126^\circ$ . When combined with the wide variety of available monochromators, including vertically focussing Si(111) and Si(115), this will allow researchers great flexibility in the choice of experimental resolution.

The powder diffractometer has an 800-wire, curved, position-sensitive detector built by Division Leti, Grenoble. The radius of the detector is 1.5 m and the angular spacing of the wires is  $0.1^\circ$ . The detector thus spans a range of  $80^\circ$  in scattering angle and it can be positioned to  $0.001^\circ$ . It can be rotated to allow data collection over the complete range of scattering angles,  $0^\circ$  to  $140^\circ$  and at angles between the wire positions. An oscillating collimator is positioned between the specimen and detector. In the highest resolution configuration  $\Delta d/d$  will be 0.1%.

To familiarize Canadian scientists with the Rietveld method and to introduce them to the capabilities of the new powder diffractometer, a Workshop on Neutron Powder Diffraction was held at Chalk River Laboratories on May 30/31<sup>st</sup>, 1991. Sponsored by the Canadian Institute for Neutron Scattering, by AECL Research and by the Natural Sciences and Engineering Research Council, the Workshop was organized by B. M. Powell and B. H. Torrie (Waterloo). It attracted 35 participants from academia and industry. Guest lecturers were A. K. Cheetham (Oxford), R. B. Von Dreele (Los

## MEETING REPORTS

PICXAM - Pacific International Conference on X-Ray Analytical Methods. Workshops: 7-9 August 1991, University of Hawaii at Hilo, Hawaii. Congress: 12-16 August 1991, Hilton Hawaiian Village, Honolulu.

The Congress was preceded by 22 half-day workshop sessions, each with a different organizer, fitted into 2-1/2 days and attracting 185 registrants.

Special sessions were included on microtomography, thin-film analysis, and lattice defects. The overall organizer of the Workshops was Prof. Deane K. Smith (US) who noted with satisfaction that the attendance numbers were similar for all sessions, which indicated that the varied topics matched the varied interests of the attendees. A more detailed report is to appear in the journal Powder Diffraction.

The Congress was organized by the Denver Conference group, the Australian X-Ray Analytical Association, and the X-ray Analysis Group of the Japan Society for Analytical Chemistry. It was provisioned as a means of improving the channels of communication and cooperation among the respective groups and, by all accounts, has done that very successfully. PICXAM was attended by about 180 Americans, 40 Australians, 50 Japanese, and 100 others (mostly Europeans). Each of the five morning sessions consisted of a plenary lecture followed by five concurrent sessions of oral presentations. Three different concurrent poster sessions on each of three afternoons presented more than 200 posters.

From the powder diffraction point of view, the range and extent of powder calculation tools, indexing tools, etc. were a surprise to an Australian observer. There was an emphasis on whole-pattern approaches in both qualitative and quantitative analyses which were not Rietveld based. An overall appraisal of the conference was that structure-based methods (pattern simulation, Rietveld methods, indexing, use of electron diffraction and crystal databases) appear to have taken center stage.

All observers were impressed by the fascinating scenic environment that is Hawaii. On Friday, many of the Workshop participants visited Mount Kilauea, "the world's only drive-in volcano".

The Editor of this Newsletter gives thanks, and offers apologies for any misrepresentations, to Tony Raftery (Australia), Helein D. Hitchcock (US), and Deane K. Smith (US), who have kindly permitted him to prepare the above by excerpting and paraphrasing from their much longer reports submitted to Powder Diffraction.

Alamos), E. Prince (NIST) and V. G. Young Jr. (Iowa State). The format of the Workshop had formal lectures each morning with the afternoon spent in "hands-on" solutions of set Rietveld refinement problems utilizing the code GSAS. Since 18 terminals were provided to access the four VAX computers on which GSAS was installed, all the Workshop participants were able to get extensive experience in the use of the code.

B. M. Powell

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## STATUS OF CPD PROJECTS

The first phase of the Round Robin on Rietveld Refinement has been completed and a manuscript submitted to the J. Appl. Cryst. for publication. (See summary article herein.) Work continues on phase 2.

The project to develop and operate a Program Information Exchange Bank has produced its first palpable result, a massive publication in the J. Appl. Cryst. (See brief summary article herein.) Periodic updates are planned.

Preparations for the meeting on 'Accuracy in Powder Diffraction II' to be held 26-29 May 1992 at NIST in the USA, are proceeding well. The second circular, with names and topics of invited lecturers, is due out in early December. Readers are reminded that the IUCr has provided some money for grants to young scientists to help them get to the meeting. For meeting information and a grant application form, write to Dr. E. Prince, Reactor Radiation Division, NIST, Gaithersburg, MD 20899, USA.

Preparations for the Summer School on the Rietveld Method in Cieszyn, Poland, on 13-15 August 1992 are on schedule. Some IUCr money for travel/tuition grants to young scientists is available. Write to Prof. Bojarski at the address shown on the back page.

The CPD is a co-organizer of the Fourth International School of Crystallography: Computational Methods in X-ray Powder Diffraction Analysis to be held in Aswan, Egypt in January 1993. CPD members Dr. J. I. Langford and Dr. D. Louer are members of the program committee. The organizing and local chairman is Prof. Karimat El-Sayed, Physics Department, Faculty of Science, Ain Shams University, P.O.B. 8014, Masaken Nassr, Nassr City, Cairo, EGYPT

Readers are encouraged to suggest other needed projects that could be carried out effectively by the Commission on Powder Diffraction. Suggestions should be sent to the Secretary, Dr. R. J. Hill at his address shown on the back page.

The scientific program of the meeting was divided into seven sections with the number of papers shown:

Electron diffraction: 8  
Crystal structure determination: 14  
Thinlayers: 6  
Qualitative and quantitative phase analysis: 9  
In-situ measurements: 2  
Real structure of crystalline materials: 23  
Software and hardware in crystallography: 7

Both oral and poster presentations were features and a PC software demonstration was organized.

Some 75 attendees, mostly from Czechoslovakia, enjoyed the beautiful meeting site (mineral springs Herlany) and the perfect work of the organizing committee chaired by Tomas Havlik of the Technical University Kosice.

Jaroslav Fiala

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## ICDD X-RAY CLINIC

In 1990, the ICDD International Center for Diffraction Data (ICDD) decided to continue the running of the "SUNY" X-ray Clinics, initiated in the mid 1960s by the late Henry Chessin. The second of these ICDD sponsored X-ray diffraction Clinics was held at the Pennsylvania State University at University Park in June; and the first X-ray Fluorescence Clinic was held at Swarthmore College in July. Each of the clinics was held in two one-week sessions, directed at beginners for the first weeks and advanced topics for the second weeks. Attendance for the four weeks was XRD first week 38; XRD second week: 15; XRF first week 23; and XRF second week 23.

Based on the responses from the attendee critique sheets, the first week of XRD ran very smoothly and most of the bugs are now ironed out. The comments from most of the attendees were very positive. While the second week of XRD presented more of a problem due to the wide diversity in the background and interests of the participants, it seems that we were able to satisfactorily cover most of the needs. Both weeks of XRF went very smoothly, and this is to be expected since virtually the whole of the original SUNY Clinic XRF staff were utilized.

Ron Jenkins, ICDD

During the course of the past ten years the International Centre for Diffraction Data has sponsored a number of "Round Robin" tests to evaluate the quality of experimental X-ray diffraction data, and to gauge the effectiveness of certain "routine" procedures employed, such as data base searching, indexing and profile fitting. The latest of this series, called the Instrument Parameter Round Robin, was designed to evaluate, among other things, relative angularly-dependent sensitivity differences between diffractometers. Previous experiments have indicated that even perfectly aligned diffractometers of the same generic type, do not necessarily give the same set of relative intensities. One objective of the round robin was to quantify the magnitude of the experimental differences between data sets, and to demonstrate a means for external calibration of diffractometers, so that digitized diffraction intensity data obtained from different instruments could be compared directly.

A total of 137 reference samples were sent out, and 56 users submitted data. The diffractometers used represented a wide range of manufacturers and models, and each of the four major manufacturers were well represented - Philips (31), Siemens (12), Scintag (8), and Rigaku (6). In addition, there were 4 miscellaneous "other types", including one synchrotron. While most users were either from the US or Canada, there was international participation from Australia, Bulgaria, China, Germany, France, Israel, South Africa, and the Netherlands.

The main conclusion of the Round Robin is that even though there are wide variations in the sensitivity of a given diffractometer as a function of diffraction angle, these sensitivity variations can be modelled and a calibration curve established. ICDD is strongly recommending that all users run the new NIST Instrument Sensitivity Standard, SRM 1976, to establish the sensitivity curve for their particular powder diffractometer, and that they append this curve to any archived experimental pattern. Such a procedure will allow future comparisons to be made from instrument to instrument. As has been concluded in other round robins, a major problem in this field remains the poor alignment of instruments. We would reiterate that calibration curves should be routinely determined (however, these should not be used for the sole purpose of correcting for a badly aligned diffractometer). Unusual calibration curves are cause for immediate investigation and rectification of the root problem.

Ron Jenkins, ICDD

## ROUND ROBIN ON RIETVELD REFINEMENT: A CPD Project

The first part of the Rietveld Refinement Round Robin undertaken by the Commission on Powder Diffraction has now been completed and submitted to J. Applied Crystallography for publication. In Part I, 23 participants provided the results of in-house Rietveld refinements of  $\text{PbSO}_4$  using constant-wavelength X-ray and neutron 'standard' data sets collected by the CPD. Analysis of the results provided information about (i) the range and effect of various strategies of Rietveld refinement, and (ii) the precision and accuracy of the derived parameters.

The wide variation in the values of the agreement indices obtained in these studies highlights the need for standardization of the refinement strategies and of the classes of data included in the algorithms used for assessing the fit. The major factors limiting the accuracy of the derived crystal structure parameters were (i) use of insufficiently flexible peak shape and/or background functions, (ii) truncation of the high-angle data from the refinement, (iii) non-inclusion of a sufficiently wide range of diffraction angles on either side of the peak centroid and, additionally for X-rays, (iv) simultaneous release of atomic site-occupancy and displacement parameters.

For the X-ray data, the atomic coordinate and isotropic displacement parameters obtained for the Pb and S atoms were precise and were in reasonable agreement with the values derived from single-crystal studies (viz., the spread of coordinates was in the range 0.007-0.042Å). On the other hand, the 'light' O atom parameters showed relatively poor precision and had values that were spread 0.12-0.19Å about the weighted mean. Despite the much lower intrinsic resolution of the neutron data, the coordinates and anisotropic displacement parameters obtained for the Pb and S atoms were very precise and had a relatively narrow distribution about the single-crystal results, namely, 0.004-0.020Å for the coordinates. The spread of coordinates for the lighter S atom was correspondingly larger, namely 0.024-0.043Å, about the same as that obtained from the X-ray data.

Thus, this investigation provides reason for concern; it is clear that results of possibly high precision, but low accuracy are not uncommon in Rietveld analysis. Furthermore, the disparity between individual refinements can be expected to increase when, unlike here, the analyses are undertaken using data sets collected under diverse experimental conditions. This latter aspect is the subject of Part II of the Round Robin.

The broad range of refinement strategies and results encountered argue strongly for greater communication between practitioners of the Rietveld method regarding 'proper' practices. Indeed, many users of the Rietveld method would be well advised to take substantially greater care in their refinement process. Part of the problem appears to be the very 'forgiving' nature of the Rietveld method, together with the assumption that many data sets are plagued by preferred orientation and difficult-to-model peak shapes. Under these circumstances, some practitioners are not as critical of obviously poor, even bizarre, results and ascribe them to the limitations of the data. As this Round Robin has shown, good procedures can provide excellent results if time and care are taken.

R. J. Hill

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## PROGRAM INFORMATION EXCHANGE BANK: A CPD Project

The first product of the CPD's Program-Information-Exchange-Bank project has now appeared. It is an annotated compilation of computer programs for powder diffraction analyses, categorized by purpose. Program names, sources, language, form and cost information are provided, along with comments of documentation and support, for more than 280 programs. For each category, there is some general discussion of what is needed and available for studies that fall into each of the 21 categories. The compilation was produced by Prof. D. K. Smith, CPD Consultant, for the CPD with some late and very welcome assistance from Dr. Syb Gorter, who had been working independently along similar lines. It is now published as a report to the CPD from Smith and Gorter as "Powder Diffraction Information Program 1990 Program List" in J. Appl. Cryst. 24,369-402. Professor Smith and the CPD intend that the compilation shall be updated and republished periodically, provided that the PD community find it sufficiently useful.

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## NEWS FROM JAPAN

A special issue on "The Powder Diffraction Method" is to be published as the April 1992 issue of the Journal of the Crystallographic Society of Japan. Topics to be covered include uses of the Rietveld method with both X-ray and neutron sources, instrumentation, TDS correction, time-resolved studies, incommensurate structure analysis, studies with specimens under high pressures, and ab-initio structure determination from powder diffraction data.

H. Toraya

# FUTURE MEETINGS OF INTEREST TO POWDER DIFFRACTIONISTS

Powder diffractionists are invited to send notices of forthcoming meetings to the next editor of the CPD Newsletter, Dr. D. Louër, at his address shown on the back page.

- 2-7 Dec 1991 Materials Research Society Fall Meeting. Boston, Mass., USA. (M. Gell, MRS, 9800 McNight Road, Suite 327, Pittsburgh, PA 15237, USA).
- 17-19 Dec 1991 Crystallography of Magnetic and Semiconducting Multilayers Part of the Condensed Matter and Materials Physics Meeting, Birmingham, (UK) (Dr. C. Gough, School of Physics and Space Research, Edgbaston, Birmingham B15 2TT, UK).
- 31 March 1992 British Crystallographic Assoc. Spring Meeting. Liverpool, UK. (Dr. Marjorie Harding, Chem. Dept., Liverpool Univ., PO Box 147, Liverpool L69 3BX, UK).
- 9-12 April 1992 12th European Physical Society General Conf. Condensed Matter, Prague. Czechoslovakia. (Dr. V. Smid, Institute of Phys., **Czech. Acad. Sciences**. Cukrovarnicka 10, 16200 Praha 6, CZECHOSLOVAKIA).
- Spr./summer 1992 HDC-2 Hungarian Diffraction Conference.
- 26-29 May 1992 Accuracy in Powder Diffraction II, National Institute of Standards and Technology, Gaithersburg, Maryland. USA (Dr. E. Prince, Reactor Radiation Division. NIST, Gaithersburg, MD 20899, USA. e-mail: prince@enh.nist.gov).
- 1-7 June 1992 IUCr School on Crystallographic Computing. Veszprem, Hungary. (Dr. Kalman Simon, Hungarian Chemical Society, H-1027-Budapest, Fou. 68 HUNGARY).
- 30 Jul-1 Aug 92 EPDIC-2 Second European Powder Diffraction Conference, Enschede, The Netherlands (Dr. T. Ryan, Philips Analytical, Lelyweg 1, NL-7602 EA Almelo, **THE NETHERLANDS**).
- 2-7 Aug 1992 14th European Crystallographic Meeting **E** (ECM-14) Twente, The Netherlands. (Dr. H.J. Bruins Slot. CAOS/CAMM Center, Univ. of Nijmegen, **THE NETHERLANDS**).
- 9-14 Aug 1992 American Crystallographic Association Annual Meeting, Pittsburgh, PA. USA. (Marcia J. Vair, ACA. P. O. Box % Ellicott Station, Buffalo, N.Y. 14205-0096, USA).
- 9-12 Aug 1992 XVth Conference on Applied Crystallography, Cieszyn, Poland. (Dr. Danuta Stroz, Inst. Phys. & Chem. Metals, Silesian University, ul. Bankowa 12, 40-007 Katowice, **POLAND**).
- 13-15 Aug 1992 Rietveld Summer School RSS-92. Cieszyn, Poland (Dr. Danuta Stroz, Inst. Phys. & Chem. Metals, Silesian University, ul. Bankowa 12, 40-007 Katowice, **POLAND**).
- Oct 1992 SGK, Swiss Society of Crystallography, Annual Meeting. Basel. (Prof. H. Stockli Evans, Institute de Chemie, Université de Neuchatel, 51 avenue de Bellevaux, CH-2000 Neuchatel, **SWITZERLAND**).
- 14-16 Nov 1992 1st Crystallography Conference Of the Asian Crystallographic Association. Singapore. Contact: Prof. N. Kasai, Applied Crystallography, Osaka U., 2-1 Yamadoka Suita, Osaka 565, JAPAN. For program info: Dr. E.N. Maslen, Crystallography Centre, U. of Western Australia, Nedlands **6009**, WA, **AUSTRALIA**.
- Jan 1992 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@egfrucvx.bitnet**).
- 29 Mar - 2 Apr 1993 BCA Meeting Manchester, UK (Dr. Brian Beagley, UMIST).
- 23-28 May 1993 American Crystallographic Assoc. Meeting. Albuquerque, New Mexico, USA. Dr. Allen Larson, LANSCE H805, Los Alamos Nat'l Laboratory, Los Alamos, NM 87455, USA).
- 18-26 July 1993 10th International Clay conference Adelaide, South Australia. (10th ICC Secretariat: Elliservice Convention Management. Po Box 753 Norwood, South Australia, **AUSTRALIA** 5067).
- 21-29 Aug 1993 XVth IUCr General Assembly and International Congress of Crystallography. Beijing, China. (Prof. M. C. Shao, Inst. of Physical Chemistry, Dept. of Chemistry, Peking U., Beijing 100871, **CHINA**).

## To be on the MAILING LIST FOR CPD NEWSLETTERS

If you would like to receive a personal copy of future issues of this newsletter, please make sure that your name is on our mailing list by completing a copy of this form and mailing it to the CPD Secretary, Dr. R. J. Hill, at his address shown below.

To the IUCr Commission on Powder Diffraction:

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My address has changed to that given below:

The following named person might appreciate receiving the CPD Newsletter:

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**Please mail the completed form to** Dr. R. J. Hill, Div. Mineral Chemistry, CSIRO, PO Box 124, Port Melbourne, Victoria 3207, AUSTRALIA

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## CALL FOR CONTRIBUTIONS TO THE CPD NEWSLETTERS

The next issue of the CPD Newsletter will be edited by Dr. D. Louër to appear in the spring of 1992. He would greatly appreciate contributions from readers on matters of interest to the powder diffraction community, e.g., meetings reports, future meetings, developments in instruments, techniques, and computer programs, and news of general interest. Please send articles and suggestions directly to him at: Cristallogchimie, Univ. Rennes I, Av. GI Leclerc, 35042 Rennes, FRANCE.

Many thanks,  
R. A. Young, Editor for this Newsletter

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